Appendix to:
An Analysis of the Sources and Sinks for Criegee Intermediates: An Extended Computational Study

A thesis submitted in partial fulfilment of the requirements for the award of

Doctor of Philosophy.

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By

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Contents

1.0 Supplementary Information for Chapter 3: Ozonolysis of Alkenes

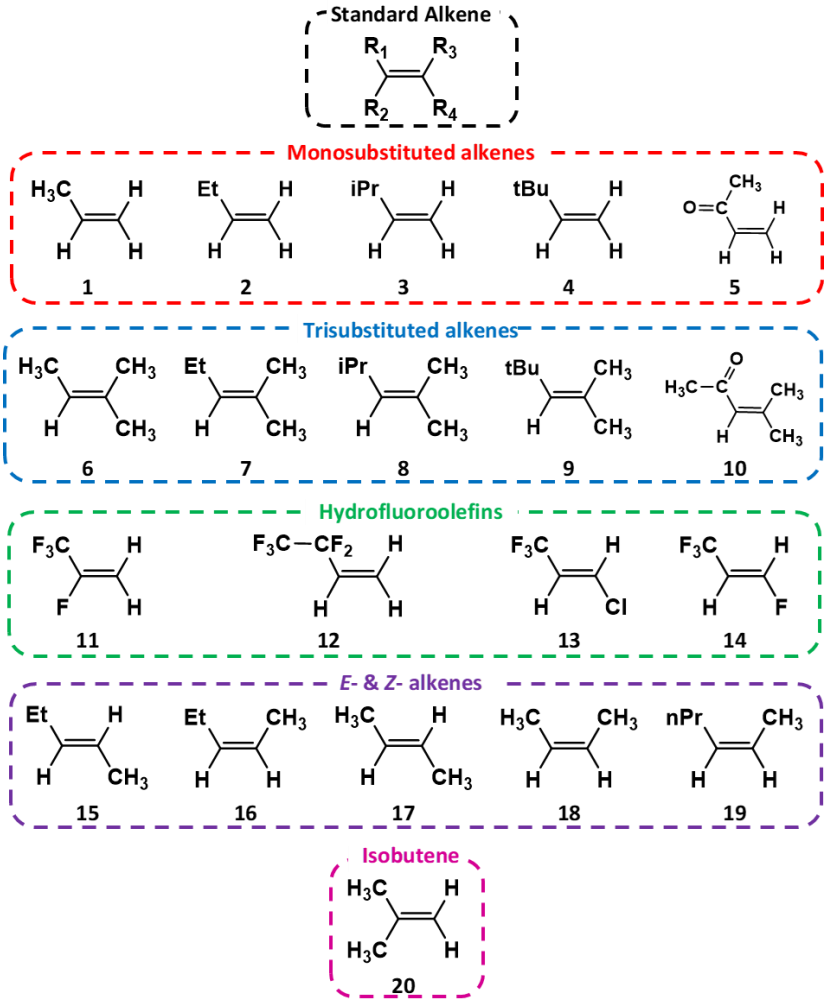


*Figure 1: Alkenes, labelled **1-20** and delineated by structural factors, modelled for ozonolysis analysis in this chapter.*

1.1 Equations

1.1.1 Canonical Rate Constant (k_{CAN})

To determine canonical rate constant (k_{CAN}), using Equation 1:

$$k_{CAN} = \sum(k_1/k_{-1} \times k_2) \qquad \textit{Equation 1}$$

Both types of rate constants produced by MESMER are generated from single step reactions or from pseudo-single step simulations of multistep reactions.

1.1.2 Conventional transition state theory rate constant (k_{TST})

Using either the partition functions (Q) and zero-point corrected energy (ΔZPE) values or the Gibbs free energy (ΔG) value, determined from the computational chemistry calculations, the Equations 2—7, are used to determine the conventional transition state theory rate constant (k_{TST}):

$$k_{TST} = \sum k_{TS}$$

(Equation 2)

$$k_{TS} = K_{eq} \times k_2$$

(Equation 3)

$$K_{eq} = \frac{RT}{P_0} \frac{Q_{PRC}}{Q_{R1}Q_{R2}} e^{-(\Delta ZPE_{PRC})/RT}$$

(Equation 4)

$$K_{eq} = \frac{RT}{P_0} e^{-(\Delta G_{PRC})/RT}$$

(Equation 5)

$$k_2 = \boldsymbol{\kappa} \frac{k_B T}{h} \frac{Q_{TS}}{Q_{PRC}} e^{-(\Delta ZPE_{TS} - \Delta ZPE_{PRC})/RT}$$

(Equation 6)

$$k_2 = \boldsymbol{\kappa} \frac{k_B T}{h} e^{-(\Delta G_{TS} - \Delta G_{PRC})/RT}$$

(Equation 7)

The factors in these equations are: $\boldsymbol{\kappa}$ is the tunneling constant (see section 2.6); k_B is Boltzmann constant; T is temperature; h is Planck's constant; R is the gas constant; P_0 is the pressure of the system; Q_{TS}, Q_{PRC}, Q_{R1} and Q_{R2} are the partition functions for transition state, pre-reaction complex, reactant 1 and reactant 2; ΔG_{TS} and ΔG_{PRC} are the relative molar Gibbs free energy for the transition state and pre-reaction complex, at 298 K

1.1.3 Structure activity relationships rate constant (k_{SAR})

Structure activity relationships depends on three types of groups to produce three different types of steric factors (s_0, s_1, s_2), identified in Figure 2: Disubstituted alkyl groups (s_0), α-alkyl groups (s_1) and ß-alkyl groups (s_2)

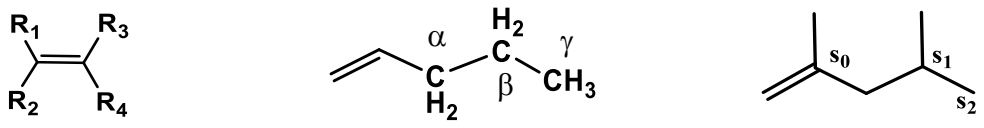


Figure 2: Alkenes R_1—R_4 substituent positions and the positions of hydrogen analogues on a substituent carbon chain labelled using Greek letters (α, ß, γ …), and the structure of 2,4-dimethyl-1-pentene labelled s_0, s_1 & s_2 according to which alkyl segment(s) causes the s_0, s_1 & s_2 steric effect in the SAR model.

To determine structure—activity relationship rate constant (k_{CAN}), use following equations. displayed in Equation 1.3, by using the number of alkyl groups attached to the >C=C< bond, which ranges from 0-4, as the total inductive factor (I). When combined with the total steric factor (S), which increases depending on the number of steric interferences in those substituent groups.

$$S = \sum s_n \qquad \textit{(Equation 8)} \qquad x = (yS) + I \qquad \textit{(Equation 9)}$$

The steric effect (S) depends on three factors: the clash between two alkyl groups at the end of an olefin bond (s_0 = 0.20); the steric interference of extra α-alkyl groups (s_1 = 0.033); and the steric interference of extra ß-alkyl groups (s_2 = 0.020).

$$\log k_{SAR}(298\,K) = (1.28 \pm 0.05)x - (18.14 \pm 0.07) \qquad \textit{(Equation 10)}$$

1.1.4 Dipole-Dipole Capture ($k_{d\text{-}d}$) and Collision Limits (k_{COLL}) of Rate Constants

The collision-limited reaction rate coefficient (k_{COLL}), is calculated using the following equations:

$$k_{COLL} = \left(\frac{8k_BT}{\pi\mu}\right)^{1/2} \pi(r_1 + r_2)^2 \qquad \textit{Equation 11} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} \qquad \textit{Equation 12}$$

k_B is the Boltzmann constant, T is the temperature, μ are the reduced mass of reactants, r_1 and r_2 are the covalent radii of reactants and, m_1 and m_2, is the masses.

The dipole–dipole capture limit ($k_{d\text{-}d}$) is calculated using the following equations:

$$k_{d\text{-}d} = C\sqrt{\pi/\mu}\ (\mu_{D1}\mu_{D2})^{(2/3)}(k_BT)^{-1/6} \qquad \textit{Equation 13}$$

μ_{D1} and μ_{D2}, the dipole moments of reactants, μ, reduced mass, k_B, the Boltzmann constant, T, temperature, and, C, isotropic, adiabatic or non-adiabatic anisotropic constant which depends on the anisotropy of the capture potential model. The C value can vary depending on whether the model adopted is isotropic (used in the main body of the thesis), adiabatic anisotropic or non-adiabatic anisotropic (C= 4.08, 2.68 and 1.953 respectively).

1.1.5 Effective Rate Constant (k_{EFF})

The Effective Rate Constant (k_{EFF}) uses the concentration of the co-reactant to determine the overall impact of a reaction:

$$k_{EFF} = k_{ME}\,[\text{co-reactant}] \qquad \textit{Equation 14}$$

1.1.6 Background to the Software Programmes: KisThELP and MESMER

In Section 1.4, the process by which many of the key kinetics and thermodynamics values, such as zero-point corrected energy and Gibbs free energy, obtained by computational chemistry calculations are used to obtain important k_{THEO} and Γ_{THEO} values is described and there are a large variety of software programmes used to estimate these reaction properties. This section will outline the function of the Kinetic and Statistical Thermodynamical Package (KiSThelP) and Master Equation Solver for Multi-Energy Well Reactions (MESMER) software used in these studies to find these molecular and reaction properties and the reasons why they were selected to undertake these projects. Whilst k_{THEO} and Γ_{THEO} values can be determined by hand using the thermochemistry equation seen in Section 1.4, these programmes can calculate these values accurately and more rapidly and provide a large array of other important features describing reaction properties. These include producing graphs of the changes in rate constant with varying temperature; and graphs of the fractional population of reactants and products over time.

The KiSThelP software programme is free, open-source and it supports Gaussian09 files allowing for its use in this study.[310] It can determine individual rate constants using either conventional transition state theory (TST), variation transition state theory and the Rice-Ramsperger-Kassel-Marcus (RRKM) rate constants.[311–315] This software also divides the individual reactions into its individual components, the pre-reaction complex equilibrium constant (K_{eq}) and the unimolecular rate constant (k_2), as well as providing a full rate coefficient value for reactions that have no pre-reaction complex. It can provide the choice of applying a Wigner or Eckart one-dimensional tunneling constant, if desired. Unlike MESMER, it displays the tunneling constant rather than simply integrating it into the rate constant.[316,317] Additionally, this software provides rate constants at different temperatures and can display these changes over the temperature profile graphically. If an alternative molecular energy is required, the input file that is formed for KiSThelP can be edited to incorporate this.

This software was selected for sCI + alcohol reactions for several reasons: the sCI + alcohol reactions are all 1-step; the software can produce raw Eckart values which can be compared to the higher level semi-classical on-the-fly tunneling factors; the produced temperature profiles can be compared to the experimental values; and it is a user-friendly piece of software. The nomenclature of this study is that if the reaction goes straight from

reaction to the final product, it is a one-step reaction. If the reaction involves a short-lived intermediate product, often a cyclic compound, it will be considered a two-step reaction with an intermediate formation step and a decomposition step. A one or two step reaction does not refer to the number of transition states at each step.

For the other chapters, another free open-source software is used and this is called the Master Equation Solver for Multi-Energy Well Reactions (MESMER). This can be used to calculate a master equation rate constant (k_{ME}) and the canonical rate constant (k_{CAN}) for one-step reactions.[312,318] For two-step reactions such as ozonolysis of alkenes, the microcanonical rate constants for each step can be used to derive the overall product branching ratio. For two-step systems, the input file needs to be adapted to a single step to determine the k_{ME}. These computations can be calculated under a variety of both atmospheric temperatures, pressures and excess reactant concentrations. MESMER is also useful because it provides a method (reverse ILT method used in Chapter 4) to find product yields for barrierless pathways, such as for the HCO + OH and CH_3 + NH exit channels for the unimolecular decompositions of CH_2OO and CH_3NH respectively.[319,320]

This piece of software is used in Chapters 3, 5 and 6 for several important reasons: that product branching ratios can be calculated from multistep reactions; it is compatible with Gaussian '09 output files; that the input files can be edited to add the relevant molecular energy without editing the input gaussian file; by producing two sets of rate constants (k_{CAN} & k_{ME}), providing a method of validating the accuracy of the results; and it has a user-friendly interface. For more details on the method of how the software was used, please see the method section for Chapter 2.

1.2 Rate Constants and Product Branching Ratios

1.2.1 Master Equation Rate Constants (k_{CAN})

The grainsize used to determine the master equation rate constants and the master equation rate constants at various temperatures are categorised in this section.

*Table 1: Calculated Master Equation Rate Constants (k_{ME}) at Standard Pressure over a variety of Temperatures for the Ozonolysis of Alkenes **1**—**20**.*

O_3 + Alkene 1		O_3 + Alkene 2		O_3 + Alkene 3	
Grainsize:	10	Grainsize:	20	Grainsize:	20
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	2.63E-18	200	9.13E-18	200	4.87E-18
275	2.04E-17	275	6.58E-17	275	3.21E-17
298	3.24E-17	298	1.03E-16	298	4.96E-17
325	5.23E-17	325	1.63E-16	325	7.82E-17
400	1.53E-16	400	4.59E-16	400	2.21E-16
O_3 + Alkene 4		O_3 + Alkene 5		O_3 + Alkene 6	
Grainsize:	10	Grainsize:	20	Grainsize:	10
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	2.26E-18	200	1.14E-17	200	3.90E-15
275	1.47E-17	275	4.90E-17	275	4.12E-15
298	2.25E-17	298	6.90E-17	298	4.34E-15
325	3.50E-17	325	9.92E-17	325	4.66E-15
400	9.50E-17	400	2.32E-16	400	5.86E-15
O_3 + Alkene 7		O_3 + Alkene 8		O_3 + Alkene 9	
Grainsize:	10	Grainsize:	15	Grainsize:	10
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	4.78E-15	200	8.86E-17	200	7.64E-17
275	4.89E-15	275	1.99E-16	275	1.95E-16
298	5.12E-15	298	2.459E-16	298	2.456E-16
325	5.46E-15	325	3.10E-16	325	3.15E-16
400	6.81E-15	400	5.54E-16	400	5.66E-16
O_3 + Alkene 10		O_3 + Alkene 11		O_3 + Alkene 12	
Grainsize:	15	Grainsize:	10	Grainsize:	25
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	4.84E-19	200	3.84E-23	200	1.20E-22
275	1.26E-18	275	4.15E-21	275	1.12E-20
298	1.57E-18	298	1.14E-20	298	2.99E-20
325	2.24E-18	325	3.15E-20	325	8.07E-20
400	6.17E-18	400	2.83E-19	400	6.97E-19
O_3 + Alkene 13		O_3 + Alkene 14		O_3 + Alkene 15	
Grainsize:	10	Grainsize:	10	Grainsize:	25
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	8.75E-23	200	2.07E-23	200	7.31E-16
275	7.18E-21	275	2.84E-21	275	1.34E-15
298	1.85E-20	298	8.11E-21	298	1.13E-15
325	4.82E-20	325	2.34E-20	325	9.64E-16

400	3.79E-19	400	2.25E-19	400	4.46E-15

O_3 + Alkene 16		O_3 + Alkene 17		O_3 + Alkene 18	
Grainsize: 15		Grainsize: 10		Grainsize: 10	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
200	1.31E-15	200	3.68E-17	200	4.41E-16
275	2.15E-15	275	1.34E-16	275	9.62E-16
298	2.48E-15	298	1.81E-16	298	1.18E-15
325	2.93E-15	325	2.48E-16	325	1.46E-15
400	4.54E-15	400	5.15E-16	400	2.50E-15

O_3 + Alkene 20	
Grainsize: 10	
T (K)	k_{ME} (cm^3 s^{-1})
200	1.04E-18
275	9.29E-18
298	1.51E-17
325	2.49E-17
400	7.60E-17

*Table 2: Calculated Master Equation Rate Constants (k_{ME}) at non-standard pressure over a select range of Temperatures for the Ozonolysis of Alkenes **4** & **5**.*

O_3 + Alkene 4		O_3 + Alkene 5	
Grainsize: 10		Grainsize: 20	
T (K)	k_{ME} (cm^3 s^{-1})	T (K)	k_{ME} (cm^3 s^{-1})
210	3.08E-18	281	9.20E-17
218	3.88E-18	284	9.55E-17
226	4.83E-18	287	9.90E-17
235	6.08E-18	289	1.01E-16
245	7.74E-18	292	1.05E-16
255	9.71E-18	295	1.09E-16
288	1.88E-17	-	-
301	2.37E-17	-	-

1.2.2 Canonical Rate Constants (k_{CAN})

Canonical Rate constants produced by MESMER are displayed in this section.

*Table 3: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **20** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

Alkene #	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	TS_{OZO} 1			TS_{OZO} 2		
			k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	2.63E-18	1.01E-10	1.37E+12	3.31E+04	1.01E-10	6.63E+11	1.26E+03
	275	2.04E-17	1.01E-10	1.04E+13	1.82E+06	1.01E-10	4.89E+12	1.38E+05
	298	3.24E-17	1.01E-10	1.52E+13	4.11E+06	1.01E-10	7.09E+12	3.60E+05
	325	5.23E-17	1.01E-10	2.16E+13	9.24E+06	1.01E-10	1.01E+13	9.32E+05
	400	1.53E-16	1.00E-10	4.15E+13	4.89E+07	1.00E-10	1.91E+13	6.61E+06
4	200	2.26E-18	1.01E-10	1.01E+12	2.23E+04	1.01E-10	2.03E+11	6.44E+01
	275	1.47E-17	1.00E-10	4.77E+12	6.69E+05	1.00E-10	1.41E+12	8.68E+03
	298	2.25E-17	1.00E-10	6.30E+12	1.34E+06	1.00E-10	2.02E+12	2.36E+04
	325	3.50E-17	1.00E-10	8.14E+12	2.65E+06	1.00E-10	2.82E+12	6.37E+04
	400	9.50E-17	1.00E-10	1.27E+13	1.09E+07	1.00E-10	5.19E+12	4.90E+05
6	200	3.90E-15	9.99E-11	3.90E+13	1.44E+09	1.01E-10	1.21E+10	2.49E+04
	275	4.12E-15	9.99E-11	1.21E+14	4.54E+09	1.00E-10	2.89E+11	1.06E+06
	298	4.34E-15	9.99E-11	1.46E+14	5.73E+09	1.00E-10	5.33E+11	2.28E+06
	325	4.66E-15	9.99E-11	1.74E+14	7.21E+09	1.00E-10	9.59E+11	4.88E+06
	400	5.86E-15	9.99E-11	2.28E+14	1.16E+10	1.00E-10	2.97E+12	2.34E+07
9	200	7.62E-17	1.01E-10	2.79E+10	1.81E+04	1.00E-10	7.46E+10	8.01E+03
	275	1.95E-16	1.00E-10	5.32E+11	8.37E+05	1.00E-10	1.27E+12	4.63E+05
	298	2.456E-16	1.00E-10	9.35E+11	1.83E+06	1.00E-10	2.17E+12	1.06E+06
	325	3.15E-16	1.00E-10	1.60E+12	3.98E+06	1.00E-10	3.65E+12	2.41E+06
	400	5.66E-16	9.97E-11	4.50E+12	1.96E+07	9.97E-11	9.75E+12	1.30E+07
11	200	3.84E-23	1.01E-10	4.72E+07	1.79E-06	1.01E-10	4.72E+07	1.62E-05
	275	4.15E-21	1.01E-10	4.35E+08	3.03E-03	1.01E-10	4.35E+08	1.49E-02
	298	1.14E-20	1.01E-10	6.57E+08	1.39E-02	1.01E-10	6.57E+08	6.02E-02
	325	3.15E-20	1.01E-10	9.70E+08	6.29E-02	1.01E-10	9.70E+08	2.40E-01
	400	2.83E-19	1.01E-10	2.00E+09	1.42E+00	1.01E-10	2.00E+09	4.20E+00
13	200	8.75E-23	1.01E-10	2.45E+11	1.73E-01	1.00E-10	4.51E+11	7.27E-02
	275	7.18E-21	1.01E-10	8.49E+11	4.51E+01	1.00E-10	1.58E+12	2.89E+01
	298	1.85E-20	1.01E-10	1.05E+12	1.40E+02	1.00E-10	1.95E+12	9.83E+01
	325	4.82E-20	1.01E-10	1.27E+12	4.32E+02	1.00E-10	2.37E+12	3.30E+02
	400	3.79E-19	1.00E-10	1.73E+12	4.38E+03	1.00E-10	3.24E+12	4.02E+03
14	200	2.07E-23	1.00E-10	2.37E+11	2.23E-02	1.01E-10	5.51E+11	6.18E-02
	275	2.84E-21	1.00E-10	4.91E+11	6.45E+00	1.00E-10	1.55E+12	2.36E+01
	298	8.11E-21	1.00E-10	5.46E+11	2.05E+01	1.00E-10	1.83E+12	7.93E+01
	325	2.34E-20	1.00E-10	5.95E+11	6.46E+01	1.00E-10	2.12E+12	2.64E+02
	400	2.25E-19	1.00E-10	6.52E+11	6.86E+02	1.00E-10	2.64E+12	3.15E+03
17	200	3.68E-17	1.01E-10	3.48E+10	1.27E+04	Degeneracy of 2		
	275	1.34E-16	1.01E-10	9.70E+11	1.29E+06	Degeneracy of 2		
	298	1.81E-16	1.01E-10	1.85E+12	3.32E+06	Degeneracy of 2		
	325	2.48E-16	1.01E-10	3.45E+12	8.50E+06	Degeneracy of 2		
	400	5.15E-16	1.00E-10	1.15E+13	5.91E+07	Degeneracy of 2		
18	200	4.41E-16	1.01E-10	3.49E+13	1.52E+08	1.01E-10	9.08E+10	2639.8
	275	9.62E-16	1.01E-10	8.94E+13	8.37E+08	1.01E-10	6.10E+11	128231
	298	1.18E-15	1.01E-10	1.04E+14	1.18E+09	1.01E-10	8.66E+11	283266
	325	1.46E-15	1.00E-10	1.19E+14	1.67E+09	1.01E-10	1.20E+12	621017
	400	2.50E-15	1.00E-10	1.44E+14	3.39E+09	1.01E-10	2.18E+12	3.13E+06
20	200	2.08E-18	1.01E-10	9.65E+10	9.97E+02	Degeneracy of 2		

	275	1.86E-17	1.01E-10	9.03E+11	8.34E+04	Degeneracy of 2
	298	3.02E-17	1.01E-10	1.37E+12	2.06E+05	Degeneracy of 2
	325	4.99E-17	1.00E-10	2.04E+12	5.06E+05	Degeneracy of 2
	400	1.52E-16	1.00E-10	4.26E+12	3.22E+06	Degeneracy of 2

*Table 4: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **2** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 2										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	9.13E-18	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.45E+11	1.38E+04	1.01E-10	5.75E+11	1.14E+04	1.01E-10	2.05E+12	6.69E+04
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	8.45E+11	1.75E+03	1.00E-10	2.31E+12	1.15E+03	1.01E-10	1.16E+12	1.18E+04
275	6.58E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.15E+12	9.21E+05	1.01E-10	6.35E+12	7.95E+05	1.01E-10	8.63E+12	1.91E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	5.73E+12	1.64E+05	1.00E-10	1.31E+13	1.16E+05	1.00E-10	5.76E+12	5.34E+05
298	1.03E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	7.85E+12	2.17E+06	1.01E-10	1.00E+13	1.89E+06	1.01E-10	1.11E+13	3.77E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	8.16E+12	4.15E+05	1.00E-10	1.81E+13	2.98E+05	1.00E-10	7.67E+12	1.16E+06
325	1.63E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	1.17E+13	5.07E+06	1.01E-10	1.54E+13	4.47E+06	1.01E-10	1.41E+13	7.41E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	1.14E+13	1.04E+06	1.00E-10	2.43E+13	7.57E+05	1.00E-10	1.00E+13	2.50E+06
400	4.59E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	2.47E+13	2.91E+07	1.01E-10	3.49E+13	2.62E+07	1.00E-10	2.09E+13	2.98E+07
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	2.08E+13	6.90E+06	1.00E-10	4.14E+13	5.18E+06	1.00E-10	1.60E+13	1.22E+07

*Table 5: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **3** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 3										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	4.87E-18	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.01E-10	1.48E+12	4.94E+04	1.01E-10	2.13E+12	6.81E+02	1.00E-10	4.39E+12	6.98E+03
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	5.26E+12	2.43E+03	1.00E-10	1.39E+12	2.39E+03	1.00E-10	4.21E+12	4.53E+04
275	3.21E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.01E-10	1.20E+13	2.21E+06	1.00E-10	8.44E+12	5.95E+04	1.00E-10	1.51E+13	3.00E+05
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	2.38E+13	1.91E+05	1.00E-10	6.07E+12	1.41E+05	1.00E-10	1.59E+13	1.22E+06
298	4.96E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	1.77E+13	4.80E+06	1.00E-10	1.07E+13	1.48E+05	1.00E-10	1.88E+13	6.45E+05
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	3.12E+13	4.66E+05	1.00E-10	7.88E+12	3.23E+05	1.00E-10	2.00E+13	2.39E+06
325	7.82E-17	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	2.57E+13	1.03E+07	1.00E-10	1.34E+13	3.65E+05	1.00E-10	2.28E+13	1.38E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	4.01E+13	1.13E+06	1.00E-10	1.00E+13	7.35E+05	1.00E-10	2.48E+13	4.64E+06
400	2.21E-16	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 1.3**		
		1.00E-10	5.11E+13	5.02E+07	1.00E-10	1.95E+13	2.34E+06	1.00E-10	3.13E+13	6.57E+06
		TS_{OZO} 2.1			**TS_{OZO} 2.2**			**TS_{OZO} 2.3**		
		1.00E-10	6.22E+13	6.93E+06	1.00E-10	1.52E+13	3.99E+06	1.00E-10	3.55E+13	1.82E+07

*Table 6: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **7** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 7										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	4.78E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.01E-10	2.82E+13	4.19E+08	1.01E-10	2.11E+13	5.25E+04	1.01E-10	2.11E+13	5.41E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	5.15E+10	1.61E+04	1.01E-10	5.15E+10	2.02E+01	1.01E-10	5.15E+10	3.40E+05
275	4.89E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.01E-10	7.83E+13	1.32E+09	1.00E-10	7.84E+13	2.03E+06	1.00E-10	7.84E+13	1.84E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	9.45E+11	8.00E+05	1.01E-10	9.45E+11	5.03E+03	1.01E-10	9.45E+11	7.09E+06
298	5.11E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.27E+13	1.66E+09	1.00E-10	9.86E+13	4.30E+06	1.00E-10	9.86E+13	2.36E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	1.65E+12	1.78E+06	1.01E-10	1.65E+12	1.56E+04	1.01E-10	1.65E+12	1.32E+07
325	5.46E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.07E+14	2.08E+09	1.00E-10	1.22E+14	9.05E+06	1.00E-10	1.22E+14	3.02E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.82E+12	3.93E+06	1.00E-10	2.82E+12	4.78E+04	1.00E-10	2.82E+12	2.44E+07
400	6.82E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.34E+14	3.32E+09	1.00E-10	1.73E+14	4.21E+07	1.00E-10	1.73E+14	5.05E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.83E+12	2.01E+07	1.00E-10	7.83E+12	4.84E+05	1.00E-10	7.83E+12	8.71E+07

*Table 7: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **8** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 8										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	8.85E-17	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	2.07E+13	1.44E+07	1.00E-10	2.07E+13	1.43E+05	1.01E-10	4.15E+14	1.18E+05
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	2.55E+11	4.67E+04	1.01E-10	2.55E+11	1.90E+02	1.01E-10	4.15E+14	9.89E+03
275	1.98E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	7.37E+13	1.08E+08	1.00E-10	7.37E+13	3.68E+06	1.00E-10	5.14E+14	3.12E+06
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	2.37E+12	1.08E+06	1.01E-10	2.37E+12	1.90E+04	1.00E-10	5.14E+14	4.46E+05
298	2.443E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.18E+13	1.62E+08	1.00E-10	9.18E+13	7.15E+06	1.00E-10	5.15E+14	6.08E+06
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.01E-10	3.60E+12	2.05E+06	1.01E-10	3.60E+12	4.85E+04	1.00E-10	5.15E+14	9.71E+05
325	3.07E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.12E+14	2.43E+08	1.00E-10	1.12E+14	1.38E+07	1.00E-10	5.06E+14	1.18E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	5.34E+12	3.86E+06	1.00E-10	5.34E+12	1.23E+05	1.00E-10	5.06E+14	2.10E+06
400	5.45E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.55E+14	5.60E+08	1.00E-10	1.55E+14	5.36E+07	1.00E-10	4.49E+14	4.60E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	1.11E+13	1.42E+07	1.00E-10	1.11E+13	8.39E+05	1.00E-10	4.49E+14	1.02E+07

*Table 8: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **12** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 12										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.20E-22	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	1.81E+12	1.27E+00	9.99E-11	1.81E+12	3.22E-03	1.00E-10	9.79E+11	3.32E-02
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	9.50E+11	4.29E-01	1.00E-10	1.11E+14	1.84E-02	1.00E-10	9.79E+11	9.67E-03
275	1.12E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	2.02E+12	1.17E+02	1.00E-10	2.02E+12	1.47E+00	1.00E-10	2.54E+12	1.95E+01
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.05E+12	8.70E+01	1.00E-10	6.83E+13	8.45E+00	1.00E-10	2.54E+12	7.62E+00
298	2.99E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.98E+12	2.95E+02	1.00E-10	1.98E+12	5.15E+00	1.00E-10	2.96E+12	7.17E+01
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.30E+12	2.57E+02	1.00E-10	5.91E+13	2.95E+01	1.00E-10	2.96E+12	2.98E+01
325	8.08E-20	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.90E+12	7.33E+02	1.00E-10	1.90E+12	1.78E+01	1.00E-10	3.37E+12	2.60E+02
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.52E+12	7.51E+02	1.00E-10	5.02E+13	1.02E+02	1.00E-10	3.37E+12	1.15E+02
400	6.97E-19	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.60E+12	4.78E+03	1.00E-10	1.60E+12	2.28E+02	1.00E-10	4.07E+12	3.71E+03
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	2.82E+12	6.83E+03	1.00E-10	3.28E+13	1.31E+03	1.00E-10	4.07E+12	1.86E+03

*Table 9: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **15** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 15										
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	7.31E-16	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	4.48E+13	2.40E+08	1.00E-10	1.76E+11	1.92E+05	1.00E-10	1.19E+14	5.30E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	6.07E+13	1.07E+07	9.98E-11	7.42E+13	9.52E+06	9.99E-11	5.15E+13	5.24E+06
275	1.34E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	1.93E+14	1.59E+09	1.00E-10	2.68E+12	6.78E+06	1.00E-10	4.67E+14	5.15E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	2.41E+14	1.56E+08	9.99E-11	2.40E+14	1.22E+08	9.99E-11	2.48E+14	8.78E+07
298	1.59E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	2.50E+14	2.33E+09	1.00E-10	4.50E+12	1.40E+07	1.00E-10	5.94E+14	8.18E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	3.08E+14	2.70E+08	9.99E-11	2.92E+14	2.05E+08	9.99E-11	3.30E+14	1.56E+08
325	1.93E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	3.17E+14	3.41E+09	1.00E-10	7.38E+12	2.89E+07	1.00E-10	7.39E+14	1.29E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.98E-11	3.84E+14	4.64E+08	9.99E-11	3.49E+14	3.44E+08	9.99E-11	4.28E+14	2.76E+08
400	3.15E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		9.99E-11	4.77E+14	7.46E+09	1.00E-10	1.89E+13	1.28E+08	1.00E-10	1.07E+15	3.33E+09
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		9.99E-11	5.59E+14	1.41E+09	9.99E-11	4.63E+14	9.92E+08	1.00E-10	6.78E+14	8.92E+08

*Table 10: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkene **16** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, & k_2)*

O_3 + Alkene 16										
T (K)	$\boldsymbol{k_{CAN}}$ ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.31E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	3.25E+13	5.96E+07	1.01E-10	3.02E+12	2.30E+03	1.01E-10	3.02E+12	3.27E+07
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.96E+11	9.28E+03	1.01E-10	2.56E+11	3.49E+00	1.01E-10	2.56E+11	9.81E+04
275	2.14E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	8.26E+13	3.55E+08	1.00E-10	1.11E+13	1.70E+05	1.00E-10	1.11E+13	1.76E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	4.39E+12	4.34E+05	1.01E-10	1.43E+12	7.66E+02	1.01E-10	1.43E+12	1.67E+06
298	2.48E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	9.61E+13	5.10E+08	1.00E-10	1.39E+13	4.07E+05	1.00E-10	1.39E+13	2.47E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	5.98E+12	9.52E+05	1.00E-10	1.96E+12	2.31E+03	1.00E-10	1.96E+12	2.98E+06
325	2.93E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.10E+14	7.30E+08	1.00E-10	1.71E+13	9.61E+05	1.00E-10	1.71E+13	3.46E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	7.96E+12	2.07E+06	1.00E-10	2.62E+12	6.88E+03	1.00E-10	2.62E+12	5.27E+06
400	4.54E-15	**TS_{ozo} 1.1**			**TS_{ozo} 1.2**			**TS_{ozo} 1.3**		
		1.00E-10	1.32E+14	1.53E+09	1.00E-10	2.40E+13	5.55E+06	1.00E-10	2.40E+13	6.91E+08
		TS_{ozo} 2.1			**TS_{ozo} 2.2**			**TS_{ozo} 2.3**		
		1.00E-10	1.33E+13	1.03E+07	1.00E-10	4.41E+12	6.54E+04	1.00E-10	4.41E+12	1.71E+07

*Table 11: Canonical Rate Constants (k_{CAN}) of Ozonolysis of Alkenes **5** & **10** based on a steady state treatment of individual canonical rate coefficients (k_1, k_{-1}, & k_2)*

O_3 + Alkene 5													
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 2.1**			**TS_{OZO} 2.2**		
		k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.14E-17	1.00E-10	4.45E+11	6.67E+02	1.01E-10	2.87E+12	1.02E+03	1.00E-10	6.45E+11	7.19E+04	1.01E-10	5.54E+11	1.06E+02
275	4.90E-17	1.00E-10	2.20E+12	4.53E+04	1.01E-10	1.22E+13	8.15E+04	1.00E-10	1.39E+12	6.36E+05	1.01E-10	4.69E+12	1.98E+04
298	6.90E-17	1.00E-10	2.93E+12	1.07E+05	1.00E-10	1.57E+13	1.99E+05	1.00E-10	1.56E+12	9.85E+05	1.01E-10	6.98E+12	5.79E+04
325	9.92E-17	1.00E-10	3.82E+12	2.50E+05	1.00E-10	1.99E+13	4.83E+05	1.00E-10	1.72E+12	1.52E+06	1.00E-10	1.02E+13	1.67E+05
400	2.32E-16	1.00E-10	6.08E+12	1.44E+06	1.00E-10	2.97E+13	2.99E+06	1.00E-10	1.92E+12	3.66E+06	1.00E-10	2.04E+13	1.49E+06
O_3 + Alkene 10													
T (K)	k_{CAN} ($cm^3\ s^{-1}$)	**TS_{OZO} 1.1**			**TS_{OZO} 1.2**			**TS_{OZO} 2.1**			**TS_{OZO} 2.2**		
		k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
200	1.42E-19	9.97E-11	3.98E+12	1.21E+03	9.98E-11	2.29E+15	2.34E+03	1.00E-10	1.60E+11	1.78E+02	1.00E-10	5.77E+14	8.55E+02
275	9.33E-19	9.98E-11	1.83E+13	4.88E+04	9.98E-11	2.95E+15	1.24E+05	1.00E-10	2.73E+12	1.79E+04	1.00E-10	5.51E+14	2.68E+04
298	1.43E-18	9.98E-11	2.40E+13	1.04E+05	9.98E-11	2.98E+15	2.79E+05	1.00E-10	4.69E+12	4.60E+04	1.00E-10	5.24E+14	5.41E+04
325	2.24E-18	9.98E-11	3.08E+13	2.19E+05	9.99E-11	2.96E+15	6.23E+05	1.00E-10	7.87E+12	1.17E+05	1.00E-10	4.89E+14	1.09E+05
400	6.29E-18	9.98E-11	4.74E+13	1.02E+06	9.99E-11	2.68E+15	3.29E+06	1.00E-10	2.12E+13	8.05E+05	1.00E-10	3.91E+14	8.05E+05

1.2.3 Product Branching Fractions (Γ_{THEO})

Complete product branching ratios (Γ_{THEO}) of ozonolysis Reactions are found herein. The branching fractions for O_3 + Alkenes **13**—**18** are displayed with new Γ_{THEO} labelling, for *anti*- & *syn*-R_1R_2COO ($\Gamma_{ANTI\text{-}R1}$ & $\Gamma_{SYN\text{-}R1}$) and *anti*- & *syn*-R_3R_4COO ($\Gamma_{ANTI\text{-}R3}$ & $\Gamma_{SYN\text{-}R3}$). One important factor is that the MESMER treatment for all other O_3 + alkene reactions expect for O_3 + Alkenes **1**, **6**, **11**, **13** & **18**, went through a single POZ conformer to determine the Γ_{THEO} values.

*Table 12: Product Branching Ratios of Ozonolysis of Alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **20**.*

T (K)	O_3 + Alkene **1**				O_3 + Alkene **6**			
	Grainsize			25	Grainsize			40
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{ANTI}	Γ_{DMFO} (1)	Γ_{DMFO} (2)	Γ_{SYN}
200	0.722	0.047	0.010	0.221	0.001	0.994	0.005	<0.001
275	0.621	0.097	0.049	0.233	0.157	0.636	0.165	0.042
298	0.452	0.157	0.115	0.276	0.216	0.509	0.203	0.072
325	0.305	0.286	0.204	0.205	0.211	0.520	0.199	0.070
400	0.536	0.139	0.094	0.232	0.231	0.478	0.209	0.081
T (K)	O_3 + Alkene **4**				O_3 + Alkene **9**			
	Grainsize			20	Grainsize			15
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{ANTI}	Γ_{DMFO} (1)	Γ_{DMFO} (2)	Γ_{SYN}
200	0.112	0.618	0.220	0.050	<0.001	<0.001	1.000	<0.001
275	0.475	0.303	0.165	0.057	0.067	0.006	0.868	0.058
298	0.470	0.303	0.168	0.059	0.114	0.010	0.778	0.098
325	0.472	0.303	0.167	0.058	0.121	0.011	0.763	0.105
400	0.460	0.304	0.174	0.062	0.130	0.014	0.742	0.114
T (K)	O_3 + Alkene **11**				O_3 + Alkene **13**			
	Grainsize			40	Grainsize			70
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	$\Gamma_{ANTI\text{-}R1}$	$\Gamma_{SYN\text{-}R1}$	$\Gamma_{ANTI\text{-}R3}$	$\Gamma_{SYN\text{-}R3}$
200	<0.001	0.524	0.476	<0.001	0.996	0.002	<0.001	0.002
275	<0.001	0.545	0.455	<0.001	0.575	0.101	0.118	0.206
298	<0.001	0.532	0.468	<0.001	0.542	0.119	0.144	0.194
325	<0.001	0.544	0.456	<0.001	0.571	0.103	0.120	0.207
400	<0.001	0.548	0.452	<0.001	0.585	0.147	0.105	0.163
T (K)	O_3 + Alkene **14**				O_3 + Alkene **17**			
	Grainsize			25	Grainsize			15
	$\Gamma_{ANTI\text{-}R1}$	$\Gamma_{SYN\text{-}R1}$	$\Gamma_{ANTI\text{-}R3}$	$\Gamma_{SYN\text{-}R3}$	Γ_{ANTI}		Γ_{SYN}	
200	0.475	0.456	0.046	0.024	0.216		0.784	
275	0.474	0.451	0.049	0.026	0.535		0.465	
298	0.473	0.450	0.050	0.027	0.520		0.480	
325	0.472	0.449	0.051	0.028	0.527		0.473	
400	0.469	0.445	0.055	0.031	0.540		0.460	
T (K)	O_3 + Alkene **18**				O_3 + Alkene **20**			
	Grainsize			40	Grainsize			15
	Γ_{ANTI}		Γ_{SYN}		Γ_{DMFO}		Γ_{FO}	
200	0.998		0.002		0.999		0.001	
275	0.879		0.121		0.828		0.172	
298	0.872		0.128		0.842		0.158	
325	0.814		0.186		0.817		0.183	
400	0.798		0.202		0.837		0.163	

*Table 13: Product Branching Ratios of Ozonolysis of Alkenes **2**, **3**, **7**, **8** & **12**.*

O_3 + Alkene **2**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.159	0.132	0.300	0.034	0.027	0.042	0.015	0.016	0.023	0.107	0.001	0.144
275	0.131	0.109	0.190	0.068	0.057	0.073	0.056	0.050	0.065	0.083	0.019	0.100
298	0.130	0.108	0.188	0.068	0.058	0.073	0.057	0.051	0.065	0.082	0.019	0.099
325	0.131	0.109	0.190	0.068	0.057	0.073	0.056	0.050	0.064	0.083	0.019	0.100
400	0.132	0.110	0.193	0.067	0.056	0.072	0.054	0.049	0.063	0.084	0.018	0.102
O_3 + Alkene **3**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.115	0.199	0.151	0.068	0.114	0.074	0.039	0.073	0.057	0.018	0.079	0.013
275	0.111	0.183	0.142	0.072	0.116	0.078	0.044	0.078	0.063	0.022	0.076	0.017
298	0.110	0.180	0.141	0.072	0.117	0.078	0.045	0.079	0.063	0.022	0.075	0.017
325	0.114	0.195	0.149	0.069	0.115	0.075	0.040	0.075	0.058	0.018	0.078	0.014
400	0.107	0.167	0.135	0.075	0.119	0.081	0.048	0.083	0.068	0.025	0.073	0.019
O_3 + Alkene **7**										Grainsize: 25		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{DMFO} (1.1)	Γ_{DMFO} (1.2)	Γ_{DMFO} (1.3)	Γ_{DMFO} (2.1)	Γ_{DMFO} (2.2)	Γ_{DMFO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.029	0.033	0.115	0.142	0.166	0.292	0.034	0.034	0.109	0.018	0.002	0.026
275	0.018	0.023	0.093	0.138	0.185	0.369	0.023	0.024	0.097	0.011	0.001	0.018
298	0.023	0.027	0.102	0.141	0.178	0.334	0.028	0.028	0.103	0.014	0.002	0.021
325	0.046	0.047	0.140	0.141	0.137	0.203	0.050	0.047	0.121	0.027	0.005	0.038
400	0.035	0.038	0.121	0.140	0.157	0.266	0.039	0.038	0.112	0.021	0.003	0.030
O_3 + Alkene **8**										Grainsize:		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{DMFO} (1.1)	Γ_{DMFO} (1.2)	Γ_{DMFO} (1.3)	Γ_{DMFO} (2.1)	Γ_{DMFO} (2.2)	Γ_{DMFO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.000	0.000	0.000	0.040	0.959	0.000	0.000	0.000	0.000	0.000	0.000	0.000
275	0.024	0.045	0.002	0.285	0.495	0.041	0.044	0.056	0.003	0.003	0.001	0.000
298	0.029	0.050	0.003	0.286	0.466	0.044	0.049	0.062	0.003	0.004	0.002	0.001
325	0.025	0.045	0.003	0.285	0.494	0.041	0.044	0.056	0.003	0.004	0.001	0.000
400	0.045	0.066	0.007	0.281	0.381	0.052	0.065	0.080	0.007	0.008	0.004	0.002
O_3 + Alkene **12**										Grainsize: 30		
T (K)	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{ANTI} (3)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (1.3)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{FO} (2.3)	Γ_{SYN} (1)	Γ_{SYN} (2)	Γ_{SYN} (3)
200	0.008	0.021	0.005	0.082	0.345	0.104	0.071	0.292	0.069	0.001	0.001	0.000
275	0.010	0.026	0.007	0.087	0.329	0.109	0.076	0.280	0.072	0.001	0.002	0.000
298	0.010	0.025	0.007	0.086	0.333	0.107	0.074	0.283	0.071	0.001	0.002	0.000
325	0.012	0.029	0.008	0.093	0.316	0.113	0.080	0.271	0.075	0.001	0.002	0.000
400	0.041	0.078	0.030	0.133	0.183	0.141	0.111	0.170	0.089	0.008	0.012	0.003

*Table 14 Product Branching Ratios of Ozonolysis of Alkenes **15** & **16**.*

						O_3 + Alkene **15**				Grainsize: 25		
T (K)	Γ_{ANTI} (1.1)	Γ_{ANTI} (1.2)	Γ_{ANTI} (1.3)	Γ_{SYN} (1.1)	Γ_{SYN} (1.2)	Γ_{SYN} (1.3)	Γ_{ANTI} (2.1)	Γ_{ANTI} (2.2)	Γ_{ANTI} (2.3)	Γ_{SYN} (2.1)	Γ_{SYN} (2.2)	Γ_{SYN} (2.3)
200	0.042	0.135	0.080	0.117	0.115	0.089	0.049	0.132	0.110	0.021	0.088	0.022
275	0.044	0.135	0.081	0.116	0.114	0.088	0.051	0.131	0.110	0.022	0.088	0.022
298	0.044	0.134	0.081	0.115	0.114	0.088	0.051	0.131	0.110	0.022	0.087	0.023
325	0.044	0.134	0.081	0.115	0.113	0.087	0.051	0.131	0.110	0.022	0.087	0.023
400	0.045	0.134	0.081	0.114	0.112	0.086	0.053	0.131	0.110	0.023	0.087	0.024
						O_3 + Alkene **16**				Grainsize:		
T (K)	Γ_{ANTI} (1.1)	Γ_{ANTI} (1.2)	Γ_{ANTI} (1.3)	Γ_{SYN} (1.1)	Γ_{SYN} (1.2)	Γ_{SYN} (1.3)	Γ_{ANTI} (2.1)	Γ_{ANTI} (2.2)	Γ_{ANTI} (2.3)	Γ_{SYN} (2.1)	Γ_{SYN} (2.2)	Γ_{SYN} (2.3)
200	0.133	0.318	0.003	0.000	0.000	0.000	0.139	0.265	0.141	0.000	0.001	0.000
275	0.144	0.221	0.040	0.011	0.022	0.001	0.160	0.192	0.150	0.022	0.030	0.008
298	0.134	0.191	0.053	0.022	0.038	0.004	0.151	0.166	0.137	0.036	0.048	0.020
325	0.140	0.207	0.046	0.016	0.030	0.003	0.155	0.180	0.144	0.029	0.038	0.014
400	0.135	0.195	0.051	0.021	0.036	0.004	0.151	0.169	0.138	0.034	0.046	0.019

*Table 15: Product Branching Ratios of Ozonolysis of Alkenes **5** & **10**.*

T (K)	O_3 + Alkene **5**							
	Grainsize				60			
	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{SYN} (1)	Γ_{SYN} (2)
200	0.008	0.028	0.011	0.597	0.028	0.314	0.001	0.014
275	0.009	0.032	0.014	0.583	0.032	0.313	0.001	0.016
298	0.012	0.035	0.017	0.571	0.036	0.310	0.002	0.018
325	0.019	0.042	0.025	0.539	0.045	0.302	0.004	0.024
400	0.038	0.066	0.048	0.438	0.076	0.283	0.011	0.041
T (K)	O_3 + Alkene **10**							
	Grainsize				60			
	Γ_{ANTI} (1)	Γ_{ANTI} (2)	Γ_{FO} (1.1)	Γ_{FO} (1.2)	Γ_{FO} (2.1)	Γ_{FO} (2.2)	Γ_{SYN} (1)	Γ_{SYN} (2)
200	0.000	0.000	0.001	0.979	0.001	0.019	0.000	0.000
275	0.005	0.019	0.053	0.679	0.035	0.207	0.000	0.003
298	0.005	0.019	0.055	0.674	0.036	0.207	0.000	0.003
325	0.006	0.020	0.057	0.669	0.037	0.208	0.000	0.003
400	0.007	0.023	0.062	0.654	0.040	0.210	0.001	0.004

1.2.4 Epoxide Related Results

Complete Rate Constants and Product Branching Ratios for Epoxide pathways simulations in Section 3.8 of the main manuscript.

*Table 16: Overall and Epoxidation Master Equation Rate Constants (k_{ME}) and Canonical Rate Constants (k_{CAN}) for O_3 + Alkene **1**. (Using B3LYP Energies)*

Rate Constants: O_3 + Alkene 1 Grainsize 20							
T (K)	k_{ME} (Total)	k_{ME} (EPO)	Total k_{CAN}	TS_{OZO} 1.1	TS_{OZO} 1.2	TS_{EPO} 1.1	TS_{EPO} 1.2
200	2.68E-16	1.56E-26	2.68E-16	2.42E-16	2.63E-17	3.59E-28	1.53E-26
275	6.00E-16	1.60E-23	6.00E-16	4.98E-16	1.02E-16	1.31E-24	1.47E-23
298	7.37E-16	7.03E-23	7.37E-16	5.97E-16	1.39E-16	7.39E-24	6.29E-23
325	9.21E-16	3.13E-22	9.21E-16	7.28E-16	1.93E-16	4.20E-23	2.71E-22
400	1.59E-15	7.71E-21	1.59E-15	1.18E-15	4.08E-16	1.66E-21	6.05E-21

*Table 17: Product Branching Ratio both all pathways including the epoxidation pathway for O_3 + Alkene **1**. (Using B3LYP Energies)*

Product Branching Ratio O_3 + Alkene 1 Grainsize 50										
	Γ_{ANTI}	Γ_{FO} (1)	Γ_{FO} (2)	Γ_{SYN}	Γ_{EPO} (1.1)	Γ_{EPO} (1.2)	Γ_{EPO} (2.1)	Γ_{EPO} (2.2)	Γ_{EPO} (2.3)	Γ_{EPO} (2.4)
200	0.616	0.140	0.102	0.142	8.65E-29	1.98E-29	4.70E-18	2.00E-16	8.52E-26	2.82E-27
275	0.566	0.157	0.128	0.149	1.25E-20	1.52E-21	1.66E-10	1.86E-09	1.91E-17	5.13E-19
298	0.578	0.154	0.120	0.149	4.42E-19	7.45E-20	2.34E-09	1.99E-08	3.43E-16	1.34E-17
325	0.566	0.157	0.128	0.149	1.25E-20	1.52E-21	1.66E-10	1.86E-09	1.91E-17	5.13E-19
400	0.450	0.199	0.183	0.168	2.88E-15	8.58E-16	1.04E-06	3.79E-06	4.10E-13	4.37E-14

*Table 18: Overall and Epoxidation Master Equation Rate Constants (k_{ME}) and Canonical Rate Constants (k_{CAN}) for O_3 + Alkene **5**. (Using B3LYP Energies)*

Rate Constants: O_3 + Alkene 5 Grainsize 20											
T (K)	k_{ME} (Total)	k_{ME} (EPO)	Total k_{CAN}	TS_{OZO} 1.1	TS_{OZO} 1.2	TS_{OZO} 2.1	TS_{OZO} 2.2	TS_{EPO} 1.1	TS_{EPO} 1.2	TS_{EPO} 1.3	TS_{EPO} 1.4
200	4.09E-17	8.44E-28	3.94E-17	2.08E-18	3.65E-19	3.68E-17	1.57E-19	5.44E-30	1.59E-28	2.72E-30	6.46E-28
275	1.23E-16	2.36E-24	1.29E-16	1.39E-17	3.65E-18	1.09E-16	1.96E-18	5.62E-26	7.11E-25	2.74E-26	1.50E-24
298	1.60E-16	1.16E-23	1.72E-16	2.13E-17	6.07E-18	1.41E-16	3.41E-18	3.91E-25	4.17E-24	1.90E-25	7.69E-24
325	2.20E-16	6.42E-23	2.34E-16	3.31E-17	1.02E-17	1.85E-16	6.01E-18	2.74E-24	2.47E-23	1.32E-24	3.96E-23
400	5.20E-16	2.74E-21	4.89E-16	8.83E-17	3.23E-17	3.47E-16	2.09E-17	1.67E-22	1.05E-21	7.96E-23	1.27E-21

1.3 Relative Energies, Enthalpies and Gibbs Free Energies.

1.3.1 Main Computational Results

The Relative Energies, Enthalpies and Gibbs Free Energies in this section is based on the DF-LCCSD(T)-F12a molecular energy calculations, used for vast majority of analysis

*Table 19: Relative Energies of O_3 + Alkene **1** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-18.43	-14.65	-13.38	21.63
TSOzo1	5.45	11.59	8.51	56.97
POZ1	-254.53	-235.22	-240.87	-186.41
PRC2	-18.27	-14.82	-13.21	19.76
TSOzo2	9.87	15.96	12.93	61.14
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TSpoz1	-241.46	-223.97	-231.14	-172.84
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TSpoz2	-241.99	-224.36	-231.40	-173.44
POZ2	-254.91	-235.70	-241.53	-186.34
POZ1	-254.53	-235.22	-240.87	-186.41
TS_{Anti} 1	-172.31	-162.77	-167.46	-114.40
C_{ANTI}	-273.71	-266.76	-267.15	-225.00
HCHO + Anti-RCHOO	-231.60	-234.74	-233.24	-233.71
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{FO} 1	-166.50	-156.71	-161.60	-108.14
$C_{FO\ 1}$	-263.60	-259.95	-258.36	-223.57
RCHO + HCHOO	-238.38	-239.30	-238.95	-241.66
POZ2	-254.91	-235.60	-241.26	-186.80
TS_{FO} 2	-164.11	-154.11	-158.96	-105.96
C_{FO} 2	-258.38	-256.17	-253.22	-227.23
	-238.38	-239.30	-238.95	-241.66
POZ2				
TS_{Syn}	-254.91	-235.70	-241.53	-186.34
C_{SYN}	-171.23	-161.14	-166.17	-112.08
HCHO + Syn-RCHOO	-275.28	-271.46	-270.32	-232.19

*Table 20: Relative Energies of O_3 + Alkene **2** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 2			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$EtCHCH_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$EtCHCH_2$ con 2 + O_3	0.28	0.64	0.34	1.35
PRC1.1	-19.79	-16.27	-14.71	19.99
TSOzo1.1	5.09	11.18	8.34	56.93
POZ1.1	-254.56	-235.71	-241.00	-185.95
PRC1.2	-20.79	-16.89	-15.71	20.57
TSOzo1.2	4.49	10.90	7.67	57.88
POZ1.2	-253.16	-234.23	-239.54	-184.52
PRC1.3	-14.74	-11.97	-9.75	20.88
TSOzo1.3	5.54	10.66	8.07	56.40
POZ1.3	-255.60	-236.90	-242.17	-187.13
PRC2.1	-17.80	-14.51	-12.66	20.10
TSOzo2.1	9.14	15.38	12.50	61.15
POZ2.1	-255.50	-236.70	-242.16	-186.33
PRC2.2	-16.74	-13.23	-11.63	22.06
TSOzo2.2	10.73	17.28	14.04	63.98
POZ2.2	-252.58	-233.64	-239.15	-183.07
PRC2.3	-15.76	-12.90	-10.73	19.93
TSOzo2.3	7.48	12.60	9.92	58.39
POZ2.3	-256.92	-238.39	-243.83	-188.04
POZ1.1	-254.56	-235.71	-241.00	-185.95
TS_{Anti} 1	-171.83	-162.54	-166.95	-113.30
C_{anti} 1	-274.18	-267.33	-267.35	-224.89
HCHO + *Anti*-EtCHOO Con 2	-230.48	-233.31	-231.68	-232.47
POZ1.2	-253.16	-234.23	-239.54	-184.52
TS_{Anti} 2	-171.97	-162.32	-166.83	-112.79
C_{anti} 2	-275.74	-269.04	-269.22	-226.30
HCHO + *Anti*-EtCHOO Con 1	-232.30	-235.39	-233.92	-233.79
POZ1.3	-255.60	-236.90	-242.17	-187.13
TS_{Anti} 3	-173.80	-164.43	-168.79	-115.45
C_{anti} 3	-272.75	-265.82	-265.83	-223.93
HCHO + *Anti*-EtCHOO Con 2	-230.48	-233.31	-231.68	-232.47
POZ1.1	-254.56	-235.71	-241.00	-185.95
TS_{FO} 1.1	-167.32	-158.01	-162.56	-108.70
C_{FO} 1.1	-262.48	-258.73	-256.68	-223.08
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ1.2	-253.16	-234.23	-239.54	-184.52
TS_{FO} 1.2	-167.10	-157.45	-162.07	-108.04
C_{FO} 1.2	-263.50	-260.77	-258.41	-226.73
HCHOO + EtCHOO Con 1	-240.75	-241.47	-241.31	-243.49
POZ1.3	-255.60	-236.90	-242.17	-187.13
TS_{FO} 1.3	-168.02	-158.53	-163.07	-109.21
C_{FO} 1.3	-267.16	-262.29	-260.89	-224.91
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ2.1	-255.50	-236.70	-242.16	-186.33
TS_{FO} 2.1	-164.73	-155.37	-159.84	-106.39
C_{FO} 2.1	-254.40	-252.39	-248.81	-229.31
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30

POZ2.2	-252.58	-233.64	-239.15	-183.07
TS_{FO} 2.2	-165.60	-155.96	-160.52	-106.68
C_{FO} 2.2	-260.15	-257.86	-254.77	-229.95
HCHOO + EtCHOO Con 1	-240.75	-241.47	-241.31	-243.49
POZ2.3	-256.92	-238.39	-243.83	-188.04
TS_{FO} 2.3	-166.18	-156.66	-161.10	-107.63
C_{FO} 2.3	-252.75	-249.15	-247.06	-213.44
HCHOO + EtCHOO Con 2	-236.82	-237.35	-236.98	-240.30
POZ2.1	-255.50	-236.70	-242.16	-186.33
TS_{Syn} 1	-172.05	-162.47	-167.22	-112.36
C_{syn} 1	-274.35	-271.35	-269.74	-231.98
HCHO + *Syn*-RCHOO Con2	-244.58	-247.65	-246.48	-246.05
POZ2.2	-252.58	-233.64	-239.15	-183.07
TS_{Syn} 2	-160.28	-150.66	-155.37	-100.89
C_{syn} 2	-262.65	-260.91	-257.37	-229.45
HCHO + *Syn*-RCHOO Con1	-242.24	-243.61	-242.67	-241.56
POZ2.3	-256.92	-238.39	-243.83	-188.04
TS_{Syn} 3	-173.28	-163.32	-168.02	-113.34
C_{syn} 3	-272.09	-267.42	-266.00	-227.72
HCHO + *Syn*-RCHOO Con1	-242.24	-243.61	-242.67	-241.56

*Table 21: Relative Energies of O_3 + Alkene **3** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 3			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
iPrCHCH$_2$ con 1 + O_3	0.00	0.00	0.00	0.00
iPrCHCH$_2$ con 2 + O_3	1.07	1.73	1.40	2.43
PRC1.1	-19.29	-15.21	-13.84	22.00
TSOzo1.1	3.23	9.81	6.80	57.01
POZ1.1	-253.05	-234.17	-239.33	-183.57
PRC1.2	-14.45	-11.80	-9.36	20.79
TSOzo1.2	5.19	10.85	8.22	57.28
POZ1.2	-255.46	-236.81	-241.95	-186.07
PRC1.3	-13.87	-10.68	-8.56	22.12
TSOzo1.3	8.62	14.68	11.81	62.10
POZ1.3	-252.61	-233.81	-238.95	-183.32
PRC2.1	-15.71	-11.95	-10.25	23.40
TSOzo2.1	10.15	16.95	13.88	64.19
POZ2.1	-252.69	-233.69	-239.03	-182.28
PRC2.2	-15.10	-12.38	-9.95	20.00
TSOzo2.2	9.23	15.06	12.27	61.70
POZ2.2	-256.81	-238.24	-243.56	-187.01
PRC2.3	-14.49	-11.16	-9.12	22.26
TSOzo2.3	12.23	18.53	15.49	66.12
POZ2.3	-252.94	-234.11	-239.49	-182.71
POZ1.1	-253.05	-234.17	-239.33	-183.57
TS_{Anti} 1	-170.80	-161.17	-165.49	-110.94
C_{anti} 1	-275.14	-268.24	-268.15	-225.11
HCHO + *Anti*-IPrCHOO Con 2	-230.57	-233.20	-231.59	-231.76
POZ1.2	-255.46	-236.81	-241.95	-186.07
TS_{Anti} 2	-173.17	-163.77	-168.03	-113.79
C_{anti} 2	-273.60	-266.66	-266.35	-224.06
HCHO + *Anti*-IPrCHOO Con 1	-229.52	-232.22	-230.41	-231.49
POZ1.3	-252.61	-233.81	-238.95	-183.32
TS_{Anti} 3	-172.03	-162.26	-166.54	-112.28
C_{anti} 3	-274.29	-267.26	-267.13	-224.58
HCHO + *Anti*-IPrCHOO Con 2	-230.57	-233.20	-231.59	-231.76
POZ1.1	-253.05	-234.17	-239.33	-183.57
TS_{FO} 1.1	-167.02	-157.49	-161.97	-107.47
C_{FO} 1.1	-269.00	-264.29	-262.91	-225.17
HCHOO + IPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ1.2	-255.46	-236.81	-241.95	-186.07
TS_{FO} 1.2	-168.20	-158.94	-163.30	-109.52
C_{FO} 1.2	-262.24	-258.42	-256.02	-222.93

HCHOO + IPrCHO Con 1	-236.77	-236.98	-236.72	-239.42
POZ1.3	-252.61	-233.81	-238.95	-183.32
TS_{FO} 1.3	-166.88	-157.28	-161.66	-107.45
C_{FO} 1.3	-261.07	-257.99	-255.31	-224.78
HCHOO + IPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ2.1	-252.69	-233.69	-239.03	-182.28
TS_{FO} 2.1	-163.47	-153.96	-158.36	-103.84
C_{FO} 2.1	-257.09	-254.73	-251.26	-229.83
HCHOO + IPrCHO Con 2	-236.77	-236.99	-236.57	-240.13
POZ2.2	-256.81	-238.24	-243.56	-187.01
TS_{FO} 2.2	-166.41	-157.12	-161.46	-107.28
C_{FO} 2.2	-257.10	-254.42	-251.05	-226.90
HCHOO + IPrCHO Con 1	-238.76	-238.97	-238.72	-241.42
POZ2.3	-252.94	-234.11	-239.49	-182.71
TS_{FO} 2.3	-165.00	-155.49	-159.79	-105.66
C_{FO} 2.3	-257.09	-254.73	-251.26	-229.83
HCHOO + IPrCHO Con 2	-238.76	-238.97	-238.72	-241.42
POZ2.1	-252.69	-233.69	-239.03	-182.28
TS_{Syn} 1	-160.09	-150.47	-155.15	-100.06
C_{syn} 1	-261.06	-259.90	-256.04	-229.02
HCHO + *Syn*-IPRCHOO Con2	-241.25	-243.13	-241.95	-240.82
POZ2.2	-256.81	-238.24	-243.56	-187.01
TS_{Syn} 2	-170.93	-161.07	-165.66	-110.04
C_{syn} 2	-273.81	-269.33	-267.78	-228.79
HCHO + *Syn*-IPRCHOO Con1	-241.25	-243.13	-241.95	-240.82
$TS_{ISO-syn}$	-214.73	-216.68	-217.74	-211.43
HCHO + *Syn*-IPRCHOO Con2	-241.25	-243.13	-241.95	-240.82
POZ2.3	-252.94	-234.11	-239.49	-182.71
TS_{Syn} 3	-159.58	-149.55	-154.14	-98.74
C_{syn} 3	-258.81	-254.77	-252.52	-216.06
HCHO + *Syn*-IPRCHOO Con1	-232.50	-233.76	-232.48	-231.33

*Table 22: Relative Energies of O_3 + Alkene **4** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 4			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-15.54	-12.97	-10.45	19.48
TSOzo1	4.65	10.25	7.70	57.57
POZ1	-253.90	-235.92	-240.68	-185.31
PRC2	-17.88	-15.34	-12.78	16.62
TSOzo2	11.41	17.26	14.55	64.78
POZ2	-254.59	-236.49	-241.47	-185.03
POZ1	-253.90	-235.92	-240.68	-185.31
TS_{Anti} 1	-173.06	-164.1	-167.98	-113.91
C_{ANTI}	-276.02	-269.74	-269.06	-227.35
HCHO + Anti-RCHOO	-231.15	-234.43	-232.32	-233.83
POZ1	-253.90	-235.92	-240.68	-185.31
TS_{FO} 1	-168.56	-159.7	-163.84	-109.85
$C_{FO\ 1}$	-269.51	-265.56	-263.43	-228.42
RCHO + HCHOO	-240.54	-241.35	-240.65	-244.73
POZ2	-254.59	-236.49	-241.47	-185.03
TS_{FO} 2	-163.64	-154.9	-158.95	-104.95
C_{FO} 2	-258.84	-257.02	-253.14	-231.57
POZ2	-254.59	-236.49	-241.47	-185.03
TS_{Syn}	-160.76	-151.5	-155.88	-100.30
C_{SYN}	-258.57	-255.77	-253.11	-217.46
HCHO + Syn-RCHOO	-233.27	-235.59	-234.04	-233.33

*Table 23: Relative Energies of O_3 + Alkene **5** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
MVK con 2 + O_3	0.00	0.00	0.00	0.00
TSmvk	22.60	20.01	18.56	21.79
MVK con 1 + O_3	2.30	1.68	1.86	1.21
PRC1.1	-15.65	-13.35	-10.69	17.58
TSiso1.1	8.19	8.12	9.06	44.3
PRC1.2	-14.31	-12.10	-9.77	21.70
PRC2.1	-15.65	-13.35	-10.69	17.58
TSiso2.1	6.90	6.49	8.00	39.3
PRC2.2	-18.75	-16.01	-14.02	19.65
PRC2.1	-15.65	-13.35	-10.69	17.58
TSiso2.2	9.27	9.13	10.25	43.1
PRC2.2	-18.75	-16.01	-14.02	19.65
PRC1.1	-15.65	-13.3	-10.69	17.58
TSOzo1.1	9.92	15.2	12.46	62.0
POZ1.1	-219.69	-203.50	-208.01	-155.52
PRC1.2	-14.31	-12.10	-9.77	21.70
TSOzo1.2	11.72	17.4	14.46	64.6
POZ1.2	-236.61	-220.08	-224.82	-171.52
PRC2.1	-10.64	-9.0	-5.61	15.95
TSOzo2.1	2.29	7.8	5.01	54.9
POZ2.1	-224.38	-208.15	-212.79	-159.25
PRC2.2	-18.75	-16.01	-14.02	19.65
TSOzo2.2	12.70	18.3	15.40	65.7
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52
TSpoz1.1	-207.86	-193.10	-199.35	-141.89
POZ2.1	-224.38	-208.15	-212.79	-159.25
POZ1.2	-236.61	-220.08	-224.82	-171.52
TSpoz1.2	-219.32	-204.50	-210.52	-153.80
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.2	-236.61	-220.08	-224.82	-171.52
TSpoz1.3	-228.72	-213.61	-220.02	-161.87
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52
TSpoz2.1	-211.57	-195.09	-202.32	-141.91
POZ1.2	-236.61	-220.08	-224.82	-171.52
POZ1.1	-236.61	-220.08	-224.82	-171.52
TSpoz2.2	-217.82	-201.56	-208.48	-148.75
POZ1.2	-239.44	-222.76	-227.65	-173.95
POZ2.1	-224.38	-208.15	-212.79	-159.25
TSpoz2.3	-212.31	-195.68	-202.99	-142.43
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ2.1	-224.38	-208.15	-212.79	-159.25
TSpoz2.4	-220.97	-204.79	-211.71	-151.75
POZ2.2	-239.44	-222.76	-227.65	-173.95
POZ1.1	-219.69	-203.50	-208.01	-155.52

TS_{Anti} 1	-140.62	-133.30	-137.01	-85.09
C_{anti} 1	-212.65	-212.56	-208.71	-186.29
HCHO + Anti-RCHOO Con 2	-191.21	-193.72	-192.92	-198.03
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{Anti} 2	-166.69	-158.76	-162.64	-110.07
C_{anti} 2	-249.38	-245.29	-244.10	-204.37
HCHO + Anti-RCHOO Con1	-213.05	-214.56	-213.99	-217.76
$TS_{ISO-ANTI}$	-188.11	-191.60	-192.68	-192.50
HCHO + Anti-RCHOO Con 2	-191.21	-193.72	-192.92	-198.03
POZ1.1	-224.38	-208.15	-212.79	-159.25
TS_{FO} 1.1	-146.22	-139.00	-142.76	-90.52
C_{FO} 1.1	-240.21	-234.56	-234.44	-190.30
HCHOO + RCHO con 1	-191.21	-193.72	-192.92	-198.03
POZ1.2	-239.44	-222.76	-227.65	-173.95
TS_{FO} 1.2	-163.33	-155.48	-159.33	-106.35
C_{FO} 1.2	-249.11	-244.23	-243.61	-201.60
HCHOO + RCHO con 2	-213.05	-214.56	-213.99	-217.76
$TS_{ISO-ALDE}$				
HCHOO + RCHO con 1	-224.38	-208.15	-212.79	-159.25
	-124.64	-118.23	-121.66	-70.22
POZ2.1	-195.65	-197.07	-192.13	-173.74
TS_{FO} 2.1	-178.76	-182.80	-181.07	-182.49
C_{FO} 2.1	-219.69	-203.50	-208.01	-155.52
HCHOO + RCHO con 1	-140.62	-133.30	-137.01	-85.09
	-212.65	-212.56	-208.71	-186.29
POZ2.2	-191.21	-193.72	-192.92	-198.03
TS_{FO} 2.2				
C_{FO} 2.2	-236.61	-220.08	-224.82	-171.52
HCHOO + RCHO con 2	-166.69	-158.76	-162.64	-110.07
	-249.38	-245.29	-244.10	-204.37
POZ2.1	-213.05	-214.56	-213.99	-217.76
TS_{Syn} 1	-188.11	-191.60	-192.68	-192.50
C_{syn} 1	-191.21	-193.72	-192.92	-198.03
HCHO + Syn-RCHOO Con2	-178.76	-182.80	-181.07	-182.49
$TS_{ISO-SYN}$	-175.10	-180.25	-180.63	-176.25
HCHO + Syn-RCHOO Con1	-202.98	-205.92	-204.89	-204.20
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{Syn} 2	-144.94	-137.01	-141.24	-88.00
C_{syn} 2	-225.90	-225.69	-222.20	-191.88

*Table 24: Relative Energies of O_3 + Alkene **6** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 6			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-12.20	-9.73	-7.64	26.04
TSOzo1	-5.62	-1.64	-3.39	44.63
POZ1	-271.15	-253.73	-259.68	-200.52
PRC2	-25.31	-22.41	-20.55	14.56
TSOzo2	-2.30	2.37	0.03	50.09
POZ2	-267.79	-250.36	-256.36	-197.69
POZ1	-271.15	-253.73	-259.68	-200.52
TSpoz1	-259.61	-244.01	-251.25	-188.39
POZ2	-267.79	-250.36	-256.36	-197.69
POZ1	-271.15	-253.73	-259.68	-200.52

TS_{Anti} 1	-189.30	-180.14	-184.97	-127.65
C_{ANTI}	-312.63	-309.87	-307.32	-275.16
$(CH_3)_2CO$ + *Anti*-CH_3CHOO	-280.30	-281.66	-280.77	-288.59
POZ1	-271.15	-253.73	-259.68	-200.52
TS_{DMFO} 1	-200.47	-191.43	-196.54	-138.13
C_{DMFO} 1	-330.72	-328.31	-326.11	-290.79
RCHO + $(CH_3)_2COO$	-296.05	-297.38	-297.35	-299.45
POZ2	-267.79	-250.36	-256.36	-197.69
TS_{DMFO} 2	-191.68	-182.27	-187.33	-129.23
C_{DMFO} 2	-326.83	-324.95	-322.60	-288.00
POZ2	-267.79	-250.36	-256.36	-197.69
TS_{Syn}	-184.69	-174.95	-180.19	-121.51
C_{SYN}	-321.21	-318.67	-315.95	-285.91
$(CH_3)_2CO$ + *Syn*-CH_3CHOO	-295.15	-295.68	-295.47	-302.28

*Table 25: Relative Energies of O_3 + Alkene **7** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 2			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$EtCHC(CH_3)_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$EtCHC(CH_3)_2$ con 2 + O_3	17.71	18.76	18.41	19.36
PRC1.1	-11.84	-9.42	-7.20	26.17
TSOzo1.1	-5.44	-0.84	-2.76	46.58
POZ1.1	-267.79	-250.50	-256.25	-195.91
PRC1.2	-12.85	-10.77	-8.46	25.04
TSOzo1.2	7.99	13.00	10.85	61.52
POZ1.2	-258.99	-241.99	-247.44	-188.94
PRC1.3	-12.85	-10.77	-8.46	25.04
TSOzo1.3	-5.83	-2.22	-4.03	45.81
POZ1.3	-270.62	-253.79	-259.37	-199.78
PRC2.1	-23.51	-20.69	-18.74	16.16
TSOzo2.1	-0.22	4.98	2.61	53.58
POZ2.1	-264.31	-247.30	-252.93	-192.89
PRC2.2	-23.51	-20.69	-18.74	16.16
TSOzo2.2	9.47	15.24	12.49	65.35
POZ2.2	-256.15	-238.92	-244.52	-185.54
PRC2.3	-23.51	-20.69	-18.74	16.16
TSOzo2.3	-4.55	-0.44	-2.69	48.56
POZ2.3	-267.99	-251.27	-256.87	-197.65
POZ1.1	-267.79	-250.50	-256.25	-195.91
TS_{Anti} 1	-180.40	-171.36	-175.98	-117.98
C_{anti} 1	-318.68	-315.65	-312.93	-278.89
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 2	-278.90	-279.79	-278.94	-287.21
POZ1.2	-258.99	-241.99	-247.44	-188.94
TS_{Anti} 2	-184.94	-175.31	-180.18	-121.25
C_{anti} 2	-310.49	-307.59	-304.76	-273.51
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 1	-280.72	-281.87	-281.18	-288.53
POZ1.3	-270.62	-253.79	-259.37	-199.78
TS_{Anti} 3	-189.88	-180.85	-185.40	-127.80
C_{anti} 3	-310.49	-307.59	-304.76	-273.51
$(CH_3)_2CO$ + *Anti*-EtCHOO Con 2	-278.90	-279.79	-278.94	-287.21

POZ1.1	-267.79	-250.50	-256.25	-195.91
TS_{DMFO} 1.1	-194.63	-186.08	-190.86	-132.13
C_{DMFO} 1.1	-328.47	-325.89	-323.49	-289.44
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ1.2	-258.99	-241.99	-247.44	-188.94
TS_{DMFO} 1.2	-198.57	-189.49	-194.50	-135.08
C_{DMFO} 1.2	-332.78	-330.40	-328.20	-292.52
$(CH_3)_2COO$ + EtCHO Con 1	-298.14	-299.11	-299.43	-301.15
POZ1.3	-270.62	-253.79	-259.37	-199.78
TS_{DMFO} 1.3	-201.33	-192.45	-197.33	-138.42
C_{DMFO} 1.3	-325.45	-323.44	-320.75	-287.65
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.1	-264.31	-247.30	-252.93	-192.89
TS_{DMFO} 2.1	-183.16	-174.26	-178.99	-120.45
C_{DMFO} 2.1	-330.14	-327.84	-325.63	-289.76
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.2	-256.15	-238.92	-244.52	-185.54
TS_{DMFO} 2.2	-184.96	-175.65	-180.49	-121.51
C_{DMFO} 2.2	-333.69	-331.27	-329.09	-293.44
$(CH_3)_2COO$ + EtCHO Con 1	-298.14	-299.11	-299.43	-301.15
POZ2.3	-267.99	-251.27	-256.87	-197.65
TS_{DMFO} 2.3	-192.15	-183.30	-187.99	-129.55
C_{DMFO} 2.3	-328.78	-326.20	-323.86	-289.29
$(CH_3)_2COO$ + EtCHO Con 2	-294.20	-295.00	-295.10	-297.96
POZ2.1	-264.31	-247.30	-252.93	-192.89
TS_{Syn} 1	-181.53	-172.18	-177.20	-117.61
C_{syn} 1	-321.93	-319.83	-317.03	-286.05
$(CH_3)_2CO$ + *Syn*-EtCHOO Con2	-292.99	-294.13	-293.74	-300.79
POZ2.2	-256.15	-238.92	-244.52	-185.54
TS_{Syn} 2	-168.80	-159.11	-164.27	-103.99
C_{syn} 2	-314.85	-311.53	-308.56	-279.01
$(CH_3)_2CO$ + *Syn*-EtCHOO Con1	-290.66	-290.09	-289.93	-296.31
POZ2.3	-267.99	-251.27	-256.87	-197.65
TS_{Syn} 3	-183.86	-174.15	-179.12	-119.90
C_{syn} 3	-317.73	-314.05	-311.41	-279.77
$(CH_3)_2CO$ + *Syn*-EtCHOO Con1	-290.66	-290.09	-289.93	-296.31

*Table 26: Relative Energies of O_3 + Alkene **8** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 3			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
iPrCHC$(CH_3)_2$ con 1 + O_3	**0.00**	**0.00**	**0.00**	**0.00**
TS_{ISOiPR}	21.71	20.69	18.30	25.03
iPrCHC$(CH_3)_2$ con 3 + O_3	18.00	19.45	19.00	19.82
iPrCHC$(CH_3)_2$ con 2 + O_3	13.39	14.17	14.01	15.65
PRC1.1	-13.44	-10.81	-8.67	26.09
TS_{ISO}	7.06	10.05	9.85	50.1
PRC1.3	4.50	8.45	10.18	45.39
PRC1.1	-13.44	-10.81	-8.67	26.09
TSOzo1.1	-1.44	3.18	1.06	52.32
POZ1.1	-267.16	-249.83	-255.59	-194.08
PRC1.2	-13.44	-10.81	-8.67	26.09
TSOzo1.2	5.96	10.86	8.65	60.07
POZ1.2	-258.98	-241.86	-247.38	-187.83
PRC1.3	4.50	8.45	10.18	45.39
TSOzo1.3	11.66	17.02	15.10	64.70
POZ1.3	-258.98	-241.01	-246.79	-185.70
PRC2.1	-19.47	-16.91	-14.56	18.09
TSOzo2.1	-0.68	4.76	2.05	55.13
POZ2.1	-258.98	-242.09	-247.64	-186.87
PRC2.2	-19.47	-16.91	-14.56	18.09
TSOzo2.2	8.12	13.79	10.99	64.45
POZ2.2	-256.16	-239.10	-244.60	-186.41
PRC2.3	-8.13	-4.61	-2.51	33.10
TSOzo2.3	14.77	20.66	18.40	69.21
POZ2.3	-252.45	-234.55	-240.32	-179.01
POZ1.1	-267.16	-249.83	-255.59	-194.08
TS_{Anti} 1	-179.85	-170.34	-175.01	-116.25
C_{anti} 1	-319.05	-315.64	-312.83	-279.01
$(CH_3)_2CO$ + *Anti*-iPrCHOO Con 2	-277.90	-278.44	-277.61	-286.25
POZ1.2	-258.98	-241.86	-247.38	-187.83
TS_{Anti} 2	-184.69	-174.86	-179.70	-120.49
C_{anti} 2	-311.14	-307.96	-305.17	-273.80
$(CH_3)_2CO$ + *Anti*-IPrCHOO Con 1	-278.95	-279.42	-278.80	-286.52
POZ1.3	-258.98	-241.01	-246.79	-185.70
TS_{Anti} 3	-170.55	-160.37	-165.34	-105.39
C_{anti} 3	-321.13	-317.73	-315.16	-280.47
$(CH_3)_2CO$ + *Anti*-IPrCHOO Con 2	-278.95	-279.42	-278.80	-286.52
POZ1.1	-267.16	-249.83	-255.59	-194.08
TS_{DMFO} 1.1	-193.44	-184.77	-189.54	-130.69
C_{DMFO} 1.1	-330.15	-327.21	-324.92	-290.14
$(CH_3)_2COO$ + IPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ1.2	-258.98	-241.86	-247.38	-187.83
TS_{DMFO} 1.2	-199.95	-190.65	-195.62	-135.72
C_{DMFO} 1.2	-330.15	-327.21	-324.92	-290.14
$(CH_3)_2COO$ + IPrCHO Con 1	-294.11	-294.36	-294.79	-297.09
POZ1.3	-258.98	-241.01	-246.79	-185.70
TS_{DMFO} 1.3	-187.62	-178.02	-183.19	-122.26
C_{DMFO} 1.3	-316.09	-312.93	-310.61	-278.63

$(CH_3)_2COO$ + IPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.1	-258.98	-242.09	-247.64	-186.87
TS_{DMFO} 2.1	-183.76	-174.87	-179.61	-120.29
C_{DMFO} 2.1	-328.56	-325.74	-323.35	-289.16
$(CH_3)_2COO$ + IPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.2	-256.16	-239.10	-244.60	-186.41
TS_{DMFO} 2.2	-184.91	-175.72	-180.36	-121.40
C_{DMFO} 2.2	-321.01	-319.33	-316.29	-288.10
$(CH_3)_2COO$ + IPrCHO Con 1	-294.11	-294.38	-294.64	-297.81
POZ2.3	-252.45	-234.55	-240.32	-179.01
TS_{DMFO} 2.3	-170.14	-160.60	-165.51	-105.56
C_{DMFO} 2.3	-325.14	-322.87	-319.93	-290.30
$(CH_3)_2COO$ + IPrCHO Con 2	-296.11	-296.36	-296.79	-299.09
POZ2.1	-258.98	-242.09	-247.64	-186.87
TS_{Syn} 1	-173.99	-163.87	-169.05	-108.17
C_{syn} 1	-318.31	-315.03	-312.23	-281.56
$(CH_3)_2CO$ + *Syn*-IPRCHOO Con2	-289.63	-289.34	-289.15	-295.58
POZ2.2	-256.16	-239.10	-244.60	-186.41
TS_{Syn} 2	-168.61	-158.48	-163.65	-102.69
C_{syn} 2	-305.52	-301.70	-298.70	-268.15
$(CH_3)_2CO$ + *Syn*-IPRCHOO Con1	-289.63	-289.34	-289.15	-295.58
POZ2.3	-258.98	-241.01	-246.79	-185.70
TS_{Syn} 3	-159.57	-150.24	-154.97	-95.77
C_{syn} 3	-312.92	-310.07	-306.91	-278.46
$(CH_3)_2CO$ + *Syn*-IPRCHOO Con1	-280.88	-279.97	-279.69	-286.09

*Table 27: Relative Energies of O_3 + Alkene **9** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 10			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-23.80	-21.19	-18.93	14.70
TSOzo1	-0.72	3.73	1.94	52.00
POZ1	-265.48	-248.24	-253.74	-193.92
PRC2	-23.22	-20.41	-18.23	16.77
TSOzo2	1.08	6.34	4.01	55.51
POZ2	-265.57	-248.45	-253.93	-193.99
POZ1	-265.48	-248.24	-253.74	-193.92
TS_{Anti} 1	-184.71	-175.09	-179.75	-121.45
C_{ANTI}	-334.98	-332.20	-329.08	-297.29
$(CH_3)_2CO$ + *Anti*-tBuCHOO	-293.11	-294.15	-293.11	-303.48
POZ1	-265.48	-248.24	-253.74	-193.92
TS_{DMFO} 1	-200.90	-191.88	-196.89	-137.50
$C_{DMFO\ 1}$	-339.76	-338.02	-334.65	-307.46
tBuCHO + $(CH_3)_2COO$	-311.47	-312.25	-312.31	-317.30
POZ2	-265.57	-248.45	-253.93	-193.99
TS_{DMFO} 2	-183.05	-174.16	-178.82	-120.51
C_{DMFO} 2	-339.76	-338.02	-334.65	-307.46
POZ2	-265.57	-248.45	-253.93	-193.99
TS_{Syn}	-169.22	-159.80	-164.50	-105.60
C_{SYN}	-320.02	-317.27	-313.99	-285.40
$(CH_3)_2CO$ + *Syn*-tBuCHOO	-295.23	-295.32	-294.84	-302.99

*Table 28: Relative Energies of O_3 + Alkene **10** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
Mes Oxy Con 2 + O_3	0.00	0.00	0.00	0.00
$TS_{MES-OXY}$	16.30	14.95	12.56	24.50
Mes Oxy Con 1 + O_3	9.26	11.12	10.32	16.32
PRC1.1	-14.80	-12.92	-10.23	22.85
TS_{PRC}1.1	-3.67	-2.37	-2.52	44.19
PRC1.2	-8.30	-4.50	-2.52	34.74
PRC1.1	-14.80	-12.92	-10.23	22.85
TSOzo1.1	7.69	12.77	9.90	67.34
POZ1.1	-238.08	-222.39	-228.17	-163.01
PRC1.2	-8.30	-4.50	-2.52	34.74
TSOzo1.2	16.42	22.20	19.24	76.83
POZ1.2	-252.19	-236.22	-242.17	-176.60
PRC2.1	-23.18	-20.60	-18.24	18.76
TSOzo2.1	4.90	10.38	7.41	65.33
POZ2.1	-237.89	-222.33	-228.10	-162.51
PRC2.2	-7.06	-3.08	-0.71	30.52
TSOzo2.2	14.67	21.02	17.79	76.57
POZ2.2	-252.78	-236.77	-242.72	-177.13
POZ1.1	-238.08	-222.39	-228.17	-163.01
TS_{Anti} 1	-150.50	-142.57	-147.17	-84.56
C_{anti} 1	-274.60	-271.57	-269.49	-230.17
$(CH_3)_2CO$ + Anti-RCHOO Con 1	-256.49	-256.79	-256.80	-257.97
POZ1.2	-252.19	-236.22	-242.17	-176.60
TS_{Anti} 2	-166.05	-157.48	-162.46	-98.13
C_{anti} 2	-284.11	-281.23	-278.92	-240.87
$(CH_3)_2CO$ + Anti-RCHOO Con 2	-241.83	-242.72	-242.55	-244.16
POZ1.1	-238.08	-222.39	-228.17	-163.01
TS_{FO} 1.1	-171.70	-163.75	-168.53	-104.90
C_{FO} 1.1	-299.10	-295.41	-294.57	-247.29
HCHOO + RCHO con 1	-245.05	-246.58	-247.08	-245.14
POZ1.2	-252.19	-236.22	-242.17	-176.60
TS_{FO} 1.2	-198.49	-189.68	-194.87	-129.68
C_{FO} 1.2	-309.06	-305.44	-304.47	-257.88
HCHOO + RCHO con 2	-266.88	-267.41	-268.15	-264.87
POZ2.1	-237.89	-222.33	-228.10	-162.51
TS_{FO} 2.1	-171.05	-162.99	-167.89	-103.43
C_{FO} 2.1	-300.77	-296.69	-296.29	-246.51
POZ2.2	-252.78	-236.77	-242.72	-177.13
TS_{FO} 2.2	-190.41	-181.46	-186.74	-120.96
C_{FO} 2.2	-307.42	-303.64	-302.64	-256.27
POZ2.1	-237.89	-222.33	-228.10	-162.51
TS_{Syn} 1	-129.70	-122.32	-126.91	-64.62
C_{syn} 1	-256.92	-254.45	-252.06	-214.15
$(CH_3)_2CO$ + Syn-RCHOO Con2	-223.63	-224.49	-224.37	-226.68
POZ2.2	-252.78	-236.77	-242.72	-177.13
TS_{Syn} 2	-157.90	-148.92	-154.39	-88.25
C_{syn} 2	-274.99	-271.85	-269.85	-231.48
$(CH_3)_2CO$ + Syn-RCHOO Con1	-247.85	-247.60	-248.19	-248.40

*Table 29: Relative Energies of O_3 + Alkene **11** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 11			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-19.53	-18.53	-14.43	-3.57
TSOzo1	26.25	31.29	28.58	80.53
POZ1	-263.99	-248.04	-252.89	-195.46
PRC2	-19.53	-18.53	-14.43	-3.57
TSOzo2	22.50	27.49	24.78	76.83
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TSpoz1	-224.01	-210.05	-215.68	-157.22
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TSpoz2	-240.38	-225.97	-231.85	-172.67
POZ2	-256.62	-241.08	-245.67	-189.02
POZ1	-263.99	-248.04	-252.89	-195.46
TS_{Anti} 1	-126.84	-120.93	-124.11	-70.70
C_{ANTI}	-210.73	-209.97	-206.04	-174.53
HCHO + *anti*-CF_3CFOO	-178.03	-181.17	-179.23	-180.35
POZ1	-263.99	-248.04	-252.89	-195.46
TS_{FO} 1	-196.69	-188.06	-192.16	-136.32
$C_{FO\ 1}$	-304.64	-297.76	-297.17	-253.94
HCHOO + CF_3CFO	-269.01	-267.38	-267.17	-270.58
POZ2	-256.62	-241.08	-245.67	-189.02
TS_{FO} 2	-195.69	-187.10	-191.14	-135.30
C_{FO} 2	-306.34	-299.06	-298.85	-254.31
POZ2	-256.62	-241.08	-245.67	-189.02
TS_{Syn}	-118.03	-112.80	-115.94	-62.60
C_{SYN}	-173.67	-175.83	-170.45	-149.89
HCHO + *Syn*-CF_3CFOO	-164.32	-168.17	-166.29	-166.18

*Table 30: Relative Energies of O_3 + Alkene **12** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 12			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
$CF_3CF_2CHCH_2$ con 1 + O_3	0.00	0.00	0.00	0.00
$CF_3CF_2CHCH_2$ con 2 + O_3	7.39	7.28	7.31	7.67
PRC1.1	-6.68	-5.40	-1.55	16.59
TSOzo1.1	20.77	26.53	23.53	75.59
POZ1.1	-226.86	-209.25	-214.02	-158.17
PRC1.2	0.61	1.85	5.68	25.05
TSOzo1.2	30.58	36.43	33.33	85.67
POZ1.2	-224.92	-207.60	-212.41	-156.91
PRC1.3	-6.68	-5.40	-1.55	16.59
TSOzo1.3	26.89	32.44	29.60	80.17
POZ1.3	-230.33	-212.87	-217.59	-161.83
PRC2.1	-10.66	-9.02	-5.60	17.00
TSOzo2.1	21.54	27.30	24.30	76.34
POZ2.1	-230.37	-212.67	-217.54	-161.02

PRC2.2	-2.89	-1.37	2.10	24.91
TSOzo2.2	34.22	40.22	37.04	89.77
POZ2.2	-227.75	-210.09	-215.11	-157.78
PRC2.3	-11.78	-10.11	-6.73	17.62
TSOzo2.3	28.77	34.26	31.44	82.30
POZ2.3	-233.19	-215.65	-220.43	-164.45
POZ1.1	-226.86	-209.25	-214.02	-158.17
TS_{Anti} 1	-120.54	-113.37	-116.88	-63.63
C_{anti} 1	-205.32	-202.11	-200.70	-160.59
HCHO + *Anti*-CF_3CF_2CHOO Con 2	-171.96	-176.50	-174.47	-175.39
POZ1.2	-224.92	-207.60	-212.41	-156.91
TS_{Anti} 2	-119.33	-112.12	-115.66	-62.00
C_{anti} 2	-194.90	-194.60	-191.29	-157.90
HCHO + *Anti*-CF_3CF_2CHOO Con 1	-171.96	-176.50	-174.47	-175.39
POZ1.3	-230.33	-212.87	-217.59	-161.83
TS_{Anti} 3	-126.06	-118.99	-122.38	-69.54
C_{anti} 3	-205.18	-201.93	-200.50	-161.01
HCHO + *Anti*-CF_3CF_2CHOO Con 2	-174.99	-179.32	-177.35	-178.73
POZ1.1	-226.86	-209.25	-214.02	-158.17
TS_{FO} 1.1	-138.19	-129.89	-133.74	-79.93
C_{FO} 1.1	-215.03	-214.07	-210.05	-190.12
HCHOO + CF_3CF_2CHO Con 2	-195.30	-196.45	-195.88	-199.17
POZ1.2	-224.92	-207.60	-212.41	-156.91
TS_{FO} 1.2	-140.15	-132.01	-135.98	-81.89
C_{FO} 1.2	-214.89	-213.82	-209.87	-188.75
HCHOO + EtCHOO Con 1	-195.30	-196.45	-195.88	-199.17
POZ1.3	-230.33	-212.87	-217.59	-161.83
TS_{FO} 1.3	-149.29	-141.02	-144.87	-90.70
C_{FO} 1.3	-214.28	-213.46	-209.41	-189.91
HCHOO + CF_3CF_2CHO Con 2	-195.78	-196.79	-196.25	-200.27
POZ2.1	-230.37	-212.67	-217.54	-161.02
TS_{FO} 2.1	-138.80	-130.45	-134.38	-79.94
C_{FO} 2.1	-211.17	-209.42	-206.10	-180.91
HCHOO + CF_3CF_2CHO Con 2	-195.30	-196.45	-195.88	-199.17
POZ2.2	-227.75	-210.09	-215.11	-157.78
TS_{FO} 2.2	-140.94	-132.63	-136.65	-81.34
C_{FO} 2.2	-216.06	-214.45	-211.33	-179.76
HCHOO + CF_3CF_2CHO Con 1	-195.30	-196.45	-195.88	-199.17
POZ2.3	-233.19	-215.65	-220.43	-164.45
TS_{FO} 2.3	-148.71	-140.27	-144.16	-89.72
C_{FO} 2.3	-219.72	-217.85	-214.89	-183.42
HCHOO + CF_3CF_2CHO Con 2	-195.78	-196.79	-196.25	-200.27
POZ2.1	-230.37	-212.67	-217.54	-161.02
TS_{Syn} 1	-109.89	-102.78	-106.53	-51.82
C_{syn} 1	-190.39	-189.36	-186.43	-150.41
HCHO + *Syn*-CF_3CF_2CHOO Con2	-166.87	-170.25	-168.75	-167.97
POZ2.2	-227.75	-210.09	-215.11	-157.78
TS_{Syn} 2	-100.18	-93.61	-97.26	-42.60
C_{syn} 2	-184.71	-185.70	-181.17	-160.08
HCHO + *Syn*-CF_3CF_2CHOO Con1	-165.85	-169.57	-168.03	-168.40
POZ2.3	-233.19	-215.65	-220.43	-164.45

TS_{Syn} 3	-112.26	-105.54	-109.12	-54.81
C_{syn} 3	-187.93	-188.49	-184.47	-155.40
HCHO + *Syn*-CF_3CF_2CHOO Con1	-165.85	-169.57	-168.03	-168.40

*Table 31: Relative Energies of O_3 + Alkene **13** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 13			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-13.43	-12.02	-8.49	15.06
TSOzo1	20.86	26.17	23.07	75.97
POZ1	-240.10	-223.91	-228.77	-172.10
PRC2	-13.46	-12.00	-8.54	16.44
TSOzo2	23.52	28.60	25.58	78.39
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TSpoz1	-225.51	-211.11	-217.19	-157.62
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TSpoz2	-207.29	-192.88	-198.81	-139.72
POZ2	-233.71	-217.82	-222.55	-166.38
POZ1	-240.10	-223.91	-228.77	-172.10
TS_{Anti} 1	-155.35	-148.12	-152.03	-97.72
C_{ANTI} 1	-257.15	-253.27	-251.49	-216.77
ClCHO + *Anti*-CF_3CHOO	-229.39	-229.48	-229.39	-233.22
POZ1	-240.10	-223.91	-228.77	-172.10
TS_{Syn} 1	-143.58	-136.39	-140.38	-85.43
C_{SYN} 1	-243.20	-238.42	-237.49	-197.24
CF_3CHO + *syn*-ClCHOO	-210.34	-209.63	-210.26	-213.55
POZ2	-233.71	-217.82	-222.55	-166.38
TS_{Anti} 1	-144.41	-137.35	-141.37	-86.45
C_{ANTI} 1	-226.39	-223.95	-221.46	-189.16
CF_3CHO + *Anti*-ClCHOO	-198.03	-199.02	-198.93	-202.71
POZ2	-233.71	-217.82	-222.55	-166.38
TS_{Syn} 2	-148.03	-141.04	-144.88	-90.29
C_{SYN} 2	-248.31	-245.43	-242.72	-213.71
ClCHO + *syn*-CF_3CHOO	-226.84	-226.10	-226.55	-228.09

*Table 32: Relative Energies of O_3 + Alkene **14** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-10.3	-9.03	-5.33	13.27
TSOzo1	25.4	30.68	27.65	79.94
POZ1	-261.9	-245.40	-250.48	-193.42
PRC2	-12.2	-10.65	-7.20	16.43
TSOzo2	24.4	29.62	26.62	78.71
POZ2	-250.4	-234.99	-239.50	-183.99
POZ1	-261.9	-245.40	-250.48	-193.42
TSpoz2	-246.7	-231.97	-238.24	-178.68
POZ2	-250.4	-234.99	-239.50	-183.99
POZ1	-261.9	-245.40	-250.48	-193.42
TS_{Anti} 1	-181.2	-173.54	-177.81	-122.87
C_{ANTI} 1	-295.0	-289.86	-288.41	-251.51
FCHO + *Anti*-CF_3CHOO	-266.8	-266.43	-266.10	-269.64
POZ1	-261.9	-245.40	-250.48	-193.42
TS_{Syn} 1	-151.2	-144.07	-147.97	-93.51
C_{SYN} 1	-237.4	-234.07	-231.81	-199.06
CF_3CHO + *syn*-FCHOO	-211.9	-211.35	-211.57	-215.26
POZ2	-250.4	-234.99	-239.50	-183.99
TS_{Anti} 1	-150.9	-143.86	-147.82	-93.28
C_{ANTI} 1	-238.5	-235.73	-233.23	-200.49
CF_3CHO + *Anti*-FCHOO	-206.6	-207.63	-207.27	-211.34
POZ2	-250.4	-234.99	-239.50	-183.99
TS_{Syn} 2	-173.7	-166.33	-170.49	-115.58
C_{SYN} 2	-286.6	-283.10	-280.36	-250.29
FCHO + *syn*-CF_3CHOO	-264.2	-263.04	-263.25	-264.51

*Table 33: Relative Energies of O_3 + Alkene **15** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 2			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
E-$EtCHCHCH_3$ con 1 + O_3	0.00	0.00	0.00	0.00
E-$EtCHCHCH_3$ con 2 + O_3	1.20	1.65	1.37	2.40
PRC1.1	-14.16	-10.58	-9.24	28.19
TSOzo1.1	-3.01	2.09	-0.20	47.81
POZ1.1	-264.53	-246.43	-251.97	-194.80
PRC1.2	-21.81	-18.70	-16.93	18.26
TSOzo1.2	-0.07	5.35	2.69	52.58
POZ1.2	-262.12	-244.07	-249.49	-192.84
PRC1.3	-13.70	-9.70	-8.70	30.32
TSOzo1.3	3.40	7.70	5.56	53.82
POZ1.3	-265.08	-247.24	-252.67	-195.93
PRC2.1	-13.71	-10.04	-8.75	28.69
TSOzo2.1	2.15	7.56	5.10	53.60
POZ2.1	-264.29	-246.06	-251.63	-194.26
PRC2.2	-12.23	-9.06	-7.44	28.56

TSOzo2.2	1.95	7.68	4.81	55.25
POZ2.2	-262.27	-244.11	-249.57	-192.52
PRC2.3	-14.98	-10.99	-9.95	28.86
TSOzo2.3	1.05	5.48	3.18	51.83
POZ2.3	-265.99	-248.17	-253.61	-196.75
POZ1.1	-264.53	-246.43	-251.97	-194.80
TS_{Anti} 1.1	-173.78	-164.51	-169.09	-113.92
C_{anti} 1.1	-295.78	-291.16	-289.70	-251.99
CH_3CHOO + *Anti*-EtCHOO Con 2	-256.77	-257.68	-257.19	-261.09
POZ1.2	-262.12	-244.07	-249.49	-192.84
TS_{Anti} 1.2	-180.34	-170.84	-175.49	-120.06
C_{anti} 1.2	-298.32	-293.64	-292.54	-253.36
CH_3CHOO + *Anti*-EtCHOO Con 1	-258.59	-259.76	-259.44	-262.41
POZ1.3	-265.08	-247.24	-252.67	-195.93
TS_{Anti} 1.3	-181.94	-172.59	-177.07	-122.47
C_{anti} 1.3	-286.48	-284.05	-280.86	-252.22
CH_3CHOO + *Anti*-EtCHOO Con 2	-256.77	-257.68	-257.19	-261.09
POZ1.1	-264.29	-246.06	-251.63	-194.26
TS_{SYN} 2.1	-182.80	-173.62	-178.37	-122.27
C_{SYN} 1.1	-297.33	-294.89	-292.58	-258.83
syn-CH_3CHOO + EtCHO Con 2	-270.87	-272.02	-272.00	-274.67
POZ1.2	-262.27	-244.11	-249.57	-192.52
TS_{SYN} 2.2	-172.06	-162.66	-167.40	-111.46
C_{SYN} 1.1	-290.57	-287.53	-284.47	-257.44
syn-CH_3CHOO + EtCHO Con 1	-268.53	-267.98	-268.19	-270.19
POZ1.3	-262.27	-244.11	-249.57	-192.52
TS_{SYN} 2.3	-183.74	-174.22	-178.92	-122.98
C_{SYN} 2.3	-300.51	-296.49	-294.34	-260.19
syn-CH_3CHOO + EtCHO Con 2	-268.53	-267.98	-268.19	-270.19
POZ2.1	-264.29	-246.06	-251.63	-194.26
TS_{Anti} 2.1	-174.25	-165.26	-169.77	-114.76
C_{anti} 2.1	-288.01	-285.05	-282.64	-249.26
Anti-CH_3CHOO + EtCHOO Con 2	-256.33	-257.17	-256.78	-260.98
POZ2.2	-262.27	-244.11	-249.57	-192.52
TS_{Anti} 2.2	-181.69	-172.47	-176.99	-121.89
C_{anti} 2.2	-288.43	-286.18	-283.60	-252.55
Anti-CH_3CHOO + EtCHOO Con 1	-260.26	-261.28	-261.11	-264.17
POZ2.3	-262.27	-244.11	-249.57	-192.52
TS_{Anti} 2.3	-181.95	-172.83	-177.26	-122.54
C_{anti} 2.3	-293.82	-289.22	-287.71	-251.74
Anti-CH_3CHOO + EtCHOO Con 2	-256.33	-257.17	-256.78	-260.98
POZ2.1	-264.53	-246.43	-251.97	-194.80
TS_{SYN} 1.1	-183.55	-174.44	-179.09	-123.53
C_{SYN} 1.1	-297.35	-294.56	-291.99	-261.11
CH_3CHOO + *syn*-EtCHO Con 2	-271.18	-271.19	-271.47	-274.67
POZ2.2	-262.12	-244.07	-249.49	-192.84
TS_{SYN} 1.2	-181.45	-171.69	-176.56	-120.22
C_{SYN} 1.2	-298.66	-296.45	-293.90	-264.20
CH_3CHOO + *syn*-EtCHO Con 1	-275.11	-275.30	-275.81	-277.86
POZ2.3	-265.08	-247.24	-252.67	-195.93
TS_{SYN} 1.3	-184.57	-175.23	-179.92	-124.15
C_{SYN} 1.3	-300.36	-297.11	-294.89	-261.99

CH_3CHOO + *syn*-EtCHO Con 2	-271.18	-271.19	-271.47	-274.67

*Table 34: Relative Energies of O_3 + Alkene **16** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 2			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
Z-$EtCHCHCH_3$ con 1 + O_3	0.00	0.00	0.00	0.00
Z-$EtCHCHCH_3$ con 2 + O_3	15.00	15.85	15.59	16.46
PRC1.1	-11.83	-8.60	-6.70	26.26
TSOzo1.1	-1.34	3.71	1.62	49.57
POZ1.1	-260.48	-242.5	-247.92	-190.5
PRC1.2	-13.46	-11.32	-8.89	21.44
TSOzo1.2	11.88	16.94	14.97	62.29
POZ1.2	-257.04	-239.32	-244.63	-186.90
PRC1.3	-13.46	-11.32	-8.89	21.44
TSOzo1.3	-3.22	0.57	-1.25	46.58
POZ1.3	-264.13	-246.36	-251.75	-194.58
PRC2.1	-16.09	-13.78	-11.35	19.34
TSOzo2.1	6.52	11.87	9.54	58.31
POZ2.1	-258.23	-240.58	-246.08	-188.18
PRC2.2	-16.09	-13.78	-11.35	19.34
TSOzo2.2	15.53	21.77	18.92	70.53
POZ2.2	-252.06	-234.07	-239.71	-181.18
PRC2.3	-16.58	-13.99	-11.48	16.53
TSOzo2.3	1.23	5.55	3.26	52.70
POZ2.3	-262.42	-244.92	-250.46	-192.94
POZ1.1	-260.48	-242.46	-247.92	-190.47
TS_{Anti} 1.1	-186.65	-177.9	-182.50	-125.5
C_{anti} 1.1	-289.58	-287.94	-285.23	-253.06
CH_3CHOO + *Anti*-EtCHOO Con 2	-261.45	-263.04	-262.51	-265.35
POZ1.2	-257.04	-239.32	-244.63	-186.90
TS_{Anti} 1.2	-181.46	-171.84	-176.74	-118.88
C_{anti} 1.2	-295.09	-293.06	-290.84	-254.98
CH_3CHOO + *Anti*-EtCHOO Con 1	-263.26	-265.12	-264.75	-266.67
POZ1.3	-264.13	-246.36	-251.75	-194.58
TS_{Anti} 1.3	-187.87	-179.02	-183.54	-127.14
C_{anti} 1.3	-292.36	-290.06	-287.68	-252.80
CH_3CHOO + *Anti*-EtCHOO Con 2	-261.45	-263.04	-262.51	-265.35
POZ2.1				
TS_{Anti} 2.1	-260.48	-242.46	-247.92	-190.47
C_{anti} 2.1	-182.06	-173.41	-178.00	-121.30
Anti-CH_3CHOO + EtCHOO Con 2	-298.86	-294.53	-293.24	-254.64
	-261.00	-262.53	-262.09	-265.23
POZ2.2				
TS_{Anti} 2.2	-257.04	-239.32	-244.63	-186.90
C_{anti} 2.2	-186.99	-177.86	-182.57	-125.68
Anti-CH_3CHOO + EtCHOO Con 1	-303.28	-299.46	-298.23	-258.47
	-264.94	-266.64	-266.42	-268.42
POZ2.3				
TS_{Anti} 2.3	-264.13	-246.36	-251.75	-194.58
C_{anti} 2.3	-188.49	-179.58	-184.20	-127.56
Anti-CH_3CHOO + EtCHOO Con 2	-298.50	-294.58	-293.02	-256.00
	-261.00	-262.53	-262.09	-265.23
POZ2.1				
TS_{SYN} 1.1	-258.23	-240.58	-246.08	-188.18

C_{SYN} 1.1	-174.21	-164.50	-169.54	-111.34
CH_3CHO + *syn*-EtCHOO Con 2	-296.40	-294.82	-292.33	-259.12
	-275.54	-277.38	-277.31	-278.93
POZ2.2				
TS_{SYN} 1.2	-252.06	-234.07	-239.71	-181.18
C_{SYN} 1.2	-161.66	-151.87	-156.96	-98.21
CH_3CHO + *syn*-EtCHOO Con 1	-295.24	-292.89	-289.78	-261.70
	-273.20	-273.34	-273.50	-274.44
POZ2.3				
TS_{SYN} 1.3	-262.42	-244.92	-250.46	-192.94
C_{SYN} 1.3	-177.70	-167.78	-172.70	-115.02
CH_3CHO + *syn*-EtCHOO Con 2	-292.52	-289.91	-287.06	-258.15
	-273.20	-273.34	-273.50	-274.44
POZ2.1				
TS_{SYN} 2.1	-258.23	-240.58	-246.08	-188.18
C_{SYN} 1.1	-178.17	-168.70	-173.64	-115.56
syn-CH_3CHOO + EtCHO Con 2	-306.12	-303.78	-301.69	-266.10
	-275.85	-276.55	-276.79	-278.93
POZ2.2				
TS_{SYN} 2.2	-252.06	-234.07	-239.71	-181.18
C_{SYN} 1.1	-171.49	-161.85	-166.69	-109.03
syn-CH_3CHOO + EtCHO Con 1	-308.42	-305.95	-303.95	-268.37
	-279.79	-280.66	-281.12	-282.12
POZ2.3				
TS_{SYN} 2.3	-262.42	-244.92	-250.46	-192.94
C_{SYN} 2.3	-178.51	-169.13	-173.92	-116.44
syn-CH_3CHOO + EtCHO Con 2	-305.23	-302.50	-300.39	-265.57

*Table 35: Relative Energies of O_3 + Alkene **17** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-26.22	-22.45	-21.34	16.40
TSOzo1	1.80	6.81	4.40	52.30
POZ1	-264.18	-245.81	-251.55	-195.30
POZ1	-264.18	-245.81	-251.55	-195.30
TS_{Anti} 1	-180.38	-170.94	-175.64	-121.33
C_{ANTI} 1	-288.19	-285.95	-283.02	-253.55
CH_3CHO + *Anti*-CH_3CHOO	-258.06	-259.47	-258.96	-262.48
POZ1	-264.18	-245.81	-251.55	-195.30
TS_{Syn} 1	-183.17	-173.65	-178.57	-123.19
C_{SYN} 1	-298.71	-296.17	-293.89	-261.60
CH_3CHO + *syn*-CH_3CHOO	-272.91	-273.49	-273.65	-276.18

*Table 36: Relative Energies of O_3 + Alkene **18** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-11.79	-8.50	-6.75	26.44
TSOzo1	-1.40	3.05	1.13	47.67
POZ1	-263.59	-245.13	-250.94	-194.21
PRC1	-17.61	-15.00	-12.59	14.73
TSOzo1	5.96	10.93	8.54	56.50
POZ1	-261.12	-242.86	-248.83	-191.86
PRC2	-263.59	-245.13	-250.94	-194.21
TSOzo2	-254.01	-237.46	-244.64	-183.50
POZ2	-261.12	-242.86	-248.83	-191.86
POZ1	-263.59	-245.13	-250.94	-194.21
TS_{Anti} 1	-187.21	-178.13	-183.01	-126.86
C_{ANTI} 1	-294.48	-292.19	-290.18	-254.43
CH_3CHO + *Anti*-CH_3CHOO	-262.58	-264.51	-264.04	-266.41
POZ1	-261.12	-242.86	-248.83	-191.86
TS_{Syn} 1	-177.65	-167.59	-172.83	-115.70
C_{SYN} 1	-307.47	-304.77	-302.95	-267.08
CH_3CHO + *syn*-CH_3CHOO	-277.44	-278.52	-278.74	-280.11

*Table 37: Relative Energies of O_3 + Alkene **20** DF-LCCSD(T)-F12a energies (kJ mol^{-1}).*

	O_3 + Alkene 14			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-19.59	-16.8	-14.60	15.70
TSOzo1	7.09	12.3	9.91	58.44
POZ1	-258.76	-241.1	-246.53	-189.89
POZ1	-258.76	-241.1	-246.53	-189.89
TS_{Anti} 1	-181.66	-172.8	-177.24	-121.97
C_{ANTI} 1	-296.33	-293.1	-291.46	-252.61
CH_3CHO + *Anti*-CH_3CHOO	-262.49	-275.6	-275.50	-274.23
POZ1	-258.76	-241.1	-246.53	-189.89
TS_{Syn} 1	-167.63	-158.4	-162.78	-108.02
C_{SYN} 1	-279.14	-275.9	-274.27	-235.42
CH_3CHO + *syn*-CH_3CHOO	-253.52	-254.7	-253.43	-261.33

1.3.2 Epoxide Results

The Relative Energies, Enthalpies and Gibbs Free Energies in this section is based on the B3LYP molecular energy calculations, used only for epoxide pathway calculations.

*Table 38: Relative Energies of O_3 + Alkene **1** using B3LYP molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-7.07	-3.29	-2.02	32.99
TSOzo1	-2.21	3.93	0.85	49.31
POZ1	-237.29	-217.98	-223.63	-169.17
PRC2	-6.03	-2.58	-0.97	32.00
TSOzo2	1.68	7.77	4.73	52.94
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TSpoz1	-223.55	-206.06	-213.23	-154.93
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TSpoz2	-225.79	-208.17	-215.21	-157.25
POZ2	-236.89	-217.68	-223.51	-168.32
POZ1	-237.29	-217.98	-223.63	-169.17
TS_{Anti} 1	-164.54	-155.00	-159.69	-106.63
C_{ANTI}	-282.66	-275.72	-276.11	-233.95
HCHO + Anti-RCHOO	-247.32	-250.46	-248.95	-249.43
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{FO} 1	-156.79	-147.01	-151.90	-98.43
$C_{FO\ 1}$	-272.72	-269.07	-267.47	-232.68
RCHO + HCHOO	-250.66	-251.58	-251.23	-253.94
POZ2	-236.89	-217.58	-223.23	-168.78
TS_{FO} 2	-154.23	-144.24	-149.08	-96.08
C_{FO} 2	-267.39	-265.18	-262.23	-236.23
POZ2	-236.89	-217.68	-223.51	-168.32
TS_{Syn}	-158.67	-148.57	-153.60	-99.51
C_{SYN}	-281.04	-277.22	-276.08	-237.95
HCHO + Syn-RCHOO	-259.26	-261.57	-260.74	-260.21
PRC1	-7.07	-3.29	-2.02	32.99
TS_{epox} 1.1	46.88	49.99	47.30	94.73
C_{epox} 1.1	-135.72	-126.87	-127.08	-87.21
PRC2	-6.03	-2.58	-0.97	32.00
TS_{epox} 1.2	38.74	42.62	39.06	89.37
C_{epox} 1.2	-132.96	-124.19	-124.22	-84.92
O2 + epoxide	-126.58	-120.8	-121.53	-113.48
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{epox} 2_1	64.20	68.04	64.86	114.97
C_{epox} 1.1	-135.72	-126.87	-127.08	-87.21
POZ2	-236.89	-217.68	-223.51	-168.32
TS_{epox} 2_2	70.90	74.06	71.13	120.52
C_{epox} 1.2	-132.96	-124.19	-124.22	-84.92
POZ1	-237.29	-218.07	-223.91	-168.72
TS_{epox} 2_3	45.43	48.86	46.12	94.74
C_{epox} 2.3	-135.49	-126.59	-126.75	-87.12

POZ2	-236.89	-217.68	-223.51	-168.32
TS_{epox} 2_4	57.32	59.78	57.08	104.88
C_{epox} 2.4	-132.34	-124.55	-123.49	-91.75

*Table 39: Relative Energies of O_3 + Alkene **5** using B3LYP molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1.1	-2.76	-0.45	2.21	30.48
TSOzo1.1	5.56	10.86	8.10	57.61
POZ1.1	-202.73	-186.54	-191.05	-138.56
PRC1.2	-1.11	1.09	3.42	34.89
TSOzo1.2	7.85	13.52	10.59	60.76
POZ1.2	-219.24	-202.70	-207.45	-154.15
PRC2.1	-2.15	-0.47	2.88	24.44
TSOzo2.1	0.27	5.79	2.99	52.88
POZ2.1	-205.35	-189.12	-193.77	-140.23
PRC2.2	-4.42	-1.67	0.31	33.98
TSOzo2.2	9.21	14.78	11.91	62.17
POZ2.2	-221.62	-204.94	-209.83	-156.13
POZ1.1	-202.73	-186.54	-191.05	-138.56
TS_{Anti} 1	-130.81	-123.57	-127.23	-75.46
C_{anti} 1	-238.71	-235.23	-234.05	-194.35
HCHO + Anti-RCHOO Con 2	-212.89	-216.96	-215.18	-215.90
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{Anti} 2	-142.25	-134.52	-138.36	-85.65
C_{anti} 2	-240.93	-240.43	-237.09	-204.96
HCHO + Anti-RCHOO Con1	-228.11	-231.59	-229.99	-230.26
POZ1.1	-202.73	-186.54	-191.05	-138.56
TS_{FO} 1.1	-133.13	-125.81	-129.52	-77.60
C_{FO} 1.1	-220.00	-219.91	-216.05	-193.63
HCHOO + RCHO con 1	-201.98	-204.49	-203.69	-208.80
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{FO} 1.2	-156.17	-148.24	-152.12	-99.55
C_{FO} 1.2	-250.85	-246.76	-245.57	-205.85
HCHOO + RCHO con 2	-223.20	-224.72	-224.15	-227.92
POZ2.1	-205.35	-189.12	-193.77	-140.23
TS_{FO} 2.1	-141.03	-133.81	-137.57	-85.33
C_{FO} 2.1	-244.38	-238.74	-238.61	-194.47
HCHOO + RCHO con 1	-201.98	-204.49	-203.69	-208.80
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{FO} 2.2	-156.06	-148.20	-152.06	-99.08
C_{FO} 2.2	-251.90	-247.03	-246.40	-204.39
HCHOO + RCHO con 2	-223.20	-224.72	-224.15	-227.92
POZ2.1	-205.35	-189.12	-193.77	-140.23
TS_{Syn} 1	-116.44	-110.02	-113.45	-62.02
C_{syn} 1	-206.38	-207.81	-202.86	-184.48
HCHO + Syn-RCHOO Con2	-192.37	-196.41	-194.68	-196.10
C_{syn} 1	-222.13	-216.96	-216.92	-173.31
HOZ2.1	-411.77	-391.87	-396.88	-342.58
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{Syn} 2	-135.75	-127.82	-132.05	-78.81
C_{syn} 2	-230.25	-230.04	-226.55	-196.23
HCHO + Syn-RCHOO Con1	-217.59	-220.53	-219.50	-218.81

PRC2.1	-2.15	-0.47	2.88	24.44
TS_{epox} 1.1	52.36	56.03	53.49	101.94
C_{epox} 2_5	-120.48	-114.34	-113.07	-77.69
PRC2.2	-4.42	-1.67	0.31	33.98
TS_{epox} 1.2	47.33	50.72	48.40	96.02
C_{epox} 2_6	-115.05	-108.63	-107.72	-70.34
PRC1.1	-2.76	-0.45	2.21	30.48
TS_{epox} 1.3	52.21	56.28	53.35	103.76
C_{epox} 1_3	-119.48	-114.13	-111.75	-85.53
PRC1.2	-1.11	1.09	3.42	34.89
TS_{epox} 1.4	42.96	47.19	44.31	94.52
C_{epox} 1_4	-113.42	-107.94	-105.80	-75.35
O2 + epoxide	-108.76	-104.92	-104.94	-98.05
O2 + epoxide	-116.19	-112.09	-112.22	-104.58
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_1	56.53	60.34	57.76	106.46
C_{epox} 2_1	-114.50	-108.78	-106.88	-77.22
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_2	64.75	67.88	65.60	113.87
C_{epox} 2_2	-120.92	-115.21	-113.23	-83.94
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_3	66.20	69.71	67.08	116.94
C_{epox} 1_3	-119.48	-114.13	-111.75	-85.53
POZ1.2	-219.24	-202.70	-207.45	-154.15
TS_{epox} 2_5	81.58	81.95	80.22	127.14
C_{epox} 2_5	-120.48	-114.34	-113.07	-77.69
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_7	104.81	105.51	103.12	153.07
C_{epox} 2_7	-118.72	-113.57	-110.94	-86.75
POZ2.2	-221.62	-204.94	-209.83	-156.13
TS_{epox} 2_8	76.04	76.45	74.43	123.74
C_{epox} 2_2	-120.92	-115.21	-113.23	-83.94

*Table 40: Relative Energies of O_3 + Alkene **1** epoxide pathways using DF-LCCSD-F12a molecular energies (kJ mol^{-1}).*

	O_3 + Alkene 1			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC1	-18.43	-14.65	-13.38	21.63
TS_{epox} 1.1	47.41	50.52	47.83	95.26
C_{epox} 1.1	-162.46	-153.61	-153.82	-113.95
PRC2	-18.27	-14.82	-13.21	19.76
TS_{epox} 1.2	39.25	43.21	39.64	89.99
C_{epox} 1.2	-165.37	-156.60	-156.63	-117.32
O2 + epoxide	-157.37	-151.64	-152.33	-144.28
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{epox} 2_1	98.09	101.93	98.76	148.86
C_{epox} 1.1	-162.46	-153.61	-153.82	-113.95
POZ2	-254.91	-235.70	-241.53	-186.34
TS_{epox} 2_2	106.67	109.82	106.89	156.28
C_{epox} 1.2	-165.37	-156.60	-156.63	-117.32
POZ1	-254.53	-235.31	-241.15	-185.96
TS_{epox} 2_3	91.11	94.54	91.80	140.42
C_{epox} 2.3	-162.57	-153.67	-153.83	-114.21
POZ2	-254.91	-235.70	-241.53	-186.34
TS_{epox} 2_4	98.78	101.24	98.54	146.34
C_{epox} 2.4	-165.37	-157.58	-156.52	-124.77

*Table 41: Relative Energies of O_3 + Alkene **5** epoxide pathways using DF-LCCSD-F12a molecular energies (kJ mol^{-1})..*

	O_3 + Alkene 5			
Stationary Point	**ΔE**	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
PRC2.1	-10.64	-8.96	-5.61	15.95
TS_{epox} 1.1	59.08	62.74	60.20	108.65
C_{epox} 2_5	-151.60	-145.46	-144.19	-108.81
PRC2.2	-18.75	-16.01	-14.02	19.65
TS_{epox} 1.2	59.17	62.56	60.23	107.86
C_{epox} 2_6	-143.07	-136.65	-135.74	-98.36
PRC1.1	-15.65	-13.35	-10.69	17.58
TS_{epox} 1.3	55.07	59.14	56.21	106.62
C_{epox} 1_3	-155.22	-149.87	-147.49	-121.28
PRC1.2	-14.31	-12.10	-9.77	21.70
TS_{epox} 1.4	49.34	53.57	50.68	100.89
C_{epox} 1_4	-148.10	-142.62	-140.48	-110.03
O2 + epoxide	-138.13	-134.29	-134.31	-127.42
O2 + epoxide	-146.69	-142.58	-142.72	-135.08
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_1	-70.49	-66.68	-69.26	-20.56
C_{epox} 2_1	-144.26	-138.54	-136.64	-106.98
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_2	-156.24	-153.10	-155.38	-107.11
C_{epox} 2_2	-153.63	-147.92	-145.94	-116.65
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_3	-155.67	-152.17	-154.80	-104.93
C_{epox} 1_3	-155.22	-149.87	-147.49	-121.28
POZ2.1	-224.38	-208.15	-212.79	-159.25
POZ1.2	-236.61	-220.08	-224.82	-171.52
TS_{epox} 2_5	103.04	103.41	101.68	148.59
C_{epox} 2_5	-151.60	-145.46	-144.19	-108.81
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_7	129.22	129.91	127.52	177.47
C_{epox} 2_7	-154.30	-149.15	-146.52	-122.33
POZ2.2	-239.44	-222.76	-227.65	-173.95
TS_{epox} 2_8	90.83	91.25	89.23	138.54
C_{epox} 2_2	-153.63	-147.92	-145.94	-116.65

1.4 Previous Literature Experimental Data

The data found in in the main thesis Table 3.2 is obtained from the data in the tables here in the appendix obtained from the following tables. Tables 1.1—1.3 contains the rate constants and OH yields for these alkene ozonolysis reactions are found here:

*Table 42: Literature Rate Constants (k_{EXP}) and OH yields of the Ozonolysis of Alkenes **1**, 2, **5**, **6** & **20**.*

Alkene	k_{EXP} (~298K) (10^{-18} cm^3 s^{-1})	ref	OH yield	ref
Propene	10.1 ± 2.5	1	0.33 ± 0.16	2
$CH_3CH=CH_2$	9.9	3	0.18 ± 0.04	4,5
(Alkene **1**)	11.1	6	0.30 ± 0.08	7
	10.0	8	0.39 ± 0.08	9
	9.6 ± 0.4	10	0.34 ± 0.03	11
	11.5 ± 1.1	12	0.33 ± 0.04	13
	10.6 ± 1.2	7		
Average	*10.4*		*0.34*	
Range	*9.6 - 11.5*	1,3,10,14–17	*0.30 - 0.39*	*2,4,5,7,9,11*
Range (± included)	*7.6 - 12.6*		*0.17 - 0.49*	
1-Butene	9.65 ± 2.5	1	0.41 ± 0.20	2
$CH_3CH_2CH=CH_2$	9.7 ± 1.9	18	0.30 ± 0.09	7
(Alkene **2**)	10.9 ± 0.8	3	0.29 ± 0.05	19
	8.8 ± 0.6	10	0.23 ± 0.04	13
	11.0 ± 3.3	15	-	
	12.4 ± 3.8	12	-	
Average	*10.4*		*0.31*	
Range	*8.8 - 12.4*	*1–4,10*	*0.23 - 0.41*	2,7,19
Range (± included)	*7.2 - 16.2*		*0.19 - 0.61*	
Methyl Vinyl Ketone	5.84 ± 0.39	20	0.13 ± 0.04	21
$CH_3C(O)CH=CH_2$	4.72 ± 0.09	22	0.16 ± 0.08	23
(Alkene **5**)	4.22 ± 0.85	10	0.16 ± 0.05	24
	4.77 ± 0.57	25	-	-
	4.5 ± 0.1	21	-	-
	5.1 ± 0.1	21	-	-
Average	*4.86*		*0.15*	
Range	*4.22 -5.84*	1,3,26	*0.13 - 0.16*	21,23,24
Range (± included)	*3.37 -6.23*		*0.08 - 0.24*	
2-methyl-2-butene	403 ± 141	1	0.98 ± 0.24	27
$CH_3CH=C(CH_3)_2$	410 ± 50	28	0.89 ± 0.37	2
(Alkene **6**)	410	29	0.93 ± 0.14	30
	396 ± 139	31	0.81 ± 0.16	32
	-	-	0.89 ± 0.22	33
	-	-	0.47 ± 0.04	28
Average	405		0.90	
Range	396 - 410	1,3,10,14–17	0.81 - 0.98	2,27,30,32,33
Range (± included)	257 - 544		0.52 - 1.26	
2-methylpropene	11.3 ± 3.0	1	0.84 ± 0.42	2
$(CH_3)_2C=CH_2$	11.1 ± 2.8	18	0.80 ± 0.10	7
(Alkene **20**)	10.8 ± 1.0	3	0.72 ± 0.12	19
	12.9	26	0.60 ± 0.06	11
Average	*11.5*	1,3,26	*0.74*	2,7,11,19
Range	*10.8 - 12.9*		*0.6 - 0.84*	
Range (± included)	*8.3 - 14.3*		*0.42 - 1.26*	

*Table 43: Literature Rate Constants (k_{EXP}) and OH yields of the Ozonolysis of Alkenes **17**, 18, **15** & **16**.*

Alkene	k_{EXP} (10^{16} cm^3 s^{-1})	ref	OH yield	ref
***E*-2-butene**	1.90 ± 0.67	1	0.64 ± 0.12	27
(Alkene **17**)	1.82 ± 0.011	3	0.64 ± 0.26	2
	2.17	14	0.24 ± 0.02	4,5
	1.81 ± 0.006	10	0.54 ± 0.11	32
	2.00 ± 0.80	15	0.19	17
	1.98	12	0.68 ± 0.09	16
	-	-	0.60 ± 0.12	7
	-	-	0.75 ± 0.19	33
	-	-	0.52 ± 0.04	34
Average	1.94	1,3,10,14–17	0.58 (0.53)	16,17
Range	1.81 – 2.17		0.52 – 0.75 (0.19 – 0.75)	
Range (± included)	1.20 – 2.80		0.43 – 0.94 (0.19 – 0.94)	
***Z*-2-butene**	1.25 ± 0.31	1	0.33 ± 0.05	27
(Alkene **18**)	1.27	3	0.41 ± 0.17	2
	1.23 ± 0.18	10	0.17 ± 0.02	4,5
	1.30 ± 0.39	15	0.33 ± 0.07	32
	1.19 (± 0.12)	12	0.39	35
	-	-	0.40	17
	-	-	0.40 ± 0.05	7
Average	1.26	1–4,10	0.38 (0.35)	1–4,10,15
Range	1.23 – 1.30		0.33 – 0.41 (0.17 – 0.41)	
Range (± included)	0.91 – 1.69		0.24 – 0.58 (0.15 – 0.58)	
***E*-2-pentene**	3.15 ± 0.95	1	0.46 ± 0.08	27
(Alkene **15**)	1.62 ± 0.06	3	-	-
	3.15	26	-	-
Average	2.39	1,3,26	0.46	27
Range	1.62 – 3.15		0.46	
Range (± included)	1.62 – 4.10		0.38 – 0.54	
***Z*-2-pentene**	3.15 ± 0.95	1	0.27 ± 0.07	27
(Alkene **16**)	1.32 ± 0.04	3	0.29 ± 0.06	27
	2.09	26	-	-
Average	1.71	1,3,26	0.28	27
Range	1.32 – 2.09		0.27 – 0.29	
Range (± included)	0.94 – 2.09		0.20 – 0.35	

*Table 44: Literature Experimental Rate Constants (k_{EXP}) range of the Ozonolysis of Alkenes **3**, **4**, **7**, **8**, **9**, **10**, **11**, **12**, **13**, **14** & **19**.*

Alkene	Alkene No	k_{EXP} (10^{-18} cm^3 s^{-1})	ref
3-methyl-1-butene	**3**	0.95 ± 0.29	1
$(CH_3)_2CHCH=CH_2$		0.73 ± 0.27	18
Average		*0.84*	1,3,26
Range		*0.73 - 0.95*	
Range (± included)		*0.46 - 1.24*	
3,3-dimethyl-1-butene	**4**	0.39 ± 0.12	1
$(CH_3)_3CCH=CH_2$		0.38 ± 0.08	18
Average		*0.385*	1,3,26
Range		*0.38 - 0.39*	
Range (± included)		*0.27 - 0.51*	
2-methyl-2-pentene	**7**	0.39 ± 0.12	1
$CH_3CH_2CH=C(CH_3)_2$		0.38 ± 0.08	36
Average		*0.385*	1,3,26
Range		*0.38 - 0.39*	
Range (± included)		*0.27 - 0.51*	
2,4-dimethyl-2-pentene $[(CH_3)_2CHCH=C(CH_3)_2]$	**8**	*223* *	37
2,4,4-trimethyl-2-pentene	**9**	1.39 ± 0.42	1
$(CH_3)_3CCH=C(CH_3)_2$		1.25 ± 0.10	2638
Average		*1.32*	1,3,26
Range		*1.25 - 1.39*	
Range (± included)		*0.97 - 1.81*	
Mesityl Oxide $(CH_3C(O)CH=C(CH_3)_2)$	**10**	0.081 ± 0.011	39
2,3,3,3-tetrafluoro-1-propene $(CF_3CF=CH_2)$	**11**	$(2.77 \pm 0.21) \times 10^{-3}$	40
3,3,4,4,4-pentafluoro-1-butene	**12**	0.211 ± 0.035	41
$CF_3CF_2CH=CH_2$		0.20 ± 0.04	42
Average		0.21	41
Range		0.16 - 0.25	
Range (± included)			
***E*-1-chloro-3,3,3-trifluoro-1-propene** (*E*-$CF_3CH=CHCl$)	**13**	$(1.46 \pm 0.12) \times 10^{-3}$	43
***E*-1,3,3,3-tetrafluoro-1-propene** (*E*-$CF_3CH=CHF$)	**14**	$(2.81 \pm 0.21) \times 10^{-3}$	44
***Z*-2-hexene**	**19**	144 ± 43	1
(*Z*-nPrCH=$CHCH_3$)		105 ± 20	3
Average		125	
Range		105 - 144	
Range (± included)		85 - 187	

The product branching fraction literature averages and ranges are in the following table:

*Table 45: The literature experimental product branching fractions of the Ozonolysis of Alkenes **1**, **2**, **3**, **4**, **5**, **6**, **8**, **9**, **12**, **13** & **20**.*

Alkene + O_3	R_1	#	Product Branching Ratio (Γ_{EXP})		Ref
			$R_1CHOO+HCHO$	$R_1CHO+HCHOO$	
Propene *	CH_3	**1**	0.60	0.40	[45]
Range			0.517 – 0.643	0.357 – 0.483	[45–47]
1-butene	Et	**2**	0.64 ± 0.04	0.36 ± 0.04	[45]
3-methyl-1-butene	iPr	**3**	0.49 ± 0.05	0.51 ± 0.05	[45]
3,3-dimethyl-1-butene	tBu	**4**	0.32 ± 0.01	0.68 ± 0.01	[45]
methyl vinyl ketone *	$CH_3C(O)$	**5**	0.22 ± 0.17	0.78 ± 0.17	[21,23]
3,3,4,4,4-pentafluoro-1-butene	CF_3CF_2-	**12**	0.739 ± 0.017	0.261 ± 0.017	[41]
Alkene + O_3		**#**	**$R_1CHOO+(CH_3)_2CO$**	**$R_1CHO+(CH_3)_2COO$**	**Ref**
2-methyl-2-butene *	CH_3	**6**	0.321	0.679	[45–47]
			0.289 – 0.387	0.613 – 0.711	[45–47]
2,4-dimethyl-2-pentene	iPr	**8**	0.82 ± 0.04	0.18 ± 0.04	[45]
2,4,4-dimethyl-2-pentene	tBu	**9**	0.82 ± 0.05	0.18 ± 0.05	[45]
	R_1	**#**	**$CF_3CHOO+ClCHO$**	**$CF_3CHO+ClCHOO$**	
***E*-1-chloro-3,3,3-trifluoro-1-propene**	CF_3	**13**	0.63 ± 0.09	0.33 ± 0.03	[48]
			$(CH_3)_2COO + HCHO$	**$HCHOO+(CH_3)_2CO$**	
2-methylpropene *	$(CH_3)_2C$	**20**	0.70	0.30	[46,49–53]
Range			0.53 – 0.77	0.23 – 0.47	

1.5 Reactant Atmospheric Abundance

The abundance and boiling points of the different atmospheric alkenes in analysed in Chapter 3 are found in the following tables

*Table 46: Atmospheric concentrations of Alkenes **1-20** (if known) under various conditions.*

Co-reactant Environment	Abundance (Original units)	Study	Ref
Ozone (O_3)			
summertime conditions - Houston	40–60 ppbv	Ryerson *et al.*	54
Can exceed	200 ppbv	Ryerson *et al.*	54
O_3 – Boreal Forest	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	55
O_3 – Tropical Forest/Rainforest	7.3×10^{11} cm^3 s^{-1}	Vereecken *et al.*	55
O_3 – Mega city	1.9×10^{12} cm^3 s^{-1}	Vereecken *et al.*	55
O_3 – Rural Europe	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	55
Propene (Alkene 1) [General Average]			
– Mega city	1.1×10^{11} cm^3 s^{-1}	Vereecken *et al.*	56
– Rural Europe	1.5×10^{9} cm^3 s^{-1}	Vereecken *et al.*	56
High ponderosapine forest	176 ppt	Rhew *et al.*	57
Low ponderosapine forest	182 ppt	Rhew *et al.*	57
Taipei Urban - Summer Daytime	0.56 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.81 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.53 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.53 ppbv	Wang *et al.*	58
Mexico City - Urban	5.93 ppb	Percival *et al.*	59
Mexico City - Industrial	10.96 ppb	Percival *et al.*	59
Chinese Max	8.2 ppb	Percival *et al.*	59
Karthmandu, Nepal	12.8 ppb	Percival *et al.*	59
Porto Alegre, Brazil	28.3 ppb	Percival *et al.*	59
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(4.7 \pm 3.7) \times 10^{8}$	Novelli *et al.*	60
1-Butene (Alkene 2) [General Average]			
– Mega city	5.7×10^{10} cm^3 s^{-1}	Vereecken *et al.*	56
– Rural Europe	5.7×10^{8} cm^3 s^{-1}	Vereecken *et al.*	56
Taipei Urban - Summer Daytime	0.14 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.18 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.12 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.13 ppbv	Wang *et al.*	58
Taipei, Taiwan	0.90 ppb	Percival *et al.*	59
Chinese Max	2.4 ppb	Percival *et al.*	59
Karachi	1.1 ppb	Percival *et al.*	59
Dallas	0.32 ppb	Percival *et al.*	59
Porto Alegre	7.8 ppb	Percival *et al.*	59
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(1.4 \pm 4.2) \times 10^{8}$	Novelli *et al.*	60
Butene (unknown)			
High ponderosapine forest	52 ppt	Rhew *et al.*	57
Low ponderosapine forest	51 ppt	Rhew *et al.*	57
3-methyl-1-butene (Alkene 3) [General Average]			
Taipei Urban - Summer Daytime	0.03 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.04 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.02 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.02 ppbv	Wang *et al.*	58
C5	0.030 ppb	Percival *et al.*	59
3,3-dimethyl-1-butene (Alkene 4) [General Average]			
c6 alkenes	0.052	Percival *et al.*	59
Methyl vinyl ketone (Alkene 5) [General Average]			
Rainforest	2.4×10^{10} cm^3 s^{-1}	Vereecken *et al.*	56

Temperate Forest		2.5×10^9 cm^3 s^{-1}	Vereecken *et al.*	56
Borneo		0.45 ppb	Percival *et al.*	59
2-methyl-2-butene (Alkene 6) [General Average]				
Taipei Urban - Summer Daytime		0.13 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time		0.21 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime		0.12 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time		0.12 ppbv	Wang *et al.*	58
Mexico City- Urban		1.69 ppbv	Percival *et al.*	59
Mexico City- Industrial		0.89 ppbv	Percival *et al.*	59
Porto Alegre Brazil		17 ppbv	Percival *et al.*	59
Seoul		1 ppbv	Percival *et al.*	59
2-methyl-2-pentene (Alkene 7) [General Average]				
Porto Alegre Brazil		4 ppbv	Percival *et al.*	59
Porto Alegre Brazil		0.017 ppbv	Percival *et al.*	59
Boston		17 ppbv	Percival *et al.*	59
C-6 alkene - Boston		0.052 ppbv	Percival *et al.*	59
2,4-dimethyl-2-pentene (Alkene 8) [General Average]				
C-7 alkene - Boston		0.007 ppbv	Percival *et al.*	59
C-7 alkene - Boston		0.003 ppbv	Percival *et al.*	59
2,4,4-trimethyl-2-pentene (Alkene 9) [General Average]				
C 8 alkene - Boston		0.019 ppbv	Percival *et al.*	59
C 8 alkene - Boston		0.004 ppbv	Percival *et al.*	59
2,3,3,3-tetrafluoro-1-propene (Alkene 11) [General Average] HFO-1234yf				
Jungfraujoch, Switzerland		3 ppq	Vollmer *et al.*	61
Dubendorf, Switzerland		136 ppq	Vollmer *et al.*	61
Global future scenario - annual	Average	0.34 pptv	Wang *et al.*	62
	Maximum	30.96 pptv	Wang *et al.*	62
China future scenario- annual	Average	2.62 pptv	Wang *et al.*	62
	Maximum	30.96 pptv	Wang *et al.*	62
USA future scenario - annual	Average	2.20 pptv	Wang *et al.*	62
	Maximum	19.44 pptv	Wang *et al.*	62
USA future scenario - summer	Average	4.19 pptv	Wang *et al.*	62
	Maximum	40.95 pptv	Wang *et al.*	62
USA future scenario - summer	Average	7.40 pptv	Luecken *et al.*	62,63
	Maximum	300.00 pptv	Luecken *et al.*	62,63
EU future scenario - annual	Average	2.73 pptv	Wang *et al.*	62
	Maximum	19.08 pptv	Wang *et al.*	62
EU future *STOCHEM* scenario - annual	Average	2.60 pptv	Henne *et al.*	62,64
	Maximum	18.00 pptv	Henne *et al.*	62,64
EU future *FLEXPART* scenario - annual	Average	1.50 pptv	Henne *et al.*	62,64
	Maximum	3.70 pptv	Henne *et al.*	62,64
North pole future scenario - annual	Average	0.40 pptv	Wang *et al.*	62
	Maximum	1.19 pptv	Wang *et al.*	62
(*E*)-1-chloro-3,3,3-trifluoro-1-propene (Alkene 13) [General Average] (HCFO-1233zd(E))				
Jungfraujoch, Switzerland		8 ppqv	Vollmer *et al.*	61
Dubendorf, Switzerland		12 ppqv	Vollmer *et al.*	61
Beijing, China		~20 ppqv	Sulbaek Andersen *et al.*	65
(*E*)-1,3,3,3-tetrafluoro-1-propene (Alkene 14) [General Average] (HFO-1234ze(E))				
Jungfraujoch, Switzerland		41 ppqv	Vollmer *et al.*	61
Dubendorf, Switzerland		928 ppqv	Vollmer *et al.*	61
(*E*)-2-pentene (Alkene 15) [General Average]				
- Mega city		1.4×10^{10} cm^3 s^{-1}	Vereecken *et al.*	56
- Rural Europe		2.0×10^7 cm^3 s^{-1}	Vereecken *et al.*	56
Taipei Urban - Summer Daytime		0.12 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time		0.21 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime		0.11 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time		0.13 ppbv	Wang *et al.*	58
Mexico City - Urban		0.74 ppbv	Percival *et al.*	59
Mexico City - Industrial		1.36 ppbv	Percival *et al.*	59
Chinese Max		5.3 ppbv	Percival *et al.*	59

(*Z*)-2-pentene (Alkene 16) [General Average]			
– Mega city	6.9×10^9 cm^3 s^{-1}	Vereecken *et al.*	56
– Rural Europe	1.7×10^7 cm^3 s^{-1}	Vereecken *et al.*	56
Taipei Urban - Summer Daytime	0.05 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.09 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.04 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.05 ppbv	Wang *et al.*	58
Mexico City - Urban	0.37 ppb	Percival *et al.*	59
Mexico City - Industrial	0.7 ppb	Percival *et al.*	59
Chinese Max	9.4 ppb	Percival *et al.*	59
(*E*)-2-butene (Alkene 17) [General Average]			
– Mega city	2.0×10^{10} cm^3 s^{-1}	Vereecken *et al.*	56
– Rural Europe	2.0×10^8 cm^3 s^{-1}	Vereecken *et al.*	56
Taipei Urban - Summer Daytime	0.10 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.16 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.08 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.09 ppbv	Wang *et al.*	58
Mexico City - Urban	1.05 ppb	Percival *et al.*	59
Mexico City - Industrial	2.48 ppb	Percival *et al.*	59
Chinese Max	3.4 ppb	Percival *et al.*	59
Karachi	0.3 ppb	Percival *et al.*	59
Dallas	0.47 ppb	Percival *et al.*	59
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(6.1 \pm 3.0) \times 10^7$	Novelli *et al.*	60
(*Z*)-2-butene (Alkene 18) [General Average]			
– Mega city	1.5×10^{10} cm^3 s^{-1}	Vereecken *et al.*	56
– Rural Europe	1.3×10^8 cm^3 s^{-1}	Vereecken *et al.*	56
Taipei Urban - Summer Daytime	0.09 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.12 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.08 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.08 ppbv	Wang *et al.*	58
Mexico City - Urban	0.83 ppb	Percival *et al.*	59
Mexico City - Industrial	1.31 ppb	Percival *et al.*	59
Chinese Max	2.7 ppb	Percival *et al.*	59
Karachi	0.2 ppb	Percival *et al.*	59
Dallas	0.24 ppb	Percival *et al.*	59
(*Z*)-2-hexene (Alkene 19) [General Average]			
Taipei Urban - Summer Daytime	0.02 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.03 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.01 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.01 ppbv	Wang *et al.*	58
Z-2-hexene in Los Angeles	0.05 — 1.04 ppb	North *et al.*	66
Boston	0.02	Percival *et al.*	59
Porto Alegre	1.6	Percival *et al.*	59
2-methylpropene or Isobutene (Alkene 20) [General Average]			
Taipei Urban - Summer Daytime	0.37 ppbv	Wang *et al.*	58
Taipei Urban - Summer Night-time	0.51 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Daytime	0.41 ppbv	Wang *et al.*	58
Taipei Urban - Autumn Night-time	0.38 ppbv	Wang *et al.*	58
Mexico City - Urban	3.04 ppb	Percival *et al.*	59
Mexico City - Industrial	5.28 ppb	Percival *et al.*	59
Chinese Max	4 ppb	Percival *et al.*	59
Porto Alegre	16.5 ppb	Percival *et al.*	59
Meadows and Coniferous forests in Bavaria (HOPE observatory)	$(4.2 \pm 2.5) \times 10^8$	Novelli *et al.*	60

*Table 47: Boiling Points of Alkenes **1—20***

No	Alkene	Boiling point (^{O}C)	Ref

1	**1-propene**	-47.7	[67]
2	**1-butene**	-6	[68]
3	**3-methyl-1-butene**	20.1	[69]
4	**3,3-dimethyl-1-butene**	41.2	[69]
5	**Methyl Vinyl Ketone (MVK)**	81	[70]
6	**2-methyl-2-butene**	37.5-38.5	[71]
7	**2-methyl-2-pentene**	67.3	[69]
8	**2,4-dimethyl-2-pentene**	83.4	[69]
9	**2,4,4-trimethyl-2-pentene**	104.9	[72]
10	**4-Methylpent-3-en-2-one (Mesityl Oxide)**	130	[73]
11	**2,3,3,3-tetrafluoro-1-propene (HFO-1234yf)**	-28	[74]
12	**3,3,4,4,4-pentafluoro-1-butene (HFO-1345fz)**	3-6	[75]
13	**(*E*)-1-chloro-3,3,3-trifluoro-1-propene (HCFO-1233zd(E))**	18.3	[76]
14	**(*E*)-1,3,3,3-tetrafluoro-1-propene (HFO-1234ze(E))**	−19	[74]
15	**(*E*)-2-pentene**	36.3	[69]
16	**(*Z*)-2-pentene**	36.9	[69]
17	**(*E*)-2-butene**	0.9	[77]
18	**(*Z*)-2-butene**	4.0	[78]
19	**(*Z*)-2-hexene**	68-70	[69]
20	**2-methylpropene (isobutene)**	-6.9	[79]

1.6 Additional Sections

1.6.1 The Impact of Alkene Interconversion on Ozonolysis Chemistry

The analysis in the main body of the Thesis in Chapter 3 involves the ozonolysis of many different alkenes there are many different types of reactions. These alkenes can be broadly divided into conformationally—restricted alkenes, which have restricted movement and symmetry mean they only have one conformer (alkenes **1**, **4**, **6**, **9**, **11**, **13**, **14**, **17**, **18** & **20**), and conformationally—flexible alkenes, which due to their size and mobility produce multiple conformers (alkenes **2**, **3**, **5**, **7**, **8**, **10**, **12**, **15**, **16** & **19**). An example these multiple conformers interconverting over an isomerisation barrier (TS_{ISO}) is seen for alkene **10**, in Figure 3.

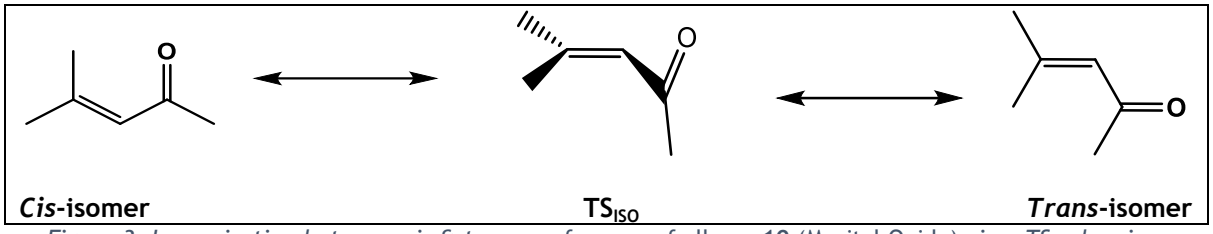


Figure 3: Isomerisation between cis & trans conformers of alkene **10** (Mesityl Oxide) *via a TS_{ISO} barrier.*

During the IRC calculations for some of these cycloaddition (TS_{OZO}) structures, the reactants that are produced are not the lowest energy conformers. In light of this, one very important factor to consider is that the TS_{ISO} barrier may provide an obstacle between the lowest energy conformer and the TS_{OZO} barrier, potentially affecting the k_{ME} values. Many TS_{ISO} barriers are small (< 5 kJ mol^{-1}), such as those seen for alkenes **2** & **15**, and so unlikely to act to be significant obstacles to reaction. However, as shown in Figure 4, there are alkenes that have larger TS_{ISO} barrier than TS_{OZO} barriers. This could be a significant issue as with O_3 + alkene **5** reaction as the TS_{ISO} barrier is between the lowest energy conformer and the lowest energy TS_{OZO} barrier.

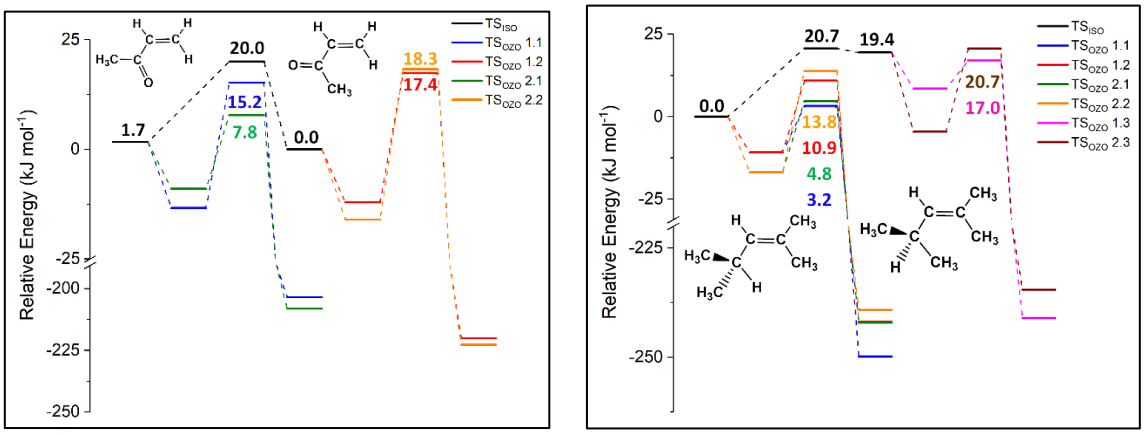


*Figure 4: Potential energy surface of the ozonolyses of alkene **5*** (on the left referred to as figure S3.xa) & *alkene **8*** (on the right referred to as figure S3.xb). *This include the different* conformers connected of *via a TS_{ISO} barrier, and which alkene conformer was produced from the IRC calculation of the TS_{OZO} step.*

To determine whether TS_{ISO} barrier could be a significant obstacle to reaction the effect of isomerisation could be tested using MESMER, which as demonstrate throughout this thesis, can determine the chemistry of multistep reactions. As it is assumed that if this alkene isomerisation has no effect on k_{ME} values then it will have no effect on Γ_{THEO} values of the final product and for that reason, only the ozonolysis step is included in this particular analysis. But, one difficulty is that including two conformers of the same raw reactant with a TS_{ISO} barrier, in a bimolecular system is beyond the capacity of MESMER. This can be circumnavigated by having within the MESMER input file, a parallel set of pre-reaction complexes augmented with the isomerisation transition states linking the two. These *augmented calculations* replicates the TS_{ISO} barrier seen between the two alkenes but by restricting it to the single bimolecular structure of the pre-reaction complexes, it is within the capacity of MESMER to process. If the obstruction caused by the TS_{ISO} barrier to the TS_{OZO} barrier is significant, the Γ_{THEO} values the POZ that is formed will drop.

The conformationally—flexible alkenes that are selected to analyse this obstructive capacity are: alkenes that have lots of bulky substituents, alkene **8** ($iPrCH=C(CH_3)_2$); and alkenes where the substituent TS_{ISO} rotation would break conjugation between >C=C< and C=O functional groups, alkenes **5** & **10** ($CH_3C(O)CH=CH_2$ & $CH_3C(O)CH=C(CH_3)_2$). A comparison of the Γ_{THEO} values of the POZ conformers comparing the *augmented calculations* with the standard MESMER treament for the cycloaddition step of the O_3 reactions with alkenes **5**, **8** & **10**, is found in Table 48.

*Table 48: Comparing different Γ_{THEO} values of the POZs from the ozonolysis of alkenes **5**, **8** & **10**, using different MESMER treatments.*

	Γ_{THEO}					
Alkene	**Alkene 5**		**Alkene 8**		**Alkene 10**	
Method	**Standard**	**Augmented**	**Standard**	**Augmented**	**Standard**	**Augmented**
Grainsize	20	20	20	20	20	20
POZ 1.1	0.053	0.053	0.723	0.723	0.301	0.301
POZ 1.2	0.018	0.019	0.032	0.032	0.006	0.007
POZ 1.3	N/A	N/A	0.005	0.005	N/A	N/A
POZ 1.1	0.916	0.916	0.234	0.234	0.686	0.685
POZ 1.2	0.012	0.012	0.006	0.006	0.007	0.007
POZ 1.3	N/A	N/A	0.001	0.001	N/A	N/A

The comparison of the standard MESMER treatment with the *augmented calculations*, appears to only diverge from each other to a negligible degree. This may be because TS_{ISO} structures always give lower ΔG barriers than the TS_{OZO} structures, as found in Appendix Section 1.3. This suggests that the standard MESMER treatment of calculating k_{ME} values, without any reference TS_{ISO} barriers, is very appropriate for determining ozonolysis

chemistry, when there are multiple alkene conformers. The standard MESMER treatment is therefore used as the standard method to calculate the k_{ME} values in Thesis Chapters 3, 4 & 6.

1.6.2 The Impact of POZ Interconversion on Ozonolysis Chemistry

In the duration of this thesis, there are many different types of reactions but these can be broadly divided into two specific types: one-step reactions, where the reactant react to produce products, not via an intermediate product; and a two-step reaction, where the reactants produce an short-lived intermediate product, usually a cyclic ozonide, which subsequently fragments, due to torsional strain and excess energy. The one-step reactions, such as sCI + alcohol reactions, are not of interest in this section, as their simplicity means the standard MESMER treatment, is not very computationally intensive for the MESMER software. However, multistep reactions in this study, such as that seen for the ozonolysis of alkene **18** (*Z*-2-butene), in Figure 5, are more complicated because they involve a cycloaddition step (TS_{OZO}) to produce a 5 member primary ozonide ring (or POZ), subsequently a POZ fragmentation step. As only the POZ fragmentation step is irreversible in this MESMER model, this makes it more costly to determine the Γ_{THEO} values as it involves calculating a lot of computationally intense *reversable reactions*.

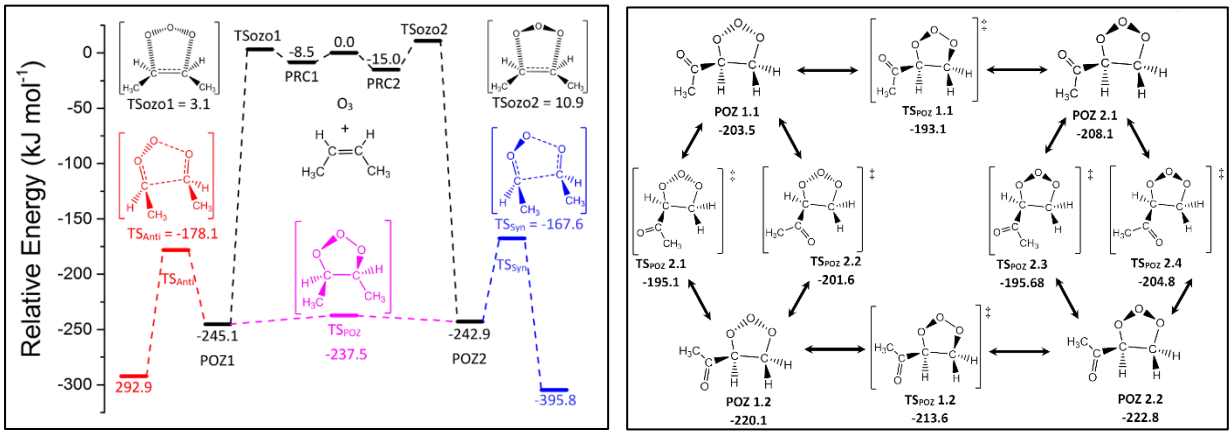


*Figure 5: Comparing the Potential Energy Surface for alkene **18** + O_3 reaction containing only one POZ isomerisation, TS_{POZ},(Figure) compared to all the different POZ conformeric isomerisation that the O_3 + alkene **5** potential energy surface would contains [relative energy in kJ mol^{-1}]*

This two-step process is seen also in Sections 5.2 & 5.3 in the main text of thesis, the **sCI** + HCHO & SO_2 reactions, which also produce short-lived intermediate products, here referred to as HOZs and SOZs respectively. While inclusion of both cycloaddition step and HOZ/SOZ decomposition does increase costs significantly, a big cost is caused by the complexity is the inclusion multiple conformers of HOZs and SOZs, which interconvert over isomerisation transition states. Nevertheless, the small size of the **sCI** + HCHO systems and

the significantly restricted nature of the interconversion in the **sCI** + SO_2 reactions, means the number of intermediate products (≤2) and isomerisation transition states (≤1), is kept low. This means only a small number of computational chemistry calculations are required to produce such intermediate structures and that the intensity of the MESMER calculations can be reduced by altering the grainsize. For more details on the sCI reactions with HCHO & SO_2 and other difficulties involved in calculations see Sections 5.2 & 5.3 in the main text of thesis. However, the alkene ozonolysis calculations in Chapter 3 & 6 can involve much larger numbers of intermediates and isomerisation transition states (see Figure 5).

Some alkene ozonolysis reactions have manageable numbers of POZ intermediates an isomerisation transition states such as alkene **17** + O_3, which has 1 × POZ without any isomerisation transition states (TS_{POZ}), or alkene **18** + O_3, (featured in figure 3.2a) which has 2 × POZs and 1 × TS_{POZ}. This means that is still possible to determine the Γ_{THEO} values using the full potential energy surface, without significant drawbacks in cost either to undertake the computational chemistry calculations or the full MESMER treatment. However this contrast significantly with the ozonolysis of alkene **5**, which produces 4 × POZs and as many as as 6 different TS_{POZ} structures. Alkene **5** + O_3 also is amongst the smaller of these "complex reactions" compared to Alkene **2** + O_3, which produces 6 × POZs and ~12 × TS_{POZ}, or Alkene **19** + O_3, which produces 18 × POZs and ~36 × TS_{POZ}. This causes significant increases in computational cost in determining the TS_{POZ} structures and goes beyond the capacity of the MESMER software to process.

In the theory, as mapped by the IRC calculations, each cycloaddition pathway produces and each POZ fragmentation pathway emerges from a particular POZ conformer. In **sCI** + SO_2 reactions this distinction is critical because the SOZ conformers often do not interconvert. But with the ozonolysis of alkenes in chapter 3 & 6, all each cycloaddition pathway and each POZ fragmentation pathway is interconnected to each POZ conformer due to the there isomersation over the TS_{POZ} barriers. However, as displayed for alkene **18** + O_3 in Figure 5, the TS_{POZ} barriers calculated for alkene ozonolysis reactions are significantly lower than both cycloaddition and POZ fragmentation barriers.

The structures of the alkenes vary significantly and if the substituent groups are different in character, such as the carbonyl R_1 substituent in the O_3 + alkene **5** reaction, could lead to higher isomerisation energy. This would imply that the POZ conformers to be chemically distinct. However, as shown in Figure 5, the TS_{POZ} barriers (-213.6 — -193.1 kJ mol^{-1}) are close in energy to POZ (-222.8 — -203.5 kJ mol^{-1}) and significantly lower in energy than both the cycloaddition barriers (7.8 — 18.3 kJ mol^{-1}) and the POZ decomposition barriers (-

158.8 — -118.2 kJ mol^{-1}). These results suggest that TS_{POZ} barrier heights are not significantly altered by the presence of the carbonyl R_1 substituent.

This indicates that these POZ conformers interconvert freely, at least to some extent, and therefore the uptake of fragmentation pathways will not discriminate between POZ conformers, to generate multiple sets of final products. This non-discrimination assumption subsequently implies that if the array of POZ conformers and TS_{POZ} barriers in the MESMER file were replaced with a single POZ conformer, with all cycloaddition channels terminating there and all POZ fragmentation pathways originating with that conformer, the same result would emerge. If this "new MESMER treatment", as it is referred to in the main body of this thesis, is true then a costs would be reduced significantly, as TS_{POZ} structures would not need to be calculated and such calculations would be significantly within the capacity of the MESMER software to process.

*Table 49: Comparing different Γ_{THEO} values of the ozonolysis of alkenes **1**, **6**, **11**, **13** & **18**, using different MESMER treatments. (different CI yields are represented using: Γ_{ANTI} for an anti-conformer; Γ_{SYN} for a syn-conformer; Γ_{FO} for yield of formaldehyde oxide; and Γ_{DMFO} for yield of dimethyl formaldehyde oxide)*

MESMER Treatment		**Full**	**New**	**Parallel**
Alkene	Channel	All POZs & TS_{POZ}	One POZ & no TS_{POZ}	Multiple POZs & no TS_{POZ}
1	**Grain size**	**25**	**20**	**20**
	Γ_{ANTI}	0.452	0.438	0.562
	Γ_{SYN}	0.276	0.239	0.256
	Γ_{FO} 1	0.157	0.175	0.080
	Γ_{FO} 2	0.115	0.148	0.102
6	**Grain size**	**70**	**40**	**40**
	Γ_{ANTI}	0.241	0.216	0.333
	Γ_{SYN}	0.050	0.072	0.053
	Γ_{DMFO} 1	0.415	0.509	0.471
	Γ_{DMFO} 2	0.294	0.203	0.143
11	**Grain size**	**80**	**40**	**60**
	Γ_{ANTI}	2.48×10^{-7}	2.49×10^{-7}	3.09×10^{-6}
	Γ_{SYN}	2.29×10^{-8}	3.31×10^{-8}	4.43×10^{-7}
	Γ_{FO} 1	0.531	0.553	0.213
	Γ_{FO} 2	0.469	0.447	0.787
13 *	**Grain size**	**70**	**40**	**60**
	$\Gamma_{ANTI-R1}$	0.542	0.604	0.811
	Γ_{SYN-R3}	0.119	0.091	0.120
	$\Gamma_{ANTI-R3}$	0.144	0.108	0.025
	Γ_{SYN-R1}	0.194	0.197	0.044
18	**Grain size**	**40**	**30**	**40**
	Γ_{ANTI}	0.872	0.817	0.976
	Γ_{SYN}	0.128	0.183	0.024

** $\Gamma_{ANTI-R1}$ is for anti-CF_3CHOO; $\Gamma_{SYN-R1\ is}$ for syn-CF_3CHOO; $\Gamma_{ANTI-R3}$ is for anti-ClCHOO; Γ_{SYN-R3} is for syn-ClCHOO*

To test this theory, the Γ_{THEO} values of various alkene ozonolysis reactions are determined using three separate treatments are run on MESMER. These 3 treatments consist of: the full MESMER treatments using all structures on the PES; channelling all cycloaddition and POZ fragmentation channels through the single lowest energy POZ structure, referred to as

the “new MESMER treatment”; and where all TS_{POZ} barriers are excluded and all cycloaddition and POZ fragmentation channels run in and out the POZ conformers that the IRC calculations produce, referred to as the “parallel MESMER treatment”. The “parallel MESMER treatment” prevents POZ interconversion and is similar to the treatment given for the **sCIs 23—26** + SO_2 reactions in chapter 5, where intermediate SOZ products cannot interconvert due to the high energetic cost. This produces essentially two analogous parallel pathways, one for POZ and one for POZ 2, which are analysed as distinct pathways within the MESMER models.

The ozonolysis of alkenes **1**, **6**, **11**, **13** & **18** ($CH_3CH=CH_2$, $CH_3CH=C(CH_3)_2$, $CF_3CF=CH_2$, *E*-$CF_3CH=CHCl$ and *Z*-$CH_3CH=CHCH_3$) reactions are used because their lack of conformational flexibility produce “simple” PESs, with only 2 × POZs and 1 or 2 × TS_{POZ} structures each. which can be used to compare these two other MESMER treatments to the *full* MESMER treatment. If the more complex alkene ozonolysis reactions were used the full MESMER treatment using all TS_{POZ} structures, would increase computational costs. This was undertaken using so many reactions, to make sure the new MESMER treatment was exhaustively tested. This comparison of the different Γ_{THEO} values produced by these MESMER treatments is seen in Table 49.

Of these different treatments, the *parallel MESMER treatment*, show a significant divergence for Γ_{THEO} values in all 5 reactions, except for the anomaly of O_3 + alkene **6** reaction. This means that the *parallel MESMER treatment*, does fundamentally lead to different chemistry and is likely to work well for the sCI + SO_2 reactions.

However the most important observation between these results is that the new MESMER treatment shows results of similar accuracy to standard MESMER treatment for all alkene ozonolysis reactions studied here. Even the most anonymous result O_3 + alkene **6** shows agreement enough to be within ~5% of the other results. Much of these degrees of error can be assumed to be due to the changes in grain size. This work was all done with the lowest possible grainsize that could be possibly processed. This exhaustive analysis of the new MESMER treatment with many different ozonolysis reactions implies that the POZs are mostly freely interconverting and can be treated as essentially one POZ conformer. This is likely because TS_{POZ} barriers are significantly lower in energy than the POZ fragmentation barriers. The high accuracy of this new MESMER treatment of channelling all cycloaddition and POZ fragmentation channels through a single POZ structure has led to it being adopted for determining the Γ_{THEO} values for most of the alkene ozonolysis reactions in chapters 3 & 6 of the main thesis. For a full review of what treatment was used and with what grainsize

was used for each Γ_{THEO} result, see Appendix section 1.2.3. Standard treatment is often used for simple alkene ozonolysis reactions to calculate the Γ_{THEO} values.

One last noteworthy observation is that during the analysis of the impact of including TS_{POZ} barriers, found here, the O_3 + Alkene **11** reaction had the highest barriers to interconversion (TS_{POZ} 1 & 2 ~ -210.1 & -226.0 kJ mol^{-1}) and this has very little impact on the overall branching ratios.

1.6.3 The Impact of CI Interconversion on Ozonolysis Chemistry

The analysis in chapter 3 produces many different CIs (and aldehydes & ketones) with various conformeric forms, but for most of these CIs the isomerisation barrier is minor (< 5 kJ mol^{-1}). It is already well established that, due to their contrasting chemistries and their high barrier to interconversion, *syn*- and *anti*-CIs are stereochemically distinct. This leads to them being treated differently in bimolecular sCI analysis (see Thesis chapters 4 & 5) and separation of their Γ_{THEO} values into Γ_{ANTI} & Γ_{SYN} values for alkene ozonolysis (see Thesis chapters 3 & 6). However, it is possible that isomerisation (TS_{ISO}) barriers, such as those seen in figure s3.x between *cis*- & *trans*-conformers of *syn*-$CH_3C(O)CHOO$, could prevent free interconversion, like that between *syn*- and *anti*-CIs.

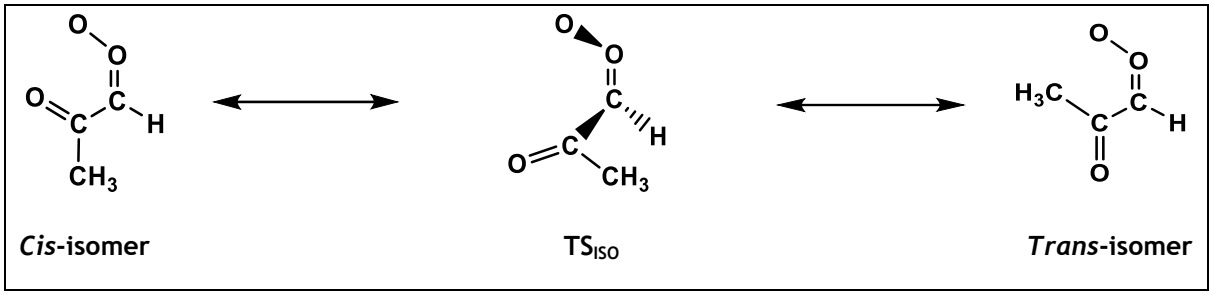


Figure S3.6: Isomerisation between cis & trans conformers of syn-*$CH_3C(O)CHOO$ via a TS_{ISO} barrier.*

Such CI interconversions are important in sCI unimolecular decomposition, as noted in Thesis Section 1.6.1, and the different *cis*- & *trans*-conformers can exhibit different bimolecular chemistry, such as that seen in Thesis Section 4.5 for alcohol reactions with isoprene-derived sCIs. In this section key CIs yielded in the alkene ozonolysis and an aldehyde ($CH_3C(O)CHO$) is also tested to see the different conformers require different classification or whether the isomers of the aldehyde interconvert post-reaction. The species selected for this comparison are CIs and aldehydes with groups that make interconversion difficult, such as bulky groups or are conjugated groups. Table 50 displays the computational energies of different conformers and the TS_{ISO} barriers of the species: $CH_3C(O)CHO$, *anti*- & *syn*-$CH_3C(O)CHOO$ and *syn*-iPrCHOO.

Table 50: The ZPE relative to lower energy conformer of divisive Criegee intermediates and aldehydes

Chemical	DF-LCCSD(T)-F12a			B3LYP		
	Con 1	TS_{ISO}	Con 2	Con 1	TS_{ISO}	Con 2
***anti*-$CH_3C(O)CHOO$**	0.0	34.2	14.1	0.0	35.3	14.6
***syn*-$CH_3C(O)CHOO$**	0.0	25.7	23.1	0.0	28.1	24.1
$CH_3C(O)CHO$	20.8	23.0	0.0	20.2	28.4	0.0
***syn*-iPrCHOO**	0.0	26.5	9.4			

With the exception of the barrier between *anti*– & *syn*–CIs, the barriers of between such CI and aldehyde conformers in this thesis are relatively small, especially given alkene ozonolysis produces significant the excess energy. Considering that the significant excess energy within a hot CIs, is that at least prior to collisional stabilisation, these different CI conformers freely interconvert (except for *anti* & *syn* conformers). Despite the fact that $CH_3C(O)CHO$ is likely to see the greater of the TS_{ISO} barriers, the barrier is still relatively small, so they are likely to freely interconvert after ozonolysis. Therefore, in the main body of this thesis does not refer to specific CI conformer branching ratios (except for *syn* and *anti* conformers), although the pathways that produce specific conformers are identified and their specific yields are noted, in Appendix Section 1.2.

1.6.4 Introduction to structure activity relationships

Whilst using experimental methods to analyse the ozonolysis of alkenes can yield accurate and reliable data, for example concerning the k_{EXP} and Γ_{EXP} values, lab-based experiments have several major drawbacks. Ozonolysis of alkenes releases large energy yields (e.g. 200-250 kJ mol^{-1} for O_3 + 2,3-dimethylbutene) that would require expensive, highly-resistant equipment to monitor the reaction directly.[80] The Criegee intermediate yields are difficult to determine because the k_{UNI} values of internally hot CIs are very high. There are even greater difficulties in determining the population of the short-lived "cold CIs", or sCIs, especially where the sCI may exhibit multiple conformers. Before the Taatjes *et al.* study in 2008, researchers tried to overcome these challenges by determining CI yields indirectly through measuring of the aldehyde/ketone by-products and the OH yields.[1,16,81] More recently however, the direct measurement of sCIs, such as *syn*- & *anti*-CH_3CHOO, have been obtained using both UV spectroscopy and infrared spectroscopy with a Herriott cell, was used to distinguish *syn*- from *anti*-sCI conformers.[82,83] Despite these recent developments, these new methods in measuring *syn*- & *anti*-sCI conformer yields have yet to be applied to measuring the experimental yields of alkene ozonolysis.

Computational methods may fill in the gaps in reactivity data which have been left by the indirect measurements of previous work, resulting in the production of a more complete picture of CI production and loss channels. Chapter 3 of this thesis demonstrates that alkenes with either small substituents (like propene) or inflexible, bulky substituents (like 2,4,4-trimethyl-2-pentene) can be computed with relatively small numbers of calculations. A study conducted by McGillen *et al.* in 2006, along with other research in the literature, found that additional alkyl groups added to substituent groups past the *β*-carbon atoms make little difference to the ozonolysis chemistry.[84,85] However, one major drawback of using computational chemistry is that accurate *ab initio* modelling of the ozonolysis of flexible middle-sized alkenes, like *cis*-2-hexene requires a very large number of calculations. This is explained and explored further in Chapter 6, along with the development of other empirical models to measure this type of *Structure-Activity Relationship* (SAR).[36,37,86]

These SAR models use well defined structural characteristics of a reactants series to estimate and predict their chemistry in a very specified reaction conditions (such as with O_3). These ansatz can be built upon either theoretical or experimental analysis. For example, McGillen *et al.*, in his 2008 model, produced a relationship between the bulk & number of substituent groups on an aliphatic alkene, and the ozonolysis rate constant (k_{O_3})

of that alkenes. This is important because, if an SAR model is reliable, it demonstrates the value to producing a chemistry-based taxonomic classification system for these types of reactions. Another reason to generate this kind of SAR modelling is to reduce the number of reactions that are undertaken in atmospheric models. One example of this is in the atmospheric models for *AtChem2*, where the sum of the tropospheric organic peroxyl radicals are often treated as one species, RO_2, because their reactions with other species, as well as their self and cross reactions, have similar chemistry. If a similar treatment can be used for the ozonolysis of alkene, as is applied with RO_2, that would significantly reduce the number of calculations and therefore the amount of computational energy required to run these models.

To the author's knowledge there are no k_{EXP} values for the O_3 + 2,4-dimethyl-2-pentene reaction in the literature, so to assess the k_{THEO} values determined for this reaction in Chapter 3 of this thesis, a rate constant derived from the SAR models (k_{SAR}) is used as a comparative tool. While the 2008 McGillen *et al*. SAR model is also used for this purpose in Chapter 6, its more important use is that it provides significant insight into the development of new models designed to calculate both the k_{THEO} & Γ_{THEO} values for the ozonolysis of long-chained alkenes, such as *cis*-2-hexene.

Structure-activity/structure-reactivity relationships have been proposed as a solution for modelling the reactions between gaseous organic compounds, including alkenes, with O_3 and other co-reactants, such as OH radicals.[87-89] Various attempts at SAR treatment to the gaseous ozonolysis of alkenes have emerged with varying degrees of success. A perturbation frontier molecular orbital (PFMO) theory derived using SAR treatment, where by the energy change between the alkene's *highest occupied molecular orbital* (HOMO) and the O_3 *lowest unoccupied molecular orbital* (LUMO) is contrasted to the $\log_{10}$ (k_{EXP}).[90-94] A derivative of this is the use of the ionization potential of the alkene as a substitute for the molecular orbitals in these SAR models.

However the successes of this model in determining a rate constant are shown to be significantly limited, as the rate constants they project for the ozonolysis of pentene and 2,4-dimethyl-3-methaylene are often out by orders of magnitude from the k_{EXP} value.[90,92,93] Explanations of these divergences and inaccuracies include steric hinderance of large substituent groups or the lack of asymmetrical orbital contributions in PFMO theory.[93,95,96] Other important factors that have been considered in SAR studies, which correlate with the rate of ozonolysis, includes the electrophilic potential of the >C=C< bond, or the Randić-type indices.[81,85,88] Many of these SAR factors have not only been correlated with

k_{O_3}, but have been observed in other alkene reactions with NO_3 and OH reactions. Unfortunately, the steric hindrance consistently causes significant divergences between k_{SAR} and k_{EXP} values.[85]

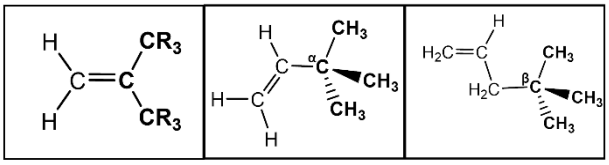


Figure 1.7: The three alkyl-substituted positions that would sterically hinder O_3 + alkene reactivity.

This led to the development of the 2008 SAR study designed mainly by McGillen *et al.*, which incorporates both the inductive and steric inputs of the alkene used into one combined factor.[37] The inputs in the SAR equation provide: the increase in reactivity of the >C=C< bond provided by each extra alkyl substituent group attached; and a steric hinderance for the reaction, which is gradually reduced as the bulkiness moves away from the >C=C< bond. In order of greatest intrusion, the alkyl groups can cause steric interference by being placed within disubstituted olefin alkene, on the α-C of a substituent, or on a ß-C of a substituent. These types of steric interference are identified in the structures of Figure 1.20 but beyond the ß-C, the steric interference , caused by extra alkyl groups, is experimentally shown to be negligible. This method has been fitted to the experimental rate constants in the literature and the theoretical results have the potential to be fitted too. It has been shown to provide a strong linear relationship (0.90—0.94) between $\log_{10}$ (k_{EXP}) and that combined factor.[36,37]

The 3 different steric interferences: a disubstituted >C= effect, an α-alkyl effect, and a ß-alkyl effect; correlate in the literature with reductions in k_{EXP} values.[37,86] The simplest example of the disubstituted >C= effect is 2-methylpropene having a lower k_{EXP} value (1.24×10^{-17} cm^3 s^{-1}) than both *cis*- and *trans*-2-butene ($1\text{-}2 \times 10^{-16}$ cm^3 s^{-1}).[37] The α-alkyl effect reduced the k_{EXP} value depending on the number of alkyl branches in α-positions in substituents, such as when 1-butene has a reduced k_{EXP} than propene (9.18 & 10.4×10^{-18} cm^3 s^{-1} respectively) due to containing an extra α-CH_3 group. A subsequent addition of an alkyl branches to the ß-position, exhibits increased steric interference of the ß-alkyl effect, as the additional a ß-CH_3 group of 1-pentene decreases the k_{EXP} value (8.74×10^{-18} cm^3 s^{-1}) compared to 1-butene.

This SAR method has been extended to include dienes, like isoprene and 1,3-butadiene, and heteroatomic alkenes, such as *E*-2-pentenoic acid, *Z*-1,2-Dichloroethene and 2-Hexen-4-one.[86] SAR methods have been adapted also to model the temperature dependence.[36]

The drawbacks of the McGillen *et al*. models produced in 2008-11 is that they only use experimental analyses and do not incorporate important computational studies. Additionally, they do not calculate product branching ratio (Γ) values for the sCIs, the aldehydes, ketones or OH by-products. The models in Chapter 6 that were derived to determine the reaction chemistry of O_3 + *cis*-2-hexene, calculates both computational k_{EXP} values and direct sCI branching ratios of the ozonolysis of medium size alkenes.

1.7 The Role of the Epoxidation in Alkene Ozonolysis

This section explores whether O_3 + Alkenes **1** & **5** can proceed via an epoxide + O_2 reaction channel and whether these competing epoxide channels have sufficient impact to warrant further investigation. Prior experimental analysis suggests the collective epoxide branching fractions (α_{EPO}) for simple acyclic alkenes are insignificant (<0.006), but that they contribute more significantly to the total reactive outcomes for conjugated dienes such as 1,3-butadiene (0.023) and isoprene (0.039 ± 0.011).[97,98] If the anticipated Γ_{THEO} values for the ozonolysis of alkenes **1**—**20** are of the same range as isoprene, the analysis in this chapter should include the relevant epoxide channels. The chemical structures of Alkenes **1** & **5** and examples of the two types of epoxide channel explored in this study are in Figure 3.29:

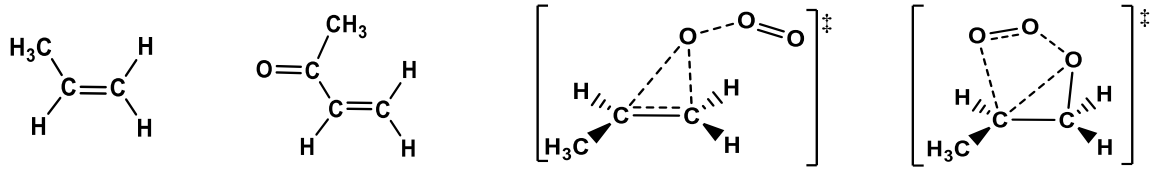


*Figure 3.8: Chemical Structures of Alkenes **1** & **5** and Example Structures of Epoxidation Channels.*

Given the low experimental α_{EPO} value for simple acyclic alkenes, a full analysis of the epoxide channels for all O_3 + mono-alkene reactions in this study are likely not necessary, so this exploratory analysis is focused on O_3 reaction with the simplest alkene, alkene **1**, to save computational cost. However, there is a prospect that the greater epoxide yields of conjugated dienes could also apply to other conjugated species, including the enones (a type of unsaturated ketones) studied in this chapter. So O_3 + alkene **5** is also examined to investigate whether enones are also more predisposed to reaction via the epoxide channels. A previous theoretical study by Li *et al.* investigated various epoxidation pathways in the O_3 + 1,3-butadiene reaction, and these calculations produced two types of mechanisms, which are referred to in this thesis as TS_{EPO} 1 and TS_{EPO} 2.[99] Figure 3.29 shows approximate templates for the O_3 + alkene **1** reaction of both the TS_{EPO} 1 channel, which generates the epoxide from the raw reactants via a single TS structure, and the TS_{EPO} 2 channel, which is a POZ fragmentation mechanism. Both epoxide channels are investigated for both O_3 + Alkenes **1** & **5** in this section and, unless otherwise stated, where there are multiple participating TS structures only the lowest energy structure is displayed.

1.7.1 Challenges with Determining the Energy of Epoxidation TS Structures

During this theoretical analysis of these epoxide pathways for O_3 + Alkenes **1** & **5**, it was noted that the relative energies of the TS_{EPO} structures calculated using *DF-LCCSD(T)-F12/aug-cc-pVTZ* were problematic, as shown in Table below. This included large differences in energy (sometimes >200 kJ mol^{-1}) between very similar TS_{EPO} structures for both alkenes **1** & **5** without any discernible reason for such an energy disparity. The TS_{EPO} 2.2 & 2.3 structures for O_3 + alkenes **5** even yielded relative energies (-153.1 & -152.2 kJ mol^{-1}) lower than the relative energy of the epoxide + O_2 final products (-138.54 kJ mol^{-1}). Many of these TS_{EPO} relative energies were even lower than those recorded for O_3 + 1,3-butadiene (33.5 & -13.4 kJ mol^{-1}), which are already favourable for an epoxide pathway.[99]

*Table 51: Examples of the variations in raw energies between DF-LCCSDT(T)-F12 and B3LYP/aug-cc-pVTZ for the same epoxidation TS structures of Ozonolysis of Alkene **1** & **5**.*

		ΔE (kJ mol^{-1})		
Alkene	**Method**	**DF-LCCSD(T)-F12**	**B3LYP**	**Difference in Relative Energy Between Methods**
1	TS_{OZO} 1	3.9	11.6	-7.7
	TS_{ANTI}	-162.8	-155.0	-7.8
	TS_{FO} 2	-154.1	-144.2	-9.9
	TS_{EPO} 1.1	50.5	50.0	0.5
	TS_{EPO} 2.1	101.9	68.0	33.9
	TS_{EPO} 2.3	94.5	48.9	45.7
5	TS_{OZO} 1.2	17.4	13.5	3.9
	TS_{ANTI} 2	-140.2	-134.5	-5.7
	TS_{FO} 2.1	-139.0	-133.8	-5.2
	TS_{EPO} 1.2	62.6	50.7	11.8
	TS_{EPO} 2.1	-66.7	60.3	-127.0
	TS_{EPO} 2.2	-153.1	67.9	-221.0
	TS_{EPO} 2.3	-152.2	69.7	-221.9
	C_{EPO} 2.1	-138.5	-108.8	-29.8

None of these faults were evident in the *B3LYP/aug-cc-pVTZ* energies, likely due to a better representation of multi-reference character. Because of this, all TS_{EPO} energies and α_{EPO} values here in Section 3.6 are based upon *B3LYP/aug-cc-pVTZ* calculations. The data in Table 6.8 provides only most severe examples of these challenging disparities in the relative energy of the TS_{EPO} structure for O_3 + alkenes **1** & **5**. The complete relative energies of all TS_{EPO} structure calculated using both the *DF-LCCSD(T)-F12/aug-cc-pVTZ* and the *B3LYP/aug-cc-pVTZ* methods in this chapter are found in Appendix 1.3.2.

1.7.2 Epoxidation During the Ozonolysis of Alkene 1 ($CH_3CH=CH_2$)

While epoxidation geometries identified in the theoretical study of O_3 + 1,3-butadiene by Li *et al.* are used as a template for the TS_{EPO} 1 & 2 structures in this study, the extra conformational flexibility of 1,3-butadiene produces overall larger numbers of TS_{EPO}

structures than those seen for O_3 + alkene **1**.[99] However, this additional conformational flexibility causing an increase in the number of TSs per channel is simply a continuation of the trend observed with both the cycloaddition and POZ fragmentation channels seen earlier in this chapter. The epoxidation of Alkene **1** by O_3 may compete with other pathways: the *direct reaction* TS_{EPO} 1.1 & 1.2 mechanism competes with the cycloaddition step (as illustrates using the lowest B3LYP/aug-cc-pVTZ energy structures in Figure 3.31), and the TS_{EPO} 2.1—2.4 structures with other POZ fragmentation channels. This means that reviewing the role of the epoxidation process in k_{ME} is just as important as reviewing the overall epoxide + O_2 branching fraction (α_{EPO}).

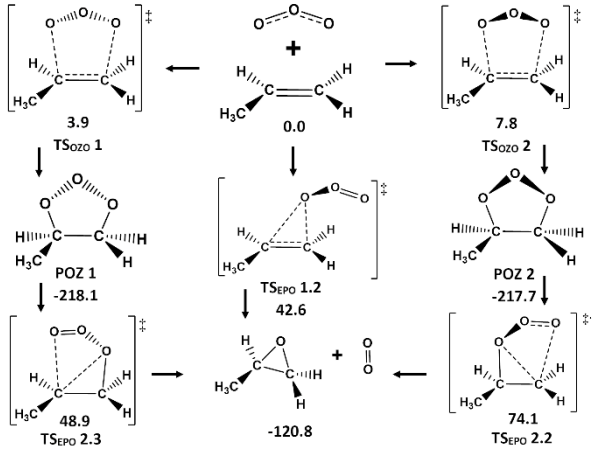


*Figure 9: Schematic of the Lowest Energy (using B3LYP/aug-cc-pVTZ energies) TS_{EPO} 1 & 2 Structures for O_3 + Alkene **1**.*

In spite of the fact that the *direct reaction* TS_{EPO} 1 barriers are lower in energy (42.6 to 50.0 kJ mol^{-1}) relative to the POZ fragmentation TS_{EPO} 2 structures (48.9 to 74.1 kJ mol^{-1}), Figure above shows that the TS_{OZO} 1 & 2 mechanisms are much more favourable to reactant uptake. This is confirmed by the k_{ME} [B3LYP] value for TS_{EPO} 1.1 & 1.2 having a very small contribution (~7.04×10^{-23} cm^3 s^{-1}) to the overall k_{ME} [B3LYP] value (7.37×10^{-16} cm^3 s^{-1}). The TS_{EPO} 2 mechanisms (48.9 to 74.1 kJ mol^{-1}) are much higher compared to other POZ fragmentation processes (-155.0 to -144.2 kJ mol^{-1}), which is reflected in the low overall epoxide branching fraction of O_3 + Alkene **1** (α_{EPO} [B3LYP] ~2.22×10^{-8}). Overall, epoxide formation has very little role in the O_3 + alkene **1** reaction.

1.7.3 Epoxidation During the Ozonolysis of Alkene 5 ($CH_3C(O)CH=CH_2$)

Alkene **5** (Methyl Vinyl Ketone) is the simplest enone and so has an *E*- and *Z*- conformers (similar to 1,3-butadiene), which differ in energy by 0.63 kJ mol^{-1}. This results in four POZs, again similar to 1,3-butadiene. This leads to a large number of epoxidation channels, the lowest of which are shown in Figure below.

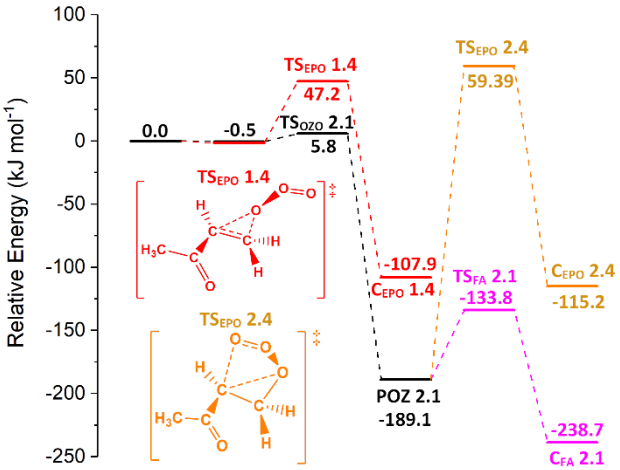


Figure 10: Limited PES comparing low energy ozonolysis and POZ decomposition pathways with lowest energy epoxidation pathways.

Figure 3.32 displays the significant disparity in energy between the TS_{EPO} 1 (47.2 to 69.7 kJ mol^{-1}) and TS_{OZO} (5.8 to 14.8 kJ mol^{-1}) or TS_{EPO} 2 (59.4 to 105.5 kJ mol^{-1}) and the other POZ breakdown pathways (-148.2 to -110.0 kJ mol^{-1}). These high barriers lead to a low k_{ME} [TS_{EPO} 1] value (1.33×10^{-23} cm^3 s^{-1}) compared to the overall B3LYP k_{ME} value (1.83×10^{-16} cm^3 s^{-1}). These high TS_{EPO} 1 barriers and similarly high TS_{EPO} 2 barriers for POZ decomposition led to a similar low α_{EPO} value for Alkene **5** (~ 7.25×10^{-8}) to that of alkene **1** (2.22×10^{-8}). Even the lowest energy TS_{EPO} 1 and TS_{EPO} 2 structures for O_3 + Alkene **5** calculated for this chapter (see Figure 3.32) are much higher than those comparative mechanism for O_3 + 1,3-butadiene calculated in a computational study by Li *et al.* (33.5 & -13.4 kJ mol^{-1}). To the author's knowledge, an α_{EPO} value has yet to be calculated for O_3 + 1,3-butadiene and the low TS_{EPO} barriers for O_3 + 1,3-butadiene may help to explain the non-negligible nature of its experimental α_{EPO} value of (~0.023).[97,98] However, despite the fact that the >C=C< bonds in both alkene **5** and 1,3-butadiene are both part of conjugated structures, the very low theoretical α_{EPO} value for O_3 + Alkene **5** suggests that ozonolysis of enones may not share the same capacity to form epoxides as do some dienes.

One noteworthy observation that requires highlighting from comparing the different TS_{EPO} structures for O_3 + Alkene **5** is that the steric interaction between the ozone group and the substituent group does not wholly dictate energy differences, as shown with the unusually low TS_{EPO} 1.4 & 2.4 barriers. The TS_{EPO} 1.4 & 2.4 structures, shown in Figure 3.33, have the similar spatial arrangement of the ketone group and the >C=C< bond being in a *Z*-orientation, in conjunction with the central oxygen in the O_3 inclined towards the $-C(O)CH_3$ substituent group. These structures, along with TS_{EPO} 2.8, have the orientations of both the electronegative oxygen atom in the ketone group and the O_3 place them into a

position where a mutual repulsion would be expected. This is the reason they are described as having “unusually low energies”.

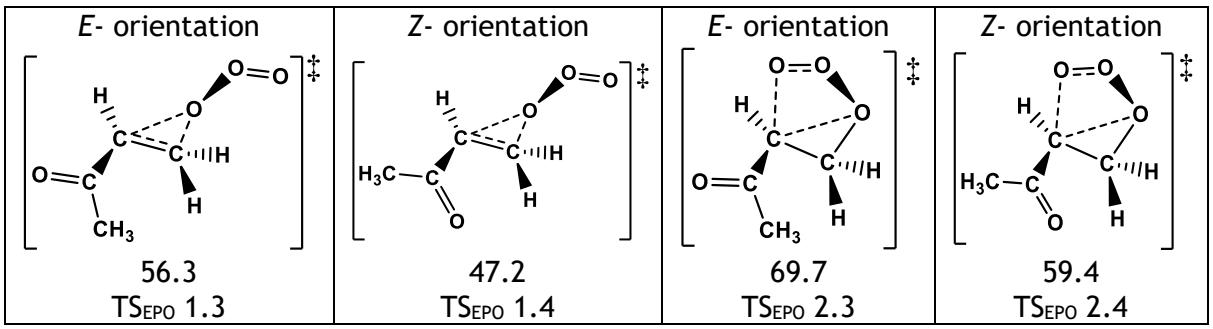


Figure 11: Comparative epoxide subchannel structures, relative B3LYP energies and E- or Z- orientation of alkene 5

If the spatial arrangement is altered slightly such as reverting the ketone group and the >C=C< bond back to an *E*-orientation, such as for TS_{EPO} 1.3 & TS_{EPO} 2.3 in Figure 3.33, a significant increase in energy is also observed. In sections 3.4.3 & 3.5.4, the TS_{OZO} 2.1 structure in O_3 reactions with both alkenes **5** & **10**, has a similar spatial arrangement for the ketone group, the >C=C< bond and the O_3, with a similarly unusually low energy. This low energy for TS_{OZO} 2.1 is also removed if the orientation of any of these groups change.

1.7.4 Summary of epoxidation channel

In summary, whilst the conjugated system of the enone does lower the energy of the epoxide pathways in some circumstances, neither Alkenes **1** or **5** have significant α_{EPO} values. Due to the very low α_{EPO} values for Alkenes **1** & **5**, this epoxide investigation has not been pursued for Alkenes **2**—**4** & **6**—**20**. Despite this, it was important to include this section of work due to the lack of information on the epoxidation pathways for enones. If this study included either isoprene or 1,3-butadiene, the epoxide channel would have been included in the investigation of these alkenes due to their high global emission profiles, such that even small branching fractions to these channels may have globally significant impacts.[100,101] To continue this area of study, a new computational approach would have to be devised for deriving the energy of the epoxide channel because of the difficulties with DF-LCCSD(T)-F12/aug-cc-pVTZ highlighted earlier.

2.0 Supplementary Information for Chapter 4: An Extended Computational Study of Criegee Intermediate—Alcohol Reactions

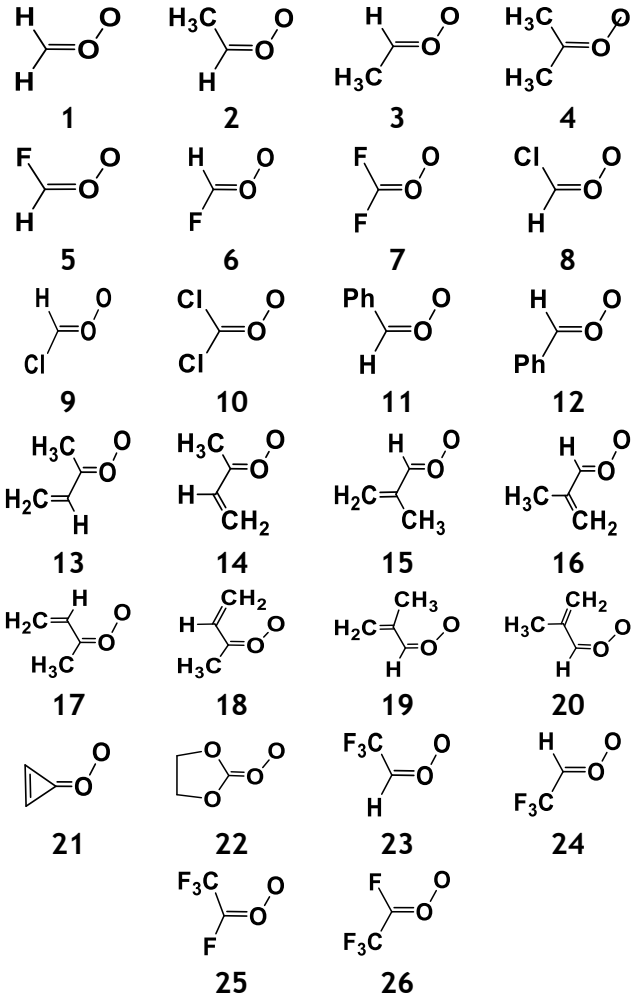


*Figure 4.12: sCIs studied labelled as **sCIs 1—26***

2.1 Dipole-Dipole Capture ($k_{d\text{-}d}$) and Collision Limits (k_{COLL}) Values

To calculate to dipole-dipole capture ($k_{d\text{-}d}$) and collision limit (k_{COLL}) values some of the following details on each reactant is required:

Table 52: Reactants Dipole moments (μ_D, Debye), mass (m, amu), radii (r, Å) and C-O-O bond ratios

Reactant	Dipole Moment (μ_D, Debye)	Mass (m, amu)	radii (r, Å)	C=O-O Bond Ratio
sCI 1	4.3104	46.005	3.209	1.078
sCI 2	4.6851	60.021	3.740	1.084
sCI 3	5.5323	60.021	4.254	1.093
sCI 4	5.4850	74.037	4.253	1.091
sCI 5	4.7113	63.996	3.257	1.113
sCI 6	3.9510	63.996	3.448	1.136
sCI 7	4.0421	81.987	3.476	1.164
sCI 8	4.2093	79.967	3.235	1.082
sCI 9	4.1271	79.967	3.823	1.104
sCI 10	3.9977	113.928	3.831	1.093
sCI 11	5.4178	122.037	6.285	1.075
sCI 12	6.3965	122.037	7.414	1.084
sCI 13	5.6440	86.037	5.264	1.065
sCI 14	5.0100	86.037	5.345	1.075
sCI 15	5.5702	86.037	5.630	1.076
sCI 16	5.5004	86.037	5.675	1.079
sCI 17	5.6349	86.037	4.730	1.070
sCI 18	4.8779	86.037	5.531	1.069
sCI 19	4.8961	86.037	4.999	1.078
sCI 20	4.7638	86.037	5.006	1.065
sCI 21	8.0393	70.005	4.635	1.186
sCI 22	9.2676	104.011	5.314	1.174
sCI 23	3.4822	113.993	4.082	1.064
sCI 24	2.5055	113.993	4.418	1.071
sCI 25	3.016	131.983	4.099	1.114
sCI 26	2.9299	131.983	4.447	1.101
MeOH	1.6556	32.026	2.829	N/A
EtOH	1.7078	46.042	3.3930	N/A
iPrOH	1.6365	60.058	4.3070	N/A

2.1.1 Gas-collision limit (k_{COLL})

Table 53: The Gas-Collision Limits for all sCI + alcohol reactions in this study at a variety of temperatures.

Reaction	Collision Limit (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + MeOH	1.36	1.59	1.66	1.73	1.92
sCI 1 + EtOH	1.47	1.72	1.79	1.87	2.08
sCI 1 + iPrOH	1.79	2.10	2.18	2.28	2.53
sCI 2 + MeOH	1.53	1.79	1.86	1.95	2.16
sCI 3 + MeOH	1.77	2.08	2.17	2.26	2.51
sCI 4 + MeOH	1.71	2.01	2.09	2.19	2.42
sCI 5 + MeOH	1.30	1.52	1.58	1.65	1.83
sCI 6 + MeOH	1.38	1.62	1.68	1.76	1.95
sCI 7 + MeOH	1.34	1.57	1.63	1.71	1.89
sCI 8 + MeOH	1.24	1.46	1.52	1.58	1.76
sCI 9 + MeOH	1.50	1.75	1.83	1.91	2.11
sCI 10 + MeOH	1.43	1.68	1.75	1.83	2.03
sCI 11 + MeOH	2.67	3.13	3.25	3.40	3.77
sCI 11 + EtOH	2.62	3.07	3.20	3.34	3.70
sCI 11 + iPrOH	2.86	3.35	3.49	3.64	4.04
sCI 12 + MeOH	3.37	3.95	4.11	4.29	4.76
sCI 12 + EtOH	3.26	3.83	3.99	4.16	4.62
sCI 12 + iPrOH	3.50	4.10	4.27	4.46	4.95
sCI 13 + MeOH	2.19	2.57	2.68	2.79	3.10
sCI 14 + MeOH	2.24	2.62	2.73	2.85	3.16
sCI 15 + MeOH	2.39	2.81	2.92	3.05	3.39
sCI 16 + MeOH	2.42	2.84	2.95	3.08	3.42
sCI 17 + MeOH	1.91	2.24	2.33	2.44	2.70
sCI 18 + MeOH	2.34	2.74	2.85	2.98	3.31
sCI 19 + MeOH	2.05	2.40	2.50	2.61	2.90
sCI 20 + MeOH	2.05	2.41	2.51	2.62	2.90
sCI 21 + MeOH	1.92	2.25	2.35	2.45	2.72
sCI 22 + MeOH	2.17	2.54	2.64	2.76	3.06
sCI 23 + MeOH	1.54	1.81	1.88	1.97	2.18
sCI 24 + MeOH	1.70	1.99	2.07	2.16	2.40
sCI 25 + MeOH	1.53	1.79	1.87	1.95	2.16
sCI 26 + MeOH	1.69	1.98	2.06	2.15	2.38

2.1.2 Isotropic Dipole-Dipole Capture Limit Values

Table 54: Isotropic Dipole-Dipole Capture Limits for all sCI + alcohol reactions in this study at a variety of temperatures.

Reaction	Isotropic $k_{d\text{-}d}$ (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + MeOH	8.71	8.26	8.15	8.03	7.76
sCI 1 + EtOH	8.05	7.64	7.53	7.43	7.17
sCI 1 + iPrOH	7.36	6.98	6.88	6.78	6.55
sCI 2 + MeOH	8.75	8.30	8.19	8.07	7.80
sCI 3 + MeOH	9.78	9.27	9.15	9.02	8.71
sCI 4 + MeOH	9.40	8.91	8.79	8.67	8.37
sCI 5 + MeOH	8.69	8.24	8.13	8.01	7.74
sCI 6 + MeOH	7.73	7.33	7.23	7.13	6.88
sCI 7 + MeOH	7.55	7.16	7.07	6.97	6.73
sCI 8 + MeOH	7.79	7.39	7.29	7.18	6.94
sCI 9 + MeOH	7.69	7.29	7.19	7.09	6.85
sCI 10 + MeOH	7.20	6.82	6.73	6.64	6.41
sCI 11 + MeOH	8.75	8.30	8.19	8.07	7.79
sCI 11 + EtOH	7.78	7.38	7.28	7.18	6.93
sCI 11 + iPrOH	6.89	6.54	6.45	6.36	6.14
sCI 12 + MeOH	9.77	9.27	9.14	9.01	8.71
sCI 12 + EtOH	8.69	8.24	8.13	8.02	7.74
sCI 12 + iPrOH	7.70	7.30	7.20	7.10	6.86
sCI 13 + MeOH	9.37	8.89	8.77	8.65	8.35
sCI 14 + MeOH	8.66	8.21	8.10	7.98	7.71
sCI 15 + MeOH	9.29	8.81	8.69	8.57	8.28
sCI 16 + MeOH	9.21	8.74	8.62	8.50	8.21
sCI 17 + MeOH	9.36	8.88	8.76	8.64	8.34
sCI 18 + MeOH	8.51	8.07	7.96	7.84	7.58
sCI 19 + MeOH	8.53	8.09	7.98	7.86	7.60
sCI 20 + MeOH	8.37	7.94	7.83	7.72	7.46
sCI 21 + MeOH	12.23	11.60	11.44	11.28	10.90
sCI 22 + MeOH	12.74	12.08	11.92	11.75	11.35
sCI 23 + MeOH	6.56	6.22	6.14	6.05	5.85
sCI 24 + MeOH	5.27	5.00	4.93	4.86	4.70
sCI 25 + MeOH	5.87	5.57	5.50	5.42	5.23
sCI 26 + MeOH	5.76	5.46	5.39	5.31	5.13

2.1.3 Adiabatic Anisotropic Dipole-Dipole Capture Limit Values

Table 55: Adiabatic anisotropic Dipole-Dipole Capture Limits for all sCI + alcohol reactions in this study at a variety of temperatures.

Reaction	Adiabatic anisotropic Isotropic $k_{d\text{-}d}$ (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + MeOH	5.72	5.42	5.35	5.27	5.10
sCI 1 + EtOH	5.29	5.02	4.95	4.88	4.71
sCI 1 + iPrOH	4.83	4.58	4.52	4.46	4.30
sCI 2 + MeOH	5.75	5.45	5.38	5.30	5.12
sCI 3 + MeOH	6.42	6.09	6.01	5.92	5.72
sCI 4 + MeOH	6.17	5.85	5.78	5.69	5.50
sCI 5 + MeOH	5.71	5.41	5.34	5.26	5.09
sCI 6 + MeOH	5.08	4.81	4.75	4.68	4.52
sCI 7 + MeOH	4.96	4.71	4.64	4.58	4.42
sCI 8 + MeOH	5.12	4.85	4.79	4.72	4.56
sCI 9 + MeOH	5.05	4.79	4.72	4.66	4.50
sCI 10 + MeOH	4.73	4.48	4.42	4.36	4.21
sCI 11 + MeOH	5.75	5.45	5.38	5.30	5.12
sCI 11 + EtOH	5.11	4.85	4.78	4.71	4.55
sCI 11 + iPrOH	5.71	5.41	5.34	5.27	5.09
sCI 12 + MeOH	6.42	6.09	6.01	5.92	5.72
sCI 12 + EtOH	4.53	4.29	4.24	4.18	4.03
sCI 12 + iPrOH	5.06	4.80	4.73	4.66	4.51
sCI 12 + MeOH	6.16	5.84	5.76	5.68	5.49
sCI 13 + MeOH	5.69	5.39	5.32	5.25	5.07
sCI 14 + MeOH	6.10	5.79	5.71	5.63	5.44
sCI 15 + MeOH	6.05	5.74	5.66	5.58	5.39
sCI 16 + MeOH	6.15	5.83	5.75	5.67	5.48
sCI 17 + MeOH	5.59	5.30	5.23	5.15	4.98
sCI 18 + MeOH	5.60	5.31	5.24	5.17	4.99
sCI 19 + MeOH	5.50	5.21	5.15	5.07	4.90
sCI 20 + MeOH	8.03	7.62	7.52	7.41	7.16
sCI 21 + MeOH	8.37	7.93	7.83	7.72	7.45
sCI 22 + MeOH	6.16	5.84	5.76	5.68	5.49
sCI 23 + MeOH	4.31	4.09	4.03	3.98	3.84
sCI 24 + MeOH	3.46	3.28	3.24	3.19	3.08
sCI 25 + MeOH	3.86	3.66	3.61	3.56	3.44
sCI 26 + MeOH	3.78	3.59	3.54	3.49	3.37

2.1.4 Non-Adiabatic anisotropic Dipole-Dipole Capture Limit Values

Table 56: Non-Adiabatic anisotropic Dipole-Dipole Capture Limits for all sCI + alcohol reactions in this study at a variety of temperatures.

Reaction	Non-Adiabatic anisotropic k_{d-d} (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + MeOH	4.17	3.95	3.90	3.84	3.71
sCI 1 + EtOH	3.85	3.66	3.61	3.55	3.43
sCI 1 + iPrOH	3.52	3.34	3.29	3.25	3.14
sCI 2 + MeOH	4.19	3.97	3.92	3.86	3.73
sCI 3 + MeOH	4.68	4.44	4.38	4.32	4.17
sCI 4 + MeOH	4.50	4.27	4.21	4.15	4.01
sCI 5 + MeOH	4.16	3.94	3.89	3.84	3.71
sCI 6 + MeOH	3.70	3.51	3.46	3.41	3.30
sCI 7 + MeOH	3.62	3.43	3.38	3.33	3.22
sCI 8 + MeOH	3.73	3.54	3.49	3.44	3.32
sCI 9 + MeOH	3.68	3.49	3.44	3.39	3.28
sCI 10 + MeOH	3.44	3.27	3.22	3.18	3.07
sCI 11 + MeOH	4.19	3.97	3.92	3.86	3.73
sCI 11 + EtOH	3.72	3.53	3.48	3.44	3.32
sCI 11 + iPrOH	3.30	3.13	3.09	3.04	2.94
sCI 12 + MeOH	4.19	3.97	3.92	3.86	3.73
sCI 12 + EtOH	4.16	3.95	3.89	3.84	3.71
sCI 12 + iPrOH	3.69	3.49	3.45	3.40	3.28
sCI 13 + MeOH	4.49	4.26	4.20	4.14	4.00
sCI 14 + MeOH	4.14	3.93	3.88	3.82	3.69
sCI 15 + MeOH	4.45	4.22	4.16	4.10	3.96
sCI 16 + MeOH	4.41	4.18	4.13	4.07	3.93
sCI 17 + MeOH	4.48	4.25	4.19	4.13	3.99
sCI 18 + MeOH	4.07	3.86	3.81	3.75	3.63
sCI 19 + MeOH	4.08	3.87	3.82	3.76	3.64
sCI 20 + MeOH	4.01	3.80	3.75	3.70	3.57
sCI 21 + MeOH	5.85	5.55	5.48	5.40	5.22
sCI 22 + MeOH	6.10	5.78	5.70	5.62	5.43
sCI 23 + MeOH	3.14	2.98	2.94	2.90	2.80
sCI 24 + MeOH	2.52	2.39	2.36	2.33	2.25
sCI 25 + MeOH	2.81	2.67	2.63	2.59	2.51
sCI 26 + MeOH	2.76	2.62	2.58	2.54	2.46

2.2 Rate Constants

2.2.1 Conventional Transition State Theory Rate Constants (k_{TST})

*Table 57: Calculated values for CIs reactions with various alcohols at 298.15K of equilibrium constant (K_{eq} in cm^3), tunnelling constant, κ_{Eckart}, unimolecular rate constant k_2 [s^{-1}],rate constant per channel k_{TS} [$cm^3\ s^{-1}$] and the overall rate constant [$cm^3\ s^{-1}$], effective tunnelling contribution [$\kappa_{contr.} = \Sigma(\Gamma x\ \kappa_{eckart})$]; **VHP channels are bold and italics***

#CI	Alcohol	#TS	K_{eq}	κ_{Eckart}	k_2	k_{TS}	Γ	k_{total}	κ_{contri}
1	MeOH	TS1	2.68×10^{-21}	1.10	3.22×10^{6}	9.45×10^{-15}	0.81	1.17×10^{-14}	1.10
		TS2	2.68×10^{-21}	1.10	7.57×10^{5}	2.23×10^{-15}	0.19		
1	EtOH	TS1.1	1.34×10^{-21}	1.08	2.01×10^{7}	2.92×10^{-14}	0.47	6.17×10^{-14}	1.09
		TS1.2	3.04×10^{-21}	1.09	7.67×10^{6}	2.54×10^{-14}	0.41		
		TS1.3	1.33×10^{-21}	1.11	5.37×10^{5}	8.02×10^{-16}	0.01		
		TS2.1	5.81×10^{-22}	1.09	5.26×10^{6}	3.32×10^{-15}	0.05		
		TS2.2	3.04×10^{-21}	1.10	8.95×10^{5}	2.99×10^{-15}	0.05		
1	iPrOH	TS1.1	2.02×10^{-21}	1.08	3.00×10^{6}	6.55×10^{-15}	0.54	1.21×10^{-14}	1.08
		TS1.2	2.02×10^{-21}	1.11	2.35×10^{5}	5.29×10^{-16}	0.04		
		TS1.3	6.62×10^{-22}	1.09	1.42×10^{6}	1.03×10^{-15}	0.08		
		TS2.1	2.02×10^{-21}	1.08	1.74×10^{6}	3.81×10^{-15}	0.31		
		TS2.2	2.02×10^{-21}	1.12	1.06×10^{5}	2.39×10^{-16}	0.02		
2	MeOH	TS1-AAAH	1.30×10^{-21}	1.17	1.1×10^{4}	1.77×10^{-17}	0.92	1.93×10^{-17}	1.17 ***25.32*** Overall : 2.54
		TS2-AAAH	1.30×10^{-21}	1.22	3.12×10^{2}	4.98×10^{-19}	0.03		
		TS1-VHP	***1.30 × 10^{-21}***	***27.74***	***8.97***	***3.24 × 10^{-19}***	0.02		
		TS2-VHP	***1.30 × 10^{-21}***	***24.29***	***24.3***	***7.69 × 10^{-19}***	0.04		
	Unimolecular decomposition			58.98	1.76	102	1.00	102	58.98
3	MeOH	TS1	2.36×10^{-20}	1.16	5.60×10^{7}	1.54×10^{-12}	0.73	2.09×10^{-12}	1.16
		TS2	2.36×10^{-20}	1.17	2.02×10^{7}	5.55×10^{-13}	0.27		
4	MeOH	TS1-AAAH	8.94×10^{-21}	1.35	4.45×10^{4}	5.39×10^{-16}	0.95	5.68×10^{-16}	1.36 ***37.32*** Overall :1.72
		TS2-AAAH	8.94×10^{-21}	1.43	1.87×10^{3}	2.38×10^{-17}	0.04		
		TS1-VHP	***8.94 × 10^{-21}***	***41.13***	***6.95***	***2.56 × 10^{-18}***	<0.01		
		TS2-VHP	***8.94 × 10^{-21}***	***34.32***	***10.6***	***3.25 × 10^{-18}***	0.01		
	Unimolecular decomposition			45.47	7.48	340	1.00	340	45.47
5	MeOH	TS1	2.06×10^{-21}	1.07	1.07×10^{8}	2.35×10^{-13}	0.31	7.62×10^{-13}	1.07
		TS2	2.06×10^{-21}	1.07	2.39×10^{8}	5.26×10^{-13}	0.69		
6	MeOH	TS1	6.98×10^{-20}	1.02	8.98×10^{9}	6.41×10^{-10}	0.74	8.66×10^{-10}	1.02
		TS2	6.98×10^{-20}	1.03	3.13×10^{9}	2.25×10^{-10}	0.26		
7	MeOH	TS	4.09×10^{-20}	1	4.79×10^{11}	1.96×10^{-8}	1.0	1.96×10^{-8}	1.0
8	MeOH	TS1	4.57×10^{-22}	1.13	1.42×10^{4}	7.32×10^{-18}	0.66	1.10×10^{-17}	1.13
		TS2	4.57×10^{-22}	1.13	7.17×10^{3}	3.71×10^{-18}	0.34		
9	MeOH	TS1	1.14×10^{-20}	1.09	4.72×10^{8}	5.88×10^{-12}	0.90	6.50×10^{-12}	1.09
		TS2	1.14×10^{-20}	1.10	4.92×10^{7}	6.17×10^{-13}	0.10		
10	MeOH	TS1	8.00×10^{-22}	1.12	2.34×10^{6}	2.10×10^{-15}	0.87	2.40×10^{-15}	1.12
		TS2	8.00×10^{-22}	1.13	3.33×10^{5}	3.01×10^{-16}	0.13		
11	MeOH	TS1	1.61×10^{-21}	1.29	8.55×10^{3}	1.78×10^{-17}	0.44	4.01×10^{-17}	1.36
		TS2	5.16×10^{-22}	1.42	3.05×10^{4}	2.23×10^{-17}	0.56		

11	EtOH	TS1.1	3.99×10^{-22}	1.28	6.68×10^{4}	3.43×10^{-17}	0.35	9.79×10^{-17}	1.31
		TS1.2	5.07×10^{-22}	1.24	6.56×10^{4}	2.87×10^{-17}	0.29		
		TS1.3	8.42×10^{-22}	1.29	5.20×10^{2}	5.64×10^{-19}	0.01		
		TS2.1	5.07×10^{-22}	1.33	2.00×10^{4}	1.35×10^{-17}	0.14		
		TS2.2	3.99×10^{-22}	1.45	3.60×10^{4}	2.08×10^{-17}	0.21		
11	iPrOH	TS1.1	7.64×10^{-22}	1.23	4.96×10^{4}	4.68×10^{-17}	0.62	7.51×10^{-17}	1.29
		TS1.2	2.77×10^{-22}	1.31	4.14×10^{3}	1.50×10^{-18}	0.02		
		TS1.3	1.18×10^{-21}	1.24	986	1.44×10^{-18}	0.02		
		TS2.1	2.77×10^{-22}	1.38	6.60×10^{4}	2.52×10^{-17}	0.34		
		TS2.2	7.64×10^{-22}	1.61	74.6	9.19×10^{-20}	<0.01		
12	MeOH	TS1	6.14×10^{-21}	1.54	1.67×10^{8}	1.58×10^{-12}	0.91	1.72×10^{-12}	1.54
		TS2	6.14×10^{-21}	1.54	1.56×10^{7}	1.48×10^{-13}	0.09		
12	EtOH	TS1.1	1.41×10^{-20}	1.65	9.94×10^{7}	2.31×10^{-12}	0.35	6.51×10^{-12}	1.53
		TS1.2	5.57×10^{-21}	1.46	4.89×10^{8}	3.99×10^{-12}	0.61		
		TS2.1	5.57×10^{-21}	1.47	1.20×10^{7}	9.81×10^{-14}	0.02		
		TS2.2	1.41×10^{-20}	1.64	4.89×10^{6}	1.13×10^{-13}	0.02		
12	iPrOH	TS1.1	9.10×10^{-21}	1.62	1.41×10^{8}	2.08×10^{-12}	0.84	2.48×10^{-12}	1.63
		TS1.2	9.10×10^{-21}	2.53	1.53×10^{6}	3.53×10^{-14}	0.01		
		TS2.1	9.10×10^{-21}	1.58	2.52×10^{7}	3.63×10^{-13}	0.15		
		TS2.2	9.10×10^{-21}	2.08	4.96×10^{5}	9.38×10^{-15}	<0.01		
13	MeOH	TS1-AAAH	2.24×10^{-22}	2.13	8.15×10^{3}	3.90×10^{-18}	0.96	4.08×10^{-18}	2.14 ***46.83*** Overall: 2.58
		TS2-AAAH	2.24×10^{-22}	2.34	2.63×10^{2}	1.38×10^{-19}	0.03		
		TS1-VHP	***2.24×10^{-22}***	***94.79***	***3.74×10^{-4}***	***7.95×10^{-24}***	<0.01		
		TS2-VHP	***2.24×10^{-22}***	***46.82***	***3.85***	***4.04×10^{-20}***	0.01		
	Unimolecular decomposition			72.30	0.312	22.6	1.00	22.6	72.30
14	MeOH	TS1-AAAH	2.45×10^{-22}	1.84	7.97×10^{4}	3.60×10^{-17}	0.98	3.68×10^{-17}	1.85 ***35.66*** Overall: 2.09
		TS2-AAAH	2.45×10^{-22}	2.44	9.40×10^{2}	5.62×10^{-19}	0.02		
		TS1-VHP	***2.45×10^{-22}***	***40.22***	***8.55***	***8.43×10^{-20}***	<0.01		
		TS2-VHP	***2.45×10^{-22}***	***33.48***	***21.5***	***1.77×10^{-19}***	<0.01		
	Unimolecular decomposition			71.77	0.301	21.6	1.00	21.6	71.77
15	MeOH	TS1	1.88×10^{-20}	1.87	2.88×10^{6}	1.01×10^{-13}	0.63	1.61×10^{-13}	1.75
		TS2	1.88×10^{-20}	1.56	2.05×10^{6}	5.99×10^{-14}	0.37		
16	MeOH	TS1	1.80×10^{-21}	1.38	1.94×10^{8}	4.83×10^{-13}	0.95	5.10×10^{-13}	1.39
		TS2	1.80×10^{-21}	1.52	9.92×10^{6}	2.72×10^{-14}	0.05		
17	MeOH	TS1	7.55×10^{-21}	1.86	6.32×10^{4}	8.86×10^{-16}	0.55	1.60×10^{-15}	2.14
		TS2	7.55×10^{-21}	2.50	3.79×10^{4}	7.15×10^{-16}	0.45		
18	MeOH	TS1	6.11×10^{-22}	1.50	3.52×10^{4}	3.22×10^{-17}	0.83	3.87×10^{-17}	1.55
		TS2	6.11×10^{-22}	1.81	5.82×10^{3}	6.46×10^{-18}	0.17		
19	MeOH	TS1	3.31×10^{-21}	1.29	4.91×10^{4}	2.09×10^{-16}	0.56	3.75×10^{-16}	1.37
		TS2	3.31×10^{-21}	1.47	3.44×10^{4}	1.67×10^{-16}	0.44		
20	MeOH	TS1	4.94×10^{-22}	1.26	7.27×10^{3}	4.53×10^{-18}	0.94	4.81×10^{-18}	1.28
		TS2	4.94×10^{-22}	1.58	3.60×10^{3}	2.80×10^{-19}	0.06		
21	MeOH	TS1	3.89×10^{-17}	1.53	4.43×10^{6}	2.63×10^{-10}	0.73	3.59×10^{-10}	1.49
		TS2	3.89×10^{-17}	1.39	1.77×10^{6}	9.58×10^{-11}	0.27		
22	MeOH	TS1	7.35×10^{-18}	1.40	4.06×10^{9}	4.19×10^{-8}	>0.99	4.20×10^{-8}	1.40
		TS2	7.35×10^{-18}	1.66	9.40×10^{6}	1.15×10^{-10}	<0.01		

2.2.2 Temperature-Dependent Graphs

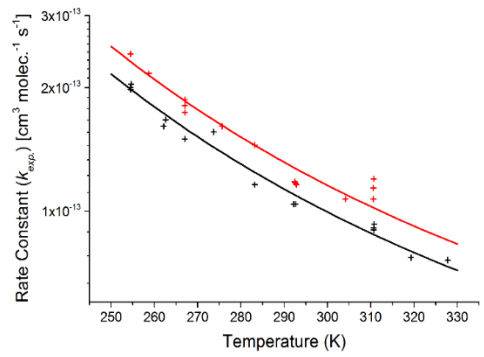
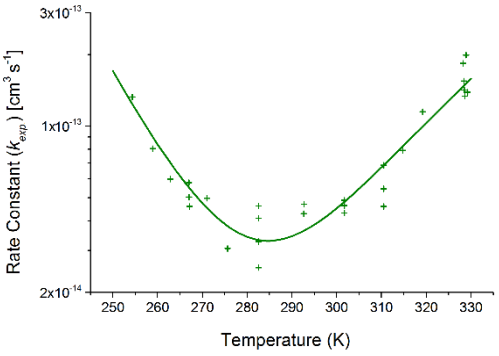
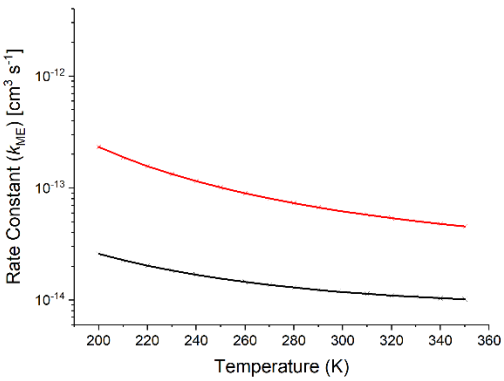
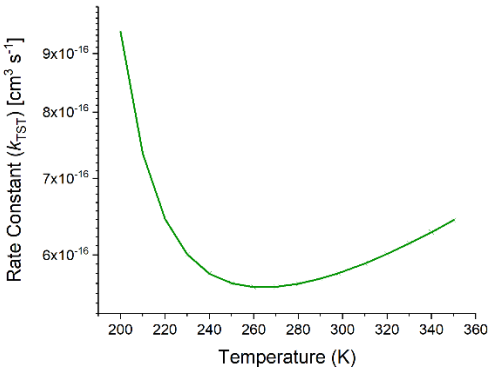
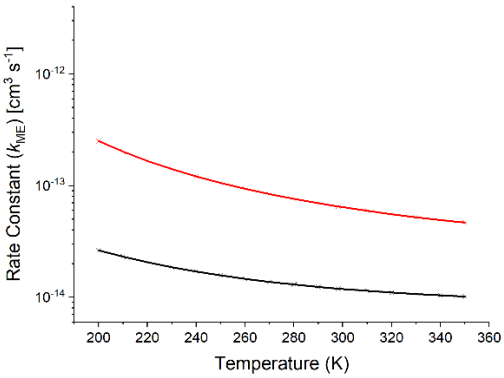
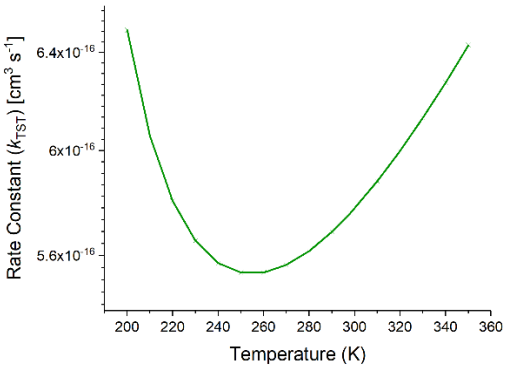
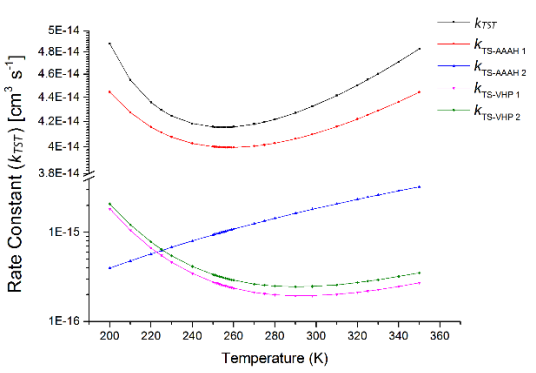
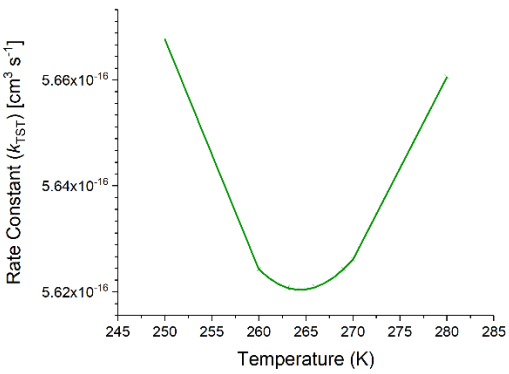
	HCHOO + MeOH/EtOH	$(CH_3)_2COO$ + MeOH
k_{EXP} 9.99 Torr		
k_{ME} New 9.99 Torr		
k_{TST} 760 Torr		
	$(CH_3)_2COO$ + MeOH by TS structure	$(CH_3)_2COO$ + MeOH point of inversion
760 Torr		

Figure 13: Table of temperature inversions at different pressures of both experimental and theoretical rate constants of HCHOO + MeOH/EtOH and $(CH_3)_2COO$ + MeOH. Conventional transition state theory rate constants used where possible at 760 Torr, otherwise Master Equation Rate constants are used.

2.2.3 Temperature-Dependent k_{TST} Values

Table 58: sCI 1 + MeOH rate components at 1 atm at different temperatures: equilibrium constant (K_{eq} in cm^3), tunnelling constant, κ_{eckart},, unimolecular rate constant (k_2 in s^{-1}), rate constant per channel (k_{total} [cm^3 s^{-1}]), the overall rate constant (k_{total} [cm^3 s^{-1}]), effective tunnelling contribution [$\kappa_{contr.} = \Sigma(\Gamma \times \kappa_{eckart})$]

T (K)	#TS	K_{eq} (cm^3)	κ_{Eckart}	k_2 (s^{-1})	k_{TS} (cm^3 s^{-1})	k_{total} (cm^3 s^{-1})	$\kappa_{contr.}$
200	TS1	4.89×10^{-19}	1.23	3.87×10^{4}	2.32×10^{-14}	2.58×10^{-14}	1.23
	TS2	4.89×10^{-19}	1.25	4.12×10^{3}	2.52×10^{-15}		
210	TS1	2.26×10^{-19}	1.20	7.40×10^{4}	2.01×10^{-14}	2.26×10^{-14}	1.21
	TS2	2.26×10^{-19}	1.22	8.84×10^{3}	2.44×10^{-15}		
220	TS1	1.12×10^{-19}	1.18	1.33×10^{5}	1.77×10^{-14}	2.01×10^{-14}	1.19
	TS2	1.12×10^{-19}	1.20	1.76×10^{4}	2.38×10^{-15}		
225	TS1	8.14×10^{-20}	1.18	1.75×10^{5}	1.67×10^{-14}	1.91×10^{-14}	1.18
	TS2	8.14×10^{-20}	1.19	2.43×10^{4}	2.35×10^{-15}		
230	TS1	5.97×10^{-20}	1.17	2.27×10^{5}	1.58×10^{-14}	1.82×10^{-14}	1.17
	TS2	5.97×10^{-20}	1.18	3.31×10^{4}	2.33×10^{-15}		
240	TS1	3.36×10^{-20}	1.15	3.70×10^{5}	1.43×10^{-14}	1.66×10^{-14}	1.15
	TS2	3.36×10^{-20}	1.16	5.88×10^{4}	2.30×10^{-15}		
250	TS1	1.98×10^{-20}	1.14	5.79×10^{5}	1.31×10^{-14}	1.53×10^{-14}	1.14
	TS2	1.98×10^{-20}	1.15	9.96×10^{4}	2.27×10^{-15}		
260	TS1	1.22×10^{-20}	1.13	8.74×10^{5}	1.21×10^{-14}	1.43×10^{-14}	1.13
	TS2	1.22×10^{-20}	1.14	1.62×10^{5}	2.25×10^{-15}		
270	TS1	7.84×10^{-21}	1.12	1.28×10^{6}	1.12×10^{-14}	1.34×10^{-14}	1.12
	TS2	7.84×10^{-21}	1.13	2.53×10^{5}	2.24×10^{-15}		
275	TS1	6.37×10^{-21}	1.11	1.53×10^{6}	1.08×10^{-14}	1.31×10^{-14}	1.12
	TS2	6.37×10^{-21}	1.12	3.13×10^{5}	2.24×10^{-15}		
280	TS1	5.21×10^{-21}	1.11	1.81×10^{6}	1.04×10^{-14}	1.27×10^{-14}	1.11
	TS2	5.21×10^{-21}	1.12	3.84×10^{5}	2.23×10^{-15}		
290	TS1	3.57×10^{-21}	1.10	2.51×10^{6}	9.88×10^{-15}	1.21×10^{-14}	1.10
	TS2	3.57×10^{-21}	1.11	5.64×10^{5}	2.33×10^{-15}		
298.15	TS1	2.68×10^{-21}	1.10	3.22×10^{6}	9.45×10^{-15}	1.17×10^{-14}	1.10
	TS2	2.68×10^{-21}	1.10	7.57×10^{5}	2.23×10^{-15}		
310	TS1	1.81×10^{-21}	1.09	4.52×10^{6}	8.92×10^{-15}	1.12×10^{-14}	1.09
	TS2	1.81×10^{-21}	1.10	1.13×10^{6}	2.24×10^{-15}		
320	TS1	1.34×10^{-21}	1.08	5.88×10^{6}	8.54×10^{-15}	1.08×10^{-14}	1.08
	TS2	1.34×10^{-21}	1.09	1.54×10^{6}	2.25×10^{-15}		
325	TS1	1.16×10^{-21}	1.08	6.67×10^{6}	8.36×10^{-15}	1.06×10^{-14}	1.08
	TS2	1.16×10^{-21}	1.09	1.79×10^{6}	2.26×10^{-15}		
330	TS1	1.01×10^{-21}	1.08	7.54×10^{6}	8.20×10^{-15}	1.05×10^{-14}	1.08
	TS2	1.01×10^{-21}	1.08	2.07×10^{6}	2.26×10^{-15}		
340	TS1	7.76×10^{-22}	1.07	9.50×10^{6}	7.91×10^{-15}	1.02×10^{-14}	1.07
	TS2	7.76×10^{-22}	1.08	2.72×10^{6}	2.28×10^{-15}		
350	TS1	6.07×10^{-22}	1.07	1.18×10^{7}	7.66×10^{-15}	1.01×10^{-14}	1.07
	TS2	6.07×10^{-22}	1.07	3.78×10^{6}	2.46×10^{-15}		
375	TS1	3.49×10^{-22}	1.06	1.93×10^{7}	7.16×10^{-15}	9.51×10^{-15}	

	TS2	3.49×10^{-22}	1.06	6.32×10^{6}	2.35×10^{-15}		1.06
400	TS1	2.18×10^{-22}	1.05	2.96×10^{7}	6.79×10^{-15}	9.21×10^{-15}	1.05
	TS2	2.18×10^{-22}	1.06	1.05×10^{7}	2.42×10^{-15}		
425	TS1	1.45×10^{-22}	1.05	4.31×10^{7}	6.53×10^{-15}	9.02×10^{-15}	1.05
	TS2	1.45×10^{-22}	1.05	1.64×10^{7}	2.49×10^{-15}		
450	TS1	1.02×10^{-22}	1.04	5.99×10^{7}	6.34×10^{-15}	8.92×10^{-15}	1.04
	TS2	1.02×10^{-22}	1.04	2.43×10^{7}	2.58×10^{-15}		
475	TS1	7.46×10^{-23}	1.04	8.03×10^{7}	6.21×10^{-15}	8.89×10^{-15}	1.04
	TS2	7.46×10^{-23}	1.04	3.45×10^{7}	2.67×10^{-15}		
500	TS1	5.68×10^{-23}	1.03	1.04×10^{8}	6.13×10^{-15}	8.90×10^{-15}	1.03
	TS2	5.68×10^{-23}	1.04	4.72×10^{7}	2.77×10^{-15}		

Table 59: CI1 + EtOH rate components at 1 atm at different temperatures: equilibrium constant (K_{eq} in cm^3 $molec^{-1}$), tunnelling constant, κ_{eckart},, unimolecular rate constant (k_2 in s^{-1}), rate constant per channel (k_{total} [cm^3 $molec^{-1}$ s^{-1}]), the overall rate constant (k_{total} [cm^3 $molec^{-1}$ s^{-1}]), effective tunnelling contribution [$\kappa_{contr.} = \Sigma(\Gamma \times \kappa_{eckart})$];

T (K)	#TS	K_{eq} (cm^3)	κ_{Eckart}	k_2 (s^{-1})	k_{TS} (cm^3 s^{-1})	k_{total} (cm^3 s^{-1})	$\kappa_{contr.}$
200	TS1.1	2.31×10^{-19}	1.19	4.49×10^{5}	1.24×10^{-13}	2.46×10^{-13}	1.20
	TS1.2	5.52×10^{-19}	1.22	1.69×10^{5}	1.13×10^{-13}		
	TS1.3	2.31×10^{-19}	1.28	2.09×10^{3}	6.17×10^{-16}		
	TS2.1	5.63×10^{-20}	1.20	6.69×10^{4}	4.53×10^{-15}		
	TS2.2	5.51×10^{-19}	1.23	6.01×10^{3}	4.09×10^{-15}		
210	TS1.1	1.08×10^{-19}	1.17	7.84×10^{5}	9.89×10^{-14}	1.98×10^{-13}	1.18
	TS1.2	2.55×10^{-19}	1.19	2.96×10^{5}	9.00×10^{-14}		
	TS1.3	1.08×10^{-19}	1.25	4.71×10^{3}	6.32×10^{-16}		
	TS2.1	2.85×10^{-20}	1.18	1.27×10^{5}	4.28×10^{-15}		
	TS2.2	2.55×10^{-19}	1.21	1.25×10^{4}	3.86×10^{-15}		
220	TS1.1	5.40×10^{-20}	1.16	1.30×10^{6}	8.11×10^{-14}	1.63×10^{-13}	1.17
	TS1.2	1.27×10^{-19}	1.17	4.91×10^{5}	7.33×10^{-14}		
	TS1.3	5.40×10^{-20}	1.22	9.82×10^{3}	6.48×10^{-16}		
	TS2.1	1.54×10^{-20}	1.17	2.27×10^{5}	4.07×10^{-15}		
	TS2.2	1.27×10^{-19}	1.19	2.43×10^{4}	3.66×10^{-15}		
225	TS1.1	3.92×10^{-20}	1.15	1.65×10^{6}	7.40×10^{-14}	1.49×10^{-13}	1.16
	TS1.2	9.20×10^{-20}	1.17	6.21×10^{5}	6.67×10^{-14}		
	TS1.3	3.92×10^{-20}	1.21	1.38×10^{4}	6.56×10^{-16}		
	TS2.1	1.16×10^{-20}	1.16	2.97×10^{5}	3.98×10^{-15}		
	TS2.2	9.19×10^{-20}	1.18	3.30×10^{4}	3.58×10^{-15}		
230	TS1.1	2.89×10^{-20}	1.14	2.06×10^{6}	6.78×10^{-14}	1.37×10^{-13}	1.15
	TS1.2	6.75×10^{-20}	1.16	7.79×10^{5}	6.09×10^{-14}		
	TS1.3	2.89×10^{-20}	1.20	1.92×10^{4}	6.65×10^{-16}		
	TS2.1	8.82×10^{-21}	1.15	3.84×10^{5}	3.90×10^{-15}		
	TS2.2	6.75×10^{-20}	1.17	4.44×10^{4}	3.51×10^{-15}		
240	TS1.1	1.63×10^{-20}	1.13	3.13×10^{6}	5.78×10^{-14}	1.17×10^{-13}	1.14
	TS1.2	3.80×10^{-20}	1.14	1.19×10^{6}	5.16×10^{-14}		
	TS1.3	1.63×10^{-20}	1.18	3.54×10^{4}	6.83×10^{-16}		
	TS2.1	5.32×10^{-21}	1.14	6.22×10^{5}	3.76×10^{-15}		
	TS2.2	3.80×10^{-20}	1.16	7.70×10^{4}	3.38×10^{-15}		
250	TS1.1	9.70×10^{-21}	1.12	4.61×10^{6}	4.99×10^{-14}	1.02×10^{-13}	1.13
	TS1.2	2.24×10^{-20}	1.13	1.75×10^{6}	4.44×10^{-14}		
	TS1.3	9.70×10^{-21}	1.17	6.20×10^{4}	7.02×10^{-16}		
	TS2.1	3.35×10^{-21}	1.13	9.67×10^{5}	3.64×10^{-15}		
	TS2.2	2.24×10^{-20}	1.14	1.28×10^{5}	3.28×10^{-15}		
260	TS1.1	6.02×10^{-21}	1.11	6.56×10^{6}	4.38×10^{-14}	8.99×10^{-14}	1.12
	TS1.2	1.39×10^{-20}	1.12	2.49×10^{6}	3.87×10^{-14}		
	TS1.3	6.02×10^{-21}	1.15	1.04×10^{5}	7.21×10^{-16}		
	TS2.1	2.19×10^{-21}	1.12	1.45×10^{6}	3.55×10^{-15}		

	TS2.2	1.38×10^{-20}	1.13	2.04×10^{5}	3.19×10^{-15}		
270	TS1.1	3.88×10^{-21}	1.10	9.09×10^{6}	3.88×10^{-14}	8.03×10^{-14}	1.11
	TS1.2	8.89×10^{-21}	1.11	3.45×10^{6}	3.42×10^{-14}		
	TS1.3	3.88×10^{-21}	1.14	1.68×10^{5}	7.42×10^{-16}		
	TS2.1	1.49×10^{-21}	1.11	2.11×10^{6}	3.47×10^{-15}		
	TS2.2	8.89×10^{-21}	1.12	3.13×10^{5}	3.12×10^{-15}		
275	TS1.1	3.16×10^{-21}	1.10	1.06×10^{7}	3.67×10^{-14}	7.66×10^{-14}	1.10
	TS1.2	7.22×10^{-21}	1.11	4.03×10^{6}	3.22×10^{-14}		
	TS1.3	3.16×10^{-21}	1.14	2.10×10^{5}	7.52×10^{-16}		
	TS2.1	1.24×10^{-21}	1.10	2.52×10^{6}	3.44×10^{-15}		
	TS2.2	7.22×10^{-21}	1.12	4.28×10^{5}	3.45×10^{-15}		
280	TS1.1	2.59×10^{-21}	1.09	1.23×10^{7}	3.48×10^{-14}	7.25×10^{-14}	1.10
	TS1.2	5.91×10^{-21}	1.10	4.68×10^{6}	3.05×10^{-14}		
	TS1.3	2.59×10^{-21}	1.13	2.61×10^{5}	7.63×10^{-16}		
	TS2.1	1.04×10^{-21}	1.10	2.98×10^{6}	3.41×10^{-15}		
	TS2.2	5.91×10^{-21}	1.11	4.66×10^{5}	3.06×10^{-15}		
290	TS1.1	1.78×10^{-21}	1.09	1.63×10^{7}	3.15×10^{-14}	6.61×10^{-14}	1.09
	TS1.2	4.05×10^{-21}	1.10	6.19×10^{6}	2.75×10^{-14}		
	TS1.3	1.78×10^{-21}	1.12	3.93×10^{5}	7.84×10^{-16}		
	TS2.1	7.47×10^{-22}	1.09	4.12×10^{6}	3.36×10^{-15}		
	TS2.2	4.05×10^{-21}	1.10	6.75×10^{5}	3.02×10^{-15}		
298.15	TS1.1	1.34×10^{-21}	1.08	2.01×10^{7}	2.92×10^{-14}	6.17×10^{-14}	1.09
	TS1.2	3.04×10^{-21}	1.09	7.67×10^{6}	2.54×10^{-14}		
	TS1.3	1.34×10^{-21}	1.11	5.37×10^{5}	8.02×10^{-16}		
	TS2.1	5.81×10^{-22}	1.09	5.26×10^{6}	3.32×10^{-15}		
	TS2.2	3.04×10^{-21}	1.10	8.95×10^{5}	2.99×10^{-15}		
310	TS1.1	9.13×10^{-22}	1.07	2.69×10^{7}	2.64×10^{-14}	5.64×10^{-14}	1.08
	TS1.2	2.06×10^{-21}	1.08	1.03×10^{7}	2.29×10^{-14}		
	TS1.3	9.13×10^{-22}	1.11	8.22×10^{5}	8.29×10^{-16}		
	TS2.1	4.15×10^{-22}	1.08	7.33×10^{6}	3.28×10^{-15}		
	TS2.2	2.06×10^{-21}	1.09	1.31×10^{6}	2.95×10^{-15}		
320	TS1.1	6.76×10^{-22}	1.07	3.38×10^{7}	2.44×10^{-14}	5.26×10^{-14}	1.08
	TS1.2	1.52×10^{-21}	1.08	1.29×10^{7}	2.11×10^{-14}		
	TS1.3	6.76×10^{-22}	1.10	1.15×10^{6}	8.52×10^{-16}		
	TS2.1	3.19×10^{-22}	1.07	9.52×10^{6}	3.26×10^{-15}		
	TS2.2	1.52×10^{-21}	1.08	1.77×10^{6}	2.93×10^{-15}		
325	TS1.1	5.87×10^{-22}	1.07	3.76×10^{7}	2.36×10^{-14}	5.10×10^{-14}	1.07
	TS1.2	1.32×10^{-21}	1.08	1.43×10^{7}	2.04×10^{-14}		
	TS1.3	5.87×10^{-22}	1.10	1.34×10^{6}	8.64×10^{-16}		
	TS2.1	2.81×10^{-22}	1.07	1.08×10^{7}	3.25×10^{-15}		
	TS2.2	1.32×10^{-21}	1.08	2.05×10^{6}	2.92×10^{-15}		

330	TS1.1	5.12×10^{-22}	1.07	4.17×10^{7}	2.28×10^{-14}	4.94×10^{-14}	1.07
	TS1.2	1.15×10^{-21}	1.07	1.59×10^{7}	1.96×10^{-14}		
	TS1.3	5.12×10^{-22}	1.09	1.57×10^{6}	8.76×10^{-16}		
	TS2.1	2.49×10^{-22}	1.07	1.21×10^{7}	3.24×10^{-15}		
	TS2.2	1.15×10^{-21}	1.08	2.35×10^{6}	2.91×10^{-15}		
340	TS1.1	3.94×10^{-22}	1.06	5.09×10^{7}	2.13×10^{-14}	4.67×10^{-14}	1.07
	TS1.2	8.83×10^{-22}	1.07	1.95×10^{7}	1.84×10^{-14}		
	TS1.3	3.94×10^{-22}	1.09	2.10×10^{6}	9.01×10^{-16}		
	TS2.1	1.99×10^{-22}	1.07	1.53×10^{7}	3.23×10^{-15}		
	TS2.2	8.82×10^{-22}	1.07	3.06×10^{6}	2.90×10^{-15}		
350	TS1.1	3.09×10^{-22}	1.06	6.14×10^{7}	2.01×10^{-14}	4.44×10^{-14}	1.06
	TS1.2	6.90×10^{-22}	1.07	2.35×10^{7}	1.72×10^{-14}		
	TS1.3	3.09×10^{-22}	1.08	2.77×10^{6}	9.26×10^{-16}		
	TS2.1	1.60×10^{-22}	1.06	1.89×10^{7}	3.22×10^{-15}		
	TS2.2	6.90×10^{-22}	1.07	3.92×10^{6}	2.89×10^{-15}		
375	TS1.1	1.79×10^{-22}	1.05	9.35×10^{7}	1.76×10^{-14}	3.99×10^{-14}	1.05
	TS1.2	3.98×10^{-22}	1.06	3.58×10^{7}	1.50×10^{-14}		
	TS1.3	1.79×10^{-22}	1.07	5.16×10^{6}	9.91×10^{-16}		
	TS2.1	9.97×10^{-23}	1.05	3.07×10^{7}	3.22×10^{-15}		
	TS2.2	3.98×10^{-22}	1.06	7.29×10^{6}	3.07×10^{-15}		
400	TS1.1	1.12×10^{-22}	1.04	1.35×10^{8}	1.58×10^{-14}	3.65×10^{-14}	1.05
	TS1.2	2.48×10^{-22}	1.05	5.17×10^{7}	1.34×10^{-14}		
	TS1.3	1.12×10^{-22}	1.06	8.87×10^{6}	1.06×10^{-15}		
	TS2.1	6.65×10^{-23}	1.05	4.67×10^{7}	3.25×10^{-15}		
	TS2.2	2.48×10^{-22}	1.05	1.12×10^{7}	2.92×10^{-15}		
425	TS1.1	7.52×10^{-23}	1.04	1.85×10^{8}	1.45×10^{-14}	3.41×10^{-14}	1.04
	TS1.2	1.65×10^{-22}	1.04	7.12×10^{7}	1.23×10^{-14}		
	TS1.3	7.52×10^{-23}	1.05	1.43×10^{7}	1.13×10^{-15}		
	TS2.1	4.69×10^{-23}	1.04	6.74×10^{7}	3.29×10^{-15}		
	TS2.2	1.65×10^{-22}	1.05	1.71×10^{7}	2.96×10^{-15}		
450	TS1.1	5.30×10^{-23}	1.03	2.46×10^{8}	1.35×10^{-14}	3.24×10^{-14}	1.04
	TS1.2	1.16×10^{-22}	1.04	9.45×10^{7}	1.14×10^{-14}		
	TS1.3	5.30×10^{-23}	1.05	2.17×10^{7}	1.21×10^{-15}		
	TS2.1	3.47×10^{-23}	1.04	9.32×10^{7}	3.36×10^{-15}		
	TS2.2	1.16×10^{-22}	1.04	2.50×10^{7}	3.02×10^{-15}		
475	TS1.1	3.90×10^{-23}	1.03	3.16×10^{8}	1.27×10^{-14}	3.12×10^{-14}	1.03
	TS1.2	8.49×10^{-23}	1.04	1.21×10^{8}	1.07×10^{-14}		
	TS1.3	3.90×10^{-23}	1.04	3.15×10^{7}	1.28×10^{-15}		
	TS2.1	2.67×10^{-23}	1.03	1.24×10^{8}	3.43×10^{-15}		
	TS2.2	8.49×10^{-23}	1.04	3.50×10^{7}	3.09×10^{-15}		
500	TS1.1	2.98×10^{-23}	1.03	3.95×10^{8}	1.21×10^{-14}	3.03×10^{-14}	1.03
	TS1.2	6.47×10^{-23}	1.03	1.52×10^{8}	1.01×10^{-14}		
	TS1.3	2.98×10^{-23}	1.04	4.41×10^{7}	1.37×10^{-15}		
	TS2.1	2.13×10^{-23}	1.03	1.61×10^{8}	3.52×10^{-15}		

	TS2.2	6.47×10^{-23}	1.03	4.73×10^{7}	3.17×10^{-15}		

Table 60: Calculated values for CI4 + MeOH at 1 atm of *equilibrium constant (K_{eq} in cm^3), tunnelling constant, κ_{eckart},, unimolecular rate constant (k_2 in s^{-1}), rate constant per channel (k_{total} [cm^3 s^{-1}]), the overall rate constant (k_{total} [cm^3 s^{-1}]), effective tunnelling contribution* [$\kappa_{contr.} = \Sigma(\Gamma \times \kappa_{eckart})$];
VHP channels are bold and italics

T (K)	TS channel	K_{eq} (cm^3)	κ_{Eckart}	k_2 (s^{-1})	k_{TS} (cm^3 s^{-1})	k_{total} (cm^3 s^{-1})	$\kappa_{contr.}$
200	TS1-AAAH	5.56×10^{-18}	2.04	51.6	5.84×10^{-16}	6.41×10^{-16}	2.22
	TS2-AAAH	5.56×10^{-18}	2.34	0.401	5.21×10^{-18}		
	TS1-VHP	***5.56×10^{-18}***	***78481***	***5.53×10^{-5}***	***2.41×10^{-17}***		
	TS2-VHP	***5.56×10^{-18}***	***49788***	***9.94×10^{-5}***	***2.75×10^{-17}***		
210	TS1-AAAH	2.15×10^{-18}	1.89	138	5.62×10^{-16}	5.98×10^{-16}	2.00
	TS2-AAAH	2.15×10^{-18}	2.14	1.37	6.28×10^{-18}		
	TS1-VHP	***2.15×10^{-18}***	***21125***	***3.04×10^{-4}***	***1.38×10^{-17}***		
	TS2-VHP	***2.15×10^{-18}***	***13886***	***5.34×10^{-4}***	***1.60×10^{-17}***		
220	TS1-AAAH	9.12×10^{-19}	1.78	337	5.46×10^{-16}	5.73×10^{-16}	1.84
	TS2-AAAH	9.12×10^{-19}	1.92	6.99	7.52×10^{-18}		
	TS1-VHP	***9.12×10^{-19}***	***4007***	***2.95×10^{-3}***	***8.77×10^{-18}***		
	TS2-VHP	***9.12×10^{-19}***	***2769***	***5.01×10^{-3}***	***1.03×10^{-17}***		
225	TS1-AAAH	6.12×10^{-19}	1.73	510	5.41×10^{-16}	5.64×10^{-16}	1.78
	TS2-AAAH	6.12×10^{-19}	1.92	6.99	8.20×10^{-18}		
	TS1-VHP	***6.12×10^{-19}***	***4007***	***2.95×10^{-3}***	***7.23×10^{-18}***		
	TS2-VHP	***6.12×10^{-19}***	***2769***	***5.01×10^{-3}***	***8.50×10^{-18}***		
230	TS1-AAAH	4.18×10^{-19}	1.69	759	5.36×10^{-16}	5.58×10^{-16}	1.73
	TS2-AAAH	4.18×10^{-19}	1.86	11.5	8.93×10^{-18}		
	TS1-VHP	***4.18×10^{-19}***	***2473***	***5.88×10^{-3}***	***6.08×10^{-18}***		
	TS2-VHP	***4.18×10^{-19}***	***1737***	***9.90×10^{-3}***	***7.19×10^{-18}***		
240	TS1-AAAH	2.06×10^{-19}	1.61	1.60×10^{3}	5.29×10^{-16}	5.50×10^{-16}	1.64
	TS2-AAAH	2.06×10^{-19}	1.76	29.1	1.05×10^{-17}		
	TS1-VHP	***2.06×10^{-19}***	***1035***	***2.14×10^{-2}***	***4.55×10^{-18}***		
	TS2-VHP	***2.06×10^{-19}***	***749***	***3.54×10^{-2}***	***5.46×10^{-18}***		
250	TS1-AAAH	1.0722×10^{-19}	1.55	3.1685×10^{3}	5.2612×10^{-16}	5.4649×10^{-16}	1.57
	TS2-AAAH	1.0722×10^{-19}	1.67	68.493	1.2298×10^{-17}		
	TS1-VHP	***1.0722×10^{-19}***	***485***	***702.36***	***3.6514×10^{-18}***		
	TS2-VHP	***1.0722×10^{-19}***	***361***	***11.432***	***4.4293×10^{-18}***		
251	TS1-AAAH	1.0077×10^{-19}	1.54	3.3825×10^{3}	5.2592×10^{-16}	5.4634×10^{-16}	1.57
	TS2-AAAH	1.0077×10^{-19}	1.67	74.326	1.2487×10^{-17}		
	TS1-VHP	***1.0077×10^{-19}***	***452***	***786.82***	***3.5840×10^{-18}***		
	TS2-VHP	***1.0077×10^{-19}***	***338***	***12.786***	***4.3528×10^{-18}***		
252	TS1-AAAH	9.4763×10^{-20}	1.54	3.6091×10^{3}	5.2576×10^{-16}	5.4623×10^{-16}	1.56
	TS2-AAAH	9.4763×10^{-20}	1.66	80.602	1.2678×10^{-17}		
	TS1-VHP	***9.4763×10^{-20}***	***422***	***880.64***	***3.5200×10^{-18}***		
	TS2-VHP	***9.4763×10^{-20}***	***316***	***14.288***	***4.2801×10^{-18}***		

253	TS1-AAAH	8.9156×10^{-20}	1.53	3.8489×10^{3}	5.2562×10^{-16}	5.4616×10^{-16}	1.56
	TS2-AAAH	8.9156×10^{-20}	1.65	87.352	1.2871×10^{-17}		
	TS1-VHP	***8.9156×10^{-20}***	***394***	***984.75***	***3.4591×10^{-18}***		
	TS2-VHP	***8.9156×10^{-20}***	***296***	***15.952***	***4.2111×10^{-18}***		
254	TS1-AAAH	8.3925×10^{-20}	1.53	4.1025×10^{3}	5.2550×10^{-16}	5.4612×10^{-16}	1.55
	TS2-AAAH	8.3925×10^{-20}	1.65	94.606	1.3067×10^{-17}		
	TS1-VHP	***8.3925×10^{-20}***	***368***	***11.002***	***3.4012×10^{-18}***		
	TS2-VHP	***8.3925×10^{-20}***	***278***	***17.794***	***4.1455×10^{-18}***		
255	TS1-AAAH	7.9040×10^{-20}	1.52	4.3706×10^{3}	5.2541×10^{-16}	5.4611×10^{-16}	1.54
	TS2-AAAH	7.9040×10^{-20}	1.64	102.40	1.3264×10^{-17}		
	TS1-VHP	***7.9040×10^{-20}***	***345***	***12.281***	***3.3461×10^{-18}***		
	TS2-VHP	***7.9040×10^{-20}***	***260***	***19.832***	***4.0833×10^{-18}***		
256	TS1-AAAH	7.4477×10^{-20}	1.52	4.6539×10^{3}	5.2535×10^{-16}	5.4613×10^{-16}	1.54
	TS2-AAAH	7.4477×10^{-20}	1.63	110.76	1.3463×10^{-17}		
	TS1-VHP	***7.4477×10^{-20}***	***323***	***13.697***	***3.2938×10^{-18}***		
	TS2-VHP	***7.4477×10^{-20}***	***245***	***22.084***	***4.0242×10^{-18}***		
257	TS1-AAAH	7.0212×10^{-20}	1.51	4.9530×10^{3}	5.2530×10^{-16}	5.4618×10^{-16}	1.53
	TS2-AAAH	7.0212×10^{-20}	1.63	119.74	1.3664×10^{-17}		
	TS1-VHP	***7.0212×10^{-20}***	***303***	***15.262***	***3.2441×10^{-18}***		
	TS2-VHP	***7.0212×10^{-20}***	***230***	***24.571***	***3.9681×10^{-18}***		
258	TS1-AAAH	6.6224×10^{-20}	1.51	5.2688×10^{3}	5.2528×10^{-16}	5.4626×10^{-16}	1.53
	TS2-AAAH	6.6224×10^{-20}	1.62	129.36	1.3867×10^{-17}		
	TS1-VHP	***6.6224×10^{-20}***	***284***	***16.993***	***3.1969×10^{-18}***		
	TS2-VHP	***6.6224×10^{-20}***	***216***	***27.315***	***3.9149×10^{-18}***		
259	TS1-AAAH	6.2492×10^{-20}	1.50	5.6020×10^{3}	5.2527×10^{-16}	5.4636×10^{-16}	1.52
	TS2-AAAH	6.2492×10^{-20}	1.61	139.67	1.4073×10^{-17}		
	TS1-VHP	***6.2492×10^{-20}***	***267***	***18.903***	***3.1521×10^{-18}***		
	TS2-VHP	***6.2492×10^{-20}***	***204***	***30.341***	***3.8644×10^{-18}***		
260	TS1-AAAH	5.8999×10^{-20}	1.50	5.9535×10^{3}	5.2529×10^{-16}	5.4650×10^{-16}	1.52
	TS2-AAAH	5.8999×10^{-20}	1.61	150.71	1.4280×10^{-17}		
	TS1-VHP	***5.8999×10^{-20}***	***251***	***21.011***	***3.1095×10^{-18}***		
	TS2-VHP	***5.8999×10^{-20}***	***192***	***33.674***	***3.8166×10^{-18}***		
270	TS1-AAAH	3.40×10^{-20}	1.45	1.07×10^{4}	5.27×10^{-16}	5.49×10^{-16}	1.47
	TS2-AAAH	3.40×10^{-20}	1.55	313	1.65×10^{-17}		
	TS1-VHP	***3.40×10^{-20}***	***142***	***0.579***	***2.79×10^{-18}***		
	TS2-VHP	***3.40×10^{-20}***	***111***	***0.915***	***3.46×10^{-18}***		
275	TS1-AAAH	2.63×10^{-20}	1.43	1.41×10^{4}	5.28×10^{-16}	5.52 × 10-16	1.45
	TS2-AAAH	2.63×10^{-20}	1.52	441	1.76×10^{-17}		
	TS1-VHP	***2.63×10^{-20}***	***109***	***0.935***	***2.69×10^{-18}***		
	TS2-VHP	***2.63×10^{-20}***	***87.0***	***1.47***	***3.35×10^{-18}***		
280	TS1-AAAH	2.05×10^{-20}	1.41	1.83×10^{4}	5.30×10^{-16}	5.54×10^{-16}	1.43
	TS2-AAAH	2.05×10^{-20}	1.50	615	1.89×10^{-17}		
	TS1-VHP	***2.05×10^{-20}***	***86.2***	***1.48***	***2.62×10^{-18}***		
	TS2-VHP	***2.05×10^{-20}***	***69.3***	***2.31***	***3.28×10^{-18}***		

290	TS1-AAAH	1.28×10^{-20}	1.38	3.03×10^{4}	5.34×10^{-16}	5.61×10^{-16}	1.39
	TS2-AAAH	1.28×10^{-20}	1.46	1.15×10^{3}	2.15×10^{-17}		
	TS1-VHP	***1.28×10^{-20}***	***56.0***	***3.56***	***2.55×10^{-18}***		
	TS2-VHP	***1.28×10^{-20}***	***46.0***	***5.48***	***3.22×10^{-18}***		
298.15	TS1-AAAH	8.94×10^{-21}	1.35	4.45×10^{4}	5.39×10^{-16}	5.68×10^{-16}	1.37
	TS2-AAAH	8.94×10^{-21}	1.43	1.87×10^{3}	2.38×10^{-17}		
	TS1-VHP	***8.94×10^{-21}***	***41.1***	***6.95***	***2.56×10^{-18}***		
	TS2-VHP	***8.94×10^{-21}***	***34.3***	***10.6***	***3.25×10^{-18}***		
310	TS1-AAAH	5.51×10^{-21}	1.32	7.51×10^{4}	5.47×10^{-16}	5.80×10^{-16}	1.34
	TS2-AAAH	5.51×10^{-21}	1.39	3.60×10^{3}	2.75×10^{-17}		
	TS1-VHP	***5.51×10^{-21}***	***27.8***	***173***	***2.65×10^{-18}***		
	TS2-VHP	***5.51×10^{-21}***	***23.7***	***26.0***	***3.39×10^{-18}***		
320	TS1-AAAH	3.77×10^{-21}	1.30	1.13×10^{5}	5.55×10^{-16}	5.92×10^{-16}	1.31
	TS2-AAAH	3.77×10^{-21}	1.36	6.02×10^{3}	3.08×10^{-17}		
	TS1-VHP	***3.77×10^{-21}***	***27.8***	***17.3***	***2.79×10^{-18}***		
	TS2-VHP	***3.77×10^{-21}***	***23.7***	***26.0***	***3.59×10^{-18}***		
325	TS1-AAAH	3.15×10^{-21}	1.29	1.38×10^{5}	5.59×10^{-16}	5.98×10^{-16}	1.30
	TS2-AAAH	3.15×10^{-21}	1.34	7.69×10^{3}	3.26×10^{-17}		
	TS1-VHP	***3.15×10^{-21}***	***18.4***	***49.6***	***2.88×10^{-18}***		
	TS2-VHP	***3.15×10^{-21}***	***16.0***	***73.5***	***3.72×10^{-18}***		
330	TS1-AAAH	2.65×10^{-21}	1.28	1.66×10^{5}	5.64×10^{-16}	6.05×10^{-16}	1.29
	TS2-AAAH	2.65×10^{-21}	1.33	9.76×10^{3}	3.45×10^{-17}		
	TS1-VHP	***2.65×10^{-21}***	***16.3***	***69.0***	***2.99×10^{-18}***		
	TS2-VHP	***2.65×10^{-21}***	***14.3***	***102***	***3.86×10^{-18}***		
340	TS1-AAAH	1.91×10^{-21}	1.26	2.39×10^{5}	5.73×10^{-16}	6.19×10^{-16}	1.28
	TS2-AAAH	1.91×10^{-21}	1.31	1.54×10^{4}	3.83×10^{-17}		
	TS1-VHP	***1.91×10^{-21}***	***13.1***	***130***	***3.25×10^{-18}***		
	TS2-VHP	***1.91×10^{-21}***	***11.6***	***190***	***4.20×10^{-18}***		
350	TS1-AAAH	1.40×10^{-21}	1.24	3.36×10^{5}	5.84×10^{-16}	6.35×10^{-16}	1.26
	TS2-AAAH	1.40×10^{-21}	1.29	2.36×10^{4}	4.25×10^{-17}		
	TS1-VHP	***1.40×10^{-21}***	***10.8***	***235***	***3.56×10^{-18}***		
	TS2-VHP	***1.40×10^{-21}***	***9.70***	***341***	***4.62×10^{-18}***		
375	TS1-AAAH	6.98×10^{-22}	1.21	7.27×10^{5}	6.14×10^{-16}	6.78×10^{-16}	1.23
	TS2-AAAH	6.98×10^{-22}	1.25	6.22×10^{4}	5.41×10^{-17}		
	TS1-VHP	***6.98×10^{-22}***	***7.31***	***907***	***4.63×10^{-18}***		
	TS2-VHP	***6.98×10^{-22}***	***6.69***	***1.29×10^{3}***	***6.01×10^{-18}***		
400	TS1-AAAH	3.84×10^{-22}	1.18	1.43×10^{6}	6.47×10^{-16}	7.29×10^{-16}	1.20
	TS2-AAAH	3.84×10^{-22}	1.21	1.45×10^{5}	6.76×10^{-17}		
	TS1-VHP	3.84×10^{-22}	5.42	2.95×10^{3}	6.15×10^{-18}		
	TS2-VHP	3.84×10^{-22}	5.04	4.11×10^{3}	7.96×10^{-18}		
425	TS1-AAAH	2.29×10^{-22}	1.16	2.58×10^{6}	6.84×10^{-16}	7.86×10^{-16}	1.18
	TS2-AAAH	2.29×10^{-22}	1.19	3.06×10^{5}	8.31×10^{-17}		
	TS1-VHP	***2.29×10^{-22}***	***4.30***	***8.36×10^{3}***	***8.22×10^{-18}***		
	TS2-VHP	***2.29×10^{-22}***	***4.04***	***1.15×10^{4}***	***1.06×10^{-17}***		

450	TS1-AAAH	1.45×10^{-22}	1.14	4.38×10^{6}	7.25×10^{-16}	8.51×10^{-16}	1.17
	TS2-AAAH	1.45×10^{-22}	1.16	5.95×10^{5}	1.01×10^{-16}		
	TS1-VHP	***1.45×10^{-22}***	***3.58***	***2.11×10^{4}***	***1.10×10^{-17}***		
	TS2-VHP	***1.45×10^{-22}***	***3.39***	***2.85×10^{4}***	***1.41×10^{-17}***		
475	TS1-AAAH	9.76×10^{-23}	1.12	7.01×10^{6}	7.70×10^{-16}	9.23×10^{-16}	1.15
	TS2-AAAH	9.76×10^{-23}	1.15	1.08×10^{6}	1.20×10^{-16}		
	TS1-VHP	***9.76×10^{-23}***	***3.08***	***4.83×10^{4}***	***1.45×10^{-17}***		
	TS2-VHP	***9.76×10^{-23}***	***2.94***	***6.45×10^{4}***	***1.85×10^{-17}***		
500	TS1-AAAH	6.87×10^{-23}	1.11	1.07×10^{7}	8.17×10^{-16}	1.00×10^{-15}	1.14
	TS2-AAAH	6.87×10^{-23}	1.13	1.84×10^{6}	1.43×10^{-16}		
	TS1-VHP	***6.87×10^{-23}***	***2.72***	***1.02×10^{5}***	***1.91×10^{-17}***		
	TS2-VHP	***6.87×10^{-23}***	***2.62***	***1.34×10^{5}***	***2.41×10^{-17}***		

2.2.4 Master Equation Rate Constants (k_{ME}) At Non-Standard Pressures

Table 61: Calculated Master Equation Rate Constants (k_{ME}) at Non-Standard Temperatures and Pressures for sCI 1 + MeOH & EtOH at Grainsize 10

sCI 1 + MeOH			sCI 1 + EtOH		
T (K)	P_0 (Torr)	k_{ME} (10^{-14} cm^3 s^{-1})	T (K)	P_0 (Torr)	k_{ME} (10^{-14} cm^3 s^{-1})
200	9.99	2.59	200	9.99	22.83
210	9.99	2.27	210	9.99	18.53
220	9.99	2.03	220	9.99	15.43
230	9.99	1.84	230	9.99	13.12
240	9.99	1.68	240	9.99	11.36
250	9.99	1.55	250	9.99	9.99
260	9.99	1.45	260	9.99	8.90
270	9.99	1.36	270	9.99	8.01
280	9.99	1.29	280	9.99	7.28
290	9.99	1.23	290	9.99	6.68
298.15	9.99	1.19	298.15	9.99	6.26
310	9.99	1.14	310	9.99	5.74
320	9.99	1.10	320	9.99	5.37
330	9.99	1.07	330	9.99	5.06
340	9.99	1.04	340	9.99	4.78
350	9.99	1.01	350	9.99	4.54
262.1	9.99	1.43	282.5	9.99	7.12
262.6	99.9	1.44	282.5	99.5	7.36
293	9.99	1.21	328.9	9.99	5.09
295	250	1.21	329.2	99.5	5.19
-	-	-	293	9.99	6.52
-	-	-	295	250	6.63

Table 62: Calculated Master Equation Rate Constants (k_{ME}) at Non-Standard Temperatures and Pressures for sCIs 1, 2 & 3 with various alcohols at Grainsize 10

#sCI	sCI structure	ROH	T (K)	P_0 (Torr)	k_{ME} (10^{-14} cm^3 s^{-1})
1	HCHOO	iPrOH	295	250	1.25×10^{-14}
2	*syn*-CH_3CHOO	MeOH	295	250	1.91×10^{-17}
3	*anti*-CH_3CHOO	MeOH	295	250	2.30×10^{-14}

Table 63: Calculated Master Equation Rate Constants (k_{ME}) at Non-Standard Temperatures and Pressures for sCl 4 + MeOH at Grainsize 10

sCl 4 + MeOH		
T (K)	**P_0 (Torr)**	**k_{ME} (10^{-16} cm^3 s^{-1})**
200	9.99	9.40
210	9.99	7.36
220	9.99	6.45
230	9.99	6.01
240	9.99	5.78
250	9.99	5.67
260	9.99	5.62429
261	9.99	5.62270
262	9.99	5.62154
263	9.99	5.62080
264	9.99	5.62046
265	9.99	5.62050
266	9.99	5.62092
267	9.99	5.62169
268	9.99	5.62283
269	9.99	5.62431
270	9.99	5.62610
280	9.99	5.66
290	9.99	5.72
298.15	9.99	5.78
310	9.99	5.90
320	9.99	6.01
330	9.99	6.14
340	9.99	6.28
350	9.99	6.44
292.2	9.99	5.74

2.2.5 Literature Experimental Rate Constants

Table 64: Experimental Rate Constant (k_{EXP}) of sCI + alcohol reactions near 298 K found in the literature.

sCI no	sCI chemical formula	Alcohol	Temperature (K)	Pressure (Torr)	Experimental Rate Constant (k_{EXP}) [$cm^3\ s^{-1}$]	Study	Ref
1	HCHOO	MeOH	292.6	9.99	1.04×10^{-13}	Orr-Ewing *et al.*	[102]
1	HCHOO	MeOH	295	250	$(1.4 \pm 0.4) \times 10^{-13}$	Murray *et al.*	[103]
1	HCHOO	EtOH	292.8	9.99	1.16×10^{-13}	Orr-Ewing *et al.*	[102]
1	HCHOO	EtOH	295	250	$(2.3 \pm 0.6) \times 10^{-13}$	Murray *et al.*	[103]
1	HCHOO	iPrOH	295	250	$(1.9 \pm 0.5) \times 10^{-13}$	Murray *et al.*	[103]
2	*syn*-CH_3CHOO	MeOH	295	250	$\leq 2 \times 10^{-17}$	Lin *et al.*	[103]
2	*syn*-CH_3CHOO	$(MeOH)_2$	298	250	$(8.0 \pm 1.0) \times 10^{-32}$	Chao *et al.*	[104]
3	*anti*-CH_3CHOO	MeOH	295	250	$(4.8 \pm 0.5) \times 10^{-12}$	Lin *et al.* & Chao *et al.*	[103,104]
4	$(CH_3)_2COO$	MeOH	295	9.99	$(4.29 \pm 0.54) \times 10^{-14}$	Orr-Ewing *et al.*	[102]
N/A	*anti*-$CH_3(CH_2)_{11}CHOO$	MeOH	296 ± 3 K	740	3.6×10^{-13}	Tobias and Ziemann	[105]
N/A	*anti*-$CH_3(CH_2)_{11}CHOO$	iPrOH	296 ± 3 K	740	8.3×10^{-13}	Tobias and Ziemann	[105]

2.2.6 Previous Literature Theoretical Rate Constants

*Table 65: Previous literature Theoretical Rate Constant (k_{THEO}) of **sCI 1** + alcohol reactions near 298 K found in the literature by other authors.*

sCI no	sCI chemical formula	Alcohol	TS	k_{TS}	Theoretical Rate Constant (k_{THEO}) [$cm^3\ s^{-1}$]	Study	Ref
1	HCHOO	MeOH	TS_{AAAH} 1	N/A	$(3.0 \pm 1.8) \times 10^{-14}$	Aroeira *et al.*	106
1	HCHOO	MeOD	TS_{AAAH} 1	N/A	$(1.2 \pm 0.8) \times 10^{-13}$	Aroeira *et al.*	106
1	HCHOO	MeOH	TS_{AAAH} 1	N/A	2.5×10^{-13}	Murray *et al.*	103
1	HCHOO	EtOH	TS_{AAAH} 1	N/A	4.8×10^{-13}	Murray *et al.*	103
1	HCHOO	iPrOH	TS_{AAAH} 1	N/A	6.6×10^{-13}	Murray *et al.*	103
1	HCHOO	MeOH	TS_{AAAH} 1	3.20×10^{-14}	1.33×10^{-13}	Lin *et al.*	103
			TS_{AAAH} 2	11.17×10^{-14}			
2	*syn*-CH_3CHOO	MeOH	TS_{AAAH} 1	2.37×10^{-18}	$k_{AAAH} \sim 8.24 \times 10^{-17}$ ($k_{VHP} \sim 9.46 \times 10^{-18}$)	Chao *et al.*	104
			TS_{AAAH} 2	8.00×10^{-17}			
			TS_{VHP} 1	6.68×10^{-18}			
			TS_{VHP} 2	2.78×10^{-18}			
		$(MeOH)_2$	$TS(MeOH)_2$ 1	6.04×10^{-32}	1.62×10^{-31}	Chao *et al.*	104
			$TS(MeOH)_2$ 2	1.68×10^{-32}			
			$TS(MeOH)_2$ 3	9.26×10^{-34}			
			$TS(MeOH)_2$ 4	8.42×10^{-32}			
2	*syn*-CH_3CHOO	MeOH	TS_{AAAH} 1	0.20×10^{-17}	9.85×10^{-17}	Lin *et al.*	103
			TS_{AAAH} 2	9.65×10^{-17}			
2	*syn*-CH_3CHOO	MeOH	TS_{AAAH} 1	5.44×10^{-16}	5.44×10^{-16}	Tang and Li	107
2	*syn*-CH_3CHOO	EtOH	TS_{AAAH} 1	9.03×10^{-16}	9.03×10^{-16}	Tang and Li	107
3	*anti*-CH_3CHOO	MeOH	TS_{AAAH} 1	2.50×10^{-12}	1.16×10^{-11}	Chao *et al.*	104
			TS_{AAAH} 2	9.14×10^{-12}			
3	*anti*-CH_3CHOO	MeOH	TS_{AAAH} 1	1.85×10^{-12}	9.53×10^{-12}	Lin *et al.*	103
			TS_{AAAH} 2	7.68×10^{-12}			
3	*anti*-CH_3CHOO	MeOH	TS_{AAAH} 1	5.72×10^{-12}	5.72×10^{-12}	Tang and Li	107
3	*anti*-CH_3CHOO	EtOH	TS_{AAAH} 1	9.74×10^{-12}	9.74×10^{-12}	Tang and Li	107
4	$(CH_3)_2CHOO$	MeOH	TS_{AAAH} 1	N/A	$(2.8 \pm 1.3) \times 10^{-16}$	Aroeira *et al.*	106
4	$(CH_3)_2CHOO$	MeOH	TS_{AAAH} 1	N/A	$(2.8 \pm 1.3) \times 10^{-15}$	Aroeira *et al.*	106

2.3 Relative Energies of sCI + Alcohol Reactions

*Table 66: Relative energies (kJ mol-1) of stationary points of sCI reaction with alcohols. All energies were chosen as the energy of the reactants (energy of CI + energy of alcohol) **ΔE; zero-point corrected energies, Δ(E+ZPE); enthalpy, ΔH (298K); and Gibbs free energies, ΔG (298K):***

CI Entry	Alcohol	Reaction Path	Stationary Point	ΔE	Δ(E+ZPE)	ΔH (298K)	ΔG (298K)
1	MeOH	TS1	CR	-34.20	-28.15	-27.78	6.71
			TS	-12.01	-3.81	-8.35	42.58
			P	-214.75	-198.11	-202.32	-153.59
		TS2	CR	-34.20	-28.15	-27.78	6.71
			TS	-7.18	0.11	-1.87	46.18
			P	-20.71	-190.54	-193.32	-145.97
	EtOH	TS1.1	CR	-34.06	-28.15	-27.49	8.43
			TS	-15.28	-7.28	-11.16	39.76
			P	-215.39	-200.32	-202.89	-154.54
		1.2	CR	-34.25	-28.65	-27.75	6.40
			TS	-15.07	-7.42	-11.36	40.12
			P	-211.68	-196.53	-199.13	-150.44
		1.3	CR	-34.06	-28.15	-27.49	8.43
			TS	-5.58	1.63	-2.35	48.74
			P	-211.31	-196.18	-198.85	-150.50
		2.1	CR	-30.75	-25.51	-24.52	10.49
			TS	-8.78	-1.55	-5.40	45.15
			P	-206.45	-192.23	-194.51	-147.41
		2.2	CR	-34.25	-28.65	-27.75	6.40
			TS	-8.26	-1.49	-5.35	45.45
			P	-205.01	-190.22	-192.68	-145.17
	iPrOH	1.1	CR	-33.89	-28.55	-27.44	7.40
			TS	-12.16	-4.51	-8.03	43.46
			P	-211.37	-196.58	-198.83	-149.92
		1.2	CR	-33.89	-28.55	-27.44	7.40
			TS	-5.04	1.69	-2.04	49.77
			P	-202.23	-187.38	-189.65	-140.70
		1.3	CR	-31.95	-26.50	-25.48	10.17
			TS	-6.81	0.37	-3.30	48.08
			P	-210.63	-195.75	-198.13	-148.99
		2.1	CR	-33.89	-28.55	-27.44	7.40
			TS	-9.77	-2.87	-6.34	44.80
			P	-204.92	-191.17	-193.01	-147.46
		2.2	CR	-33.89	-28.55	-27.44	7.40
			TS	-2.06	4.33	0.69	51.75
			P	-194.90	-180.37	-182.47	-134.96

2	Unimolecular		TS	79.36	69.57	67.51	71.62
			VHP	-83.69	-83.07	-82.10	-84.06
	MeOH	1	CR	-34.96	-29.41	-28.98	8.49
			TS	4.85	10.04	6.03	58.33
			P	-189.72	-176.18	-178.83	-129.37
		2	CR	-34.96	-29.41	-28.98	8.49
			TS	14.84	18.75	14.53	67.28
			P	-176.51	-163.37	-165.92	-118.85
		VHP1	CR	-34.96	-29.41	-28.98	8.49
			TS	38.37	28.99	24.85	76.08
			PC	-115.88	-108.59	-107.57	-72.67
			P	-83.69	-83.07	-82.10	-84.06
		VHP2	CR	-34.96	-29.41	-28.98	8.49
			TS	36.71	27.19	23.13	73.61
			PC	-118.53	-110.86	-110.05	-74.61
			P	-83.69	-83.07	-82.10	-84.06
3	MeOH	1a	CR	-40.96	-35.13	-34.72	1.32
			TS	-23.12	-17.73	-22.16	30.11
			P	-202.63	-187.14	-190.90	-139.13
		1b	CR	-40.96	-35.13	-34.72	1.32
			TS	-18.25	-13.99	-18.09	32.64
			P	-201.04	-186.44	-189.92	-139.72
4	Unimolecular		TS	75.54	66.58	64.71	68.04
			VHP	-74.62	-73.49	-72.76	-74.50
	MeOH	1	CR	-40.11	-34.42	-33.99	3.72
			TS	-0.70	1.21	-2.56	50.21
			P	-174.29	-161.77	-164.59	-113.40
		2	CR	-40.11	-34.42	-33.99	3.72
			TS	9.11	9.63	6.01	58.07
			P	-165.51	-152.36	-155.72	-102.99
		VHP 1	CR	-40.11	-34.42	-33.99	3.72
			TS	37.38	26.11	22.55	71.94
			PC	-107.34	-99.25	-98.63	-61.44
			P	-74.62	-73.49	-72.76	-74.50
		VHP 2	CR	-40.11	-34.42	-33.99	3.72
			TS	36.40	25.32	21.70	70.89
			PC	-109.44	-101.30	-100.69	-63.87
			P	-74.62	-73.49	-72.76	-74.50
5	MeOH	1	CR	-36.15	-30.42	-29.69	7.36
			TS	-20.02	-13.02	-16.71	34.56
			P	-238.17	-225.29	227.78	-179.49
		2	CR	-36.15	-30.42	-29.69	7.36
			TS	-22.09	-15.16	-18.94	32.56
			P	-244.28	-230.67	-233.60	-183.70
6	MeOH	1	CR	-44.55	-38.52	-38.33	-1.38
			TS	-41.02	-32.22	-36.51	14.83
			P	-249.04	-233.47	-236.92	-186.89
		2	CR	-44.55	-38.52	-38.33	-1.38
			TS	-37.72	-29.55	-33.89	17.45
			P	-247.58	-232.03	-235.60	-185.59
7	MeOH	1	CR	-48.01	-41.27	-41.43	-0.05
			TS	-47.25	-40.51	-43.24	6.30
			P	-298.07	-285.84	-288.96	-237.56
8	MeOH	1	CR	-29.54	-26.80	-25.51	8.91

			TS	6.98	10.09	6.65	58.24
			P	-205.40	-195.25	-197.33	-148.94
		2	CR	-29.54	-26.80	-25.51	8.91
			TS	9.30	11.91	8.40	59.93
			P	-210.83	-200.04	-202.32	-152.98
9	MeOH	1	CR	-39.09	-35.45	-34.83	0.94
			TS	-27.58	-23.11	-27.33	24.45
			P	-227.12	-214.59	-217.49	-167.97
		2	CR	-39.09	-35.45	-34.83	0.94
			TS	-20.25	-16.71	-20.75	30.06
			P	-225.97	-213.46	-216.53	-166.79
10	MeOH	1	CR	-32.10	-27.28	-26.12	9.70
			TS	-7.11	-3.60	-7.11	46.37
			P	-214.54	205.41	-206.93	-158.17
		2	CR	-32.10	-27.28	-26.12	9.70
			TS	-1.60	1.39	-2.12	51.20
			P	-222.17	-211.56	-213.75	-162.59
11	MeOH	1	CR	-27.36	-23.07	-21.46	7.96
			TS	9.61	10.40	7.14	58.54
			P	-175.91	-165.59	-167.31	-120.03
		2	CR	-25.69	-21.25	-19.56	10.80
			TS	10.89	10.09	6.87	58.22
			P	-165.93	-155.16	-156.95	-108.98
	EtOH	1.1	CR	-25.36	-21.30	-19.17	11.42
			TS	7.30	7.45	4.89	56.91
			P	-179.08	-169.23	-170.19	-122.66
		1.2	CR	-25.63	-21.42	-19.43	11.73
			TS	7.68	8.37	5.89	57.26
			P	-182.14	-172.65	-173.39	-125.80
		1.3	CR	-28.09	-24.03	-22.09	9.58
			TS	17.40	17.44	14.85	67.10
			P	-175.68	-166.18	-167.02	-119.66
		2.1	CR	-26.73	-22.45	-20.47	10.83
			TS	9.23	9.02	6.34	59.30
			P	-173.36	-163.70	-164.58	-116.95
		2.2	CR	-25.36	-21.30	-19.17	11.42
			TS	9.34	8.04	5.30	58.44
			P	-167.83	-157.69	-158.86	-108.93
	iPrOH	1.1	CR	-27.56	-23.84	-21.61	9.82
			TS	5.98	6.16	4.16	56.04
			P	-179.39	-169.98	-170.42	-121.79
		1.2	CR	-28.03	-24.34	-22.06	7.52
			TS	16.16	15.05	13.06	64.72
			P	-170.26	-160.56	-161.23	-111.93
		1.3	CR	-27.42	-23.69	-21.42	8.75
			TS	16.57	16.01	14.11	64.68
			P	-177.73	-168.66	-169.07	-122.16
		2	CR	-25.99	-22.13	-19.86	12.34
			TS	7.82	6.58	4.39	57.85
			P	-168.57	-159.55	-159.84	-114.08
		2.2	CR	-27.56	-23.84	-21.61	9.82
			TS	22.19	20.11	17.82	72.15
			P	-170.26	-160.56	-161.23	-111.93
12	MeOH	1	CR	-36.71	-31.32	-30.35	4.65

			TS	-18.09	-17.43	-20.99	30.74
			P	-186.21	-173.54	-175.97	-127.79
		2	CR	-36.71	-31.32	-30.35	4.65
			TS	-10.92	-10.91	-14.34	36.61
			P	-185.85	-173.59	-176.11	-127.21
	EtOH	1.1	CR	-37.63	-32.93	-31.30	2.59
			TS	-19.07	-19.27	-22.19	29.97
			P	-186.64	-174.94	-176.30	-128.79
		1.2	CR	-37.57	-32.42	-31.05	4.89
			TS	-21.62	-21.01	-23.94	28.31
			P	-186.64	-174.94	-176.30	-128.79
		2.1	CR	-37.57	-32.42	-31.05	4.89
			TS	-12.01	-11.81	-14.70	37.51
			P	-187.27	-175.85	-177.39	-128.51
		2.2	CR	-37.63	-32.93	-31.30	2.59
			TS	-11.73	-12.35	-15.29	37.43
			P	-183.10	-171.81	-173.36	-125.31
	iPrOH	1a	CR	-37.77	-33.25	-31.43	3.68
			TS	-20.44	-20.84	-23.33	30.19
			P	-182.34	-171.51	-172.50	-123.83
		1b	CR	-37.77	-33.25	-31.43	3.68
			TS	-8.33	-9.82	-12.28	41.39
			P	-163.87	-151.58	-153.26	-99.48
		2.1	CR	-37.77	-33.25	-31.43	3.68
			TS	-15.33	-16.01	-18.49	34.45
			P	-183.16	-172.58	-173.50	-125.34
		2.2	CR	-37.77	-33.25	-31.43	3.68
			TS	-4.97	-6.52	-9.00	44.19
			P	-175.42	-164.40	-165.50	-115.70
13	Unimolecular		TS	84.95	74.22	69.91	75.91
			VHP	-58.02	-59.29	-57.74	-62.25
	MeOH	1a	CR	-30.03	-24.65	-23.97	12.86
			TS	15.89	14.66	11.27	63.56
			P	-148.70	-138.02	-140.36	-90.16
		1b	CR	-30.03	-24.65	-23.97	12.86
			TS	25.70	23.25	19.96	72.07
			P	-145.71	-134.61	-137.29	-86.02
		VHP 1	CR	-30.03	-24.65	-23.97	12.86
			TS	71.22	58.63	55.10	105.44
			PC	-91.06	-85.58	-84.09	-50.13
			P	-58.02	-59.29	-57.74	-62.25
		VHP 2	CR	-30.03	-24.65	-23.97	12.86
			TS	48.96	36.41	32.93	82.54
			PC	-93.27	-87.36	-85.93	-52.52
			P	-58.42	-59.34	-58.03	-61.52
14	Unimolecular		TS	83.50	73.47	71.38	76.00
			VHP	-74.35	-73.48	-72.98	-73.46
	MeOH	1a	CR	-30.48	-25.18	-24.52	12.63
			TS	8.17	7.31	3.59	57.68
			P	-160.80	-149.25	-152.06	-99.43
		1b	CR	-30.48	-25.18	-24.52	12.63
			TS	20.81	18.66	15.02	68.69
			P	-144.93	-133.17	-136.04	-84.42

		VHP 1	CR	-30.48	-25.18	-24.52	12.63
			TS	44.30	32.63	28.80	80.34
			PC	-103.74	-97.53	-95.69	-67.06
			P	-74.35	-73.48	-72.98	-73.46
		VHP 2	CR	-30.48	-25.18	-24.52	12.63
			TS	42.30	30.82	27.00	78.05
			PC	-109.99	-102.18	-101.61	-64.91
			P	-74.35	-73.48	-72.98	-73.46
15	MeOH	1a	CR	-38.51	-33.16	-32.18	1.88
			TS	-10.02	-9.96	-13.49	38.04
			P	-174.32	-161.59	-164.30	-113.95
		1b	CR	-38.51	-33.16	-32.18	1.88
			TS	-8.82	-8.67	-12.13	38.88
			P	-181.82	-169.70	-172.13	-123.05
16	MeOH	1a	CR	-33.58	-28.19	-27.26	7.68
			TS	-18.00	-15.88	-20.04	33.41
			P	-189.92	-176.55	-179.58	-127.99
		1b	CR	-33.58	-28.19	-27.26	7.68
			TS	-7.99	-7.37	-11.23	40.77
			P	-181.38	-169.05	-171.59	-123.68
17	MeOH	1a	CR	-36.77	-31.88	-30.77	4.14
			TS	2.41	0.79	-2.71	49.76
			P	-162.59	-151.75	-154.43	-103.20
		1b	CR	-36.77	-31.88	-30.77	4.14
			TS	5.40	2.26	-1.05	51.03
			P	-161.52	-150.36	-153.18	-102.15
18	MeOH	1a	CR	-27.40	-22.75	-21.32	10.37
			TS	9.67	8.44	5.15	57.43
			P	-162.65	-151.93	-154.79	-102.38
		1b	CR	-27.40	-22.75	-21.32	10.37
			TS	15.97	13.25	10.15	61.88
			P	-156.92	-146.28	-149.00	-96.82
19	MeOH	1a	CR	-35.78	-30.57	-29.71	6.18
			TS	2.20	3.55	-0.10	52.43
			P	-185.19	-174.20	-176.23	-126.96
		1b	CR	-35.78	-30.57	-29.71	6.18
			TS	5.26	4.62	1.02	53.32
			P	-168.78	-156.94	-159.49	-108.11
20	MeOH	1a	CR	-25.03	-20.69	-19.06	10.90
			TS	12.39	13.42	10.02	61.88
			P	-176.07	-165.56	-167.59	-118.99
		1b	CR	-25.03	-20.69	-19.06	10.90
			TS	20.41	19.79	16.09	69.33
			P	-163.54	-152.07	-154.49	-103.87
21	MeOH	1a	CR	-63.88	-57.50	-57.78	-17.05
			TS	-29.91	-30.31	-34.25	18.03
			P	-210.19	-199.75	-202.82	-152.14
		1b	CR	-63.88	-57.50	-57.78	-17.05
			TS	-25.86	-26.67	-30.57	20.31
			P	-206.47	-196.09	-199.14	-149.17
22	MeOH	1a	CR	-60.58	-54.01	-54.06	-12.92
			TS	-44.05	-44.31	-48.33	5.26
			P	-199.45	-190.19	-192.68	-142.94
		1b	CR	-60.58	-54.01	-54.06	-12.92

			TS	-28.74	-30.14	-34.28	20.30
			P	-210.04	-199.63	-202.67	-150.85

2.4 Computational Sensitivity Study

As mentioned in Section 2.9 in the main body of this thesis, determining the validity of the computational approach, *DF-LCCSD(T)-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ* (referred to in this section as the B3LYP-*optimised* approach), is difficult as functionals, such as the B3LYP functional used in this method, purposely built and selected because they model the particular target chemical systems. Instead, the author uses two methods of indicate a confidence level for the *B3LYP-optimised* approach: a *scope of agreeability* factor (Δ_{AGREE}) or a *sensitivity variation* factor (Δ_{SENSI}).

To determine the *scope of agreeability* (Δ_{AGREE}) involves finding the relative zero-point corrected energy of the stationary points relative to the raw reactants (ΔE_{SP}) on the potential energy surface using another approach, either using data the literature or calculating the potential energy using another approach. Here the author used the *DF-LCCSD(T)-F12a/aug-cc-pVTZ//M062X/aug-cc-pVTZ* approach, as well as data from other computational studies. The difference between the ΔE_{SP} the *B3LYP-optimised* approach and the alternative approach for each stationary point is determined and then averaged across for each potential energy surface, as shown in the Equation below. This method can only be applied when comparing computational approaches

$$\Delta_{AGREE} = \frac{\sum(|\Delta E_{SP}\text{ (B3LYP-}optimised\text{ approach)} - \Delta E_{SP}\text{ (other approach)}|)}{\text{Number of stationary points considered}} \qquad \textit{Equation 15}$$

The *sensitivity variation* factor (Δ_{SENSI}), the second assessment of reliability, involves determining the relative Gibbs free energy of the TS structures derived from both experimental studies (ΔG_{EXP}) and other theoretical studies (ΔG_{THEO}). By reversing the rate constant equation below, and assuming that P_0 is assumed here to be 1 atmospheres pressure and applying the TS_{AAAH} 1 pathway branching ratio produced from this study, the ΔG_{EXP} and ΔG_{THEO} values for TS_{AAAH} 1 can be derived:

$$k_{EXP} = \boldsymbol{\kappa}\frac{k_B T}{h} \times \frac{RT}{P_0}\, e^{(-\Delta G_{exp})/RT} \qquad \textit{Equation 16}$$

$$\Delta G_{EXP}\ (TS_{AAAH}\ 1) = RT\ ln\left\{[k_{exp} \times \Gamma_{THEO}(TS_{AAAH}\ 1)] \times \frac{h}{k_B T\, \boldsymbol{\kappa}} \times \frac{P_0}{RT}\right\} \qquad \textit{Equation 17}$$

The *sensitivity variation* factor which measures differentials between Gibbs free energy barriers of different computational approaches can be derived using Equation 19. Both the *scope of agreeability* and the *sensitivity variation* factor equations feature the two

vertical straight lines surrounding a section of the equation ($|\ |$) to convert the number or expression to the absolute value.

$$\Delta_{SENSI} = \frac{\sum(|\Delta G_{TS}\,(\text{B3LYP-}\textit{optimised}\text{ approach}) - \Delta G_{TS}\,(\text{other approach})|)}{\text{Number of stationary points considered}} \qquad \textit{Equation 18}$$

Due to the nature of this method of determining the ΔG_{EXP} (TS_{AAAH} 1) values used here, any differences in the Gibbs free energy for each transition states are likely to be the same across the potential energy surface. For this reason and for the purpose of simplicity only determining and comparing the ΔG_{EXP} for the TS_{AAAH} 1 is required here is used here.

A *scope of agreeability* factor (Δ_{AGREE}) or a *sensitivity variation* factor (Δ_{SENSI}) for various sCI + alcohol reactions can be found in this section. Whereas *scope of agreeability* factor can be determined either using just transition states (as it is in the main body of the text) or all stationary points, *sensitivity variation* factor is only be derived for transition states.

Table 67: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of CH_2OO + MeOH relative to different computational chemistry approaches both from this thesis and the literature (Δ_{SENSI}).

CH_2OO + MeOH			Zero-point corrected energy (kJ mol^{-1})							Ref
Study	**Approach**		PRC	$TS_{AAAH}1$	AAAH 1	$TS_{AAAH}2$	AAAH 2	TS_{ESTER}	Ester + H_2O	
This Thesis	*DF-LCCSD-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ*	ΔE	-28.0	-3.8	-199.0	0.1	-190.6	2.9	-512.6	-
This Thesis	*DF-LCCSD-F12a/aug-cc-pVTZ//M062X/aug-cc-pVTZ*	ΔE	-27.6	-7.1	-198.8	3.2	-190.1	9.1	-514.9	-
Overall Δ_{AGREE} ±2.3		Δ_{AGREE}	-0.4	**3.2**	-0.3	**-3.1**	-0.6	**-6.2**	2.3	
Lin *et al.*	*QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)*	ΔE	-31.6	-8.7	-194.9	-4.3	-186.8	—	—	3
Overall Δ_{AGREE} ±4.2		Δ_{AGREE}	3.5	**4.8**	-4.2	**4.4**	-3.9	—	—	
Lin *et al.*	*QCISD(T)/CBS//B3LYP/aug-cc-pVTZ*	ΔE	-31.6	-21.3	-194.9	-16.7	-186.8	—	—	3
Overall Δ_{AGREE} ±9.2		Δ_{AGREE}	3.5	**17.4**	-4.2	**16.8**	-3.9	—	—	
Aroeira *et al.*	*QCISD(T)/CBS//CCSD(T)/ANO1*	ΔE	-30.3	-6.2	-194.7	—	—	—	—	4
Overall Δ_{AGREE} ±3.0		Δ_{AGREE}	2.3	**2.4**	-4.4	—	—	—	—	

Table 68: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of syn-CH_3CHOO + MeOH relative to different computational chemistry approaches both from this thesis and the literature (Δ_{SENSI}).

syn-CH_3CHOO + MeOH			Zero-point corrected energy (kJ mol^{-1})								Ref
Study	**Approach**		PRC	$TS_{AAAH}1$	AAAH1	$TS_{AAAH}2$	AAAH2	$TS_{VHP}1$	$TS_{VHP}2$	VHP	
This Thesis	*DF-LCCSD-F12a//B3LYP/aug-cc-pVTZ*	ΔE	-29.4	10.0	-176.2	18.7	-163.4	29.0	27.2	-83.1	-
Lin *et al.*	*QCISD(T)/CBS//M062X/aug-cc-pVTZ*	ΔE	-32.9	-1.6	-169.7	6.0	-156.7	—	—	—	3
Overall Δ_{AGREE} ±8.2		Δ_{AGREE}	3.5	**11.6**	-6.4	**12.7**	-6.7	—	—	—	
Chao *et al.*	*QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)*	ΔE	-33.0	8.0	-169.7	16.7	-156.7	23.3	25.5	-73.5	5
Overall Δ_{AGREE} ±4.7		Δ_{AGREE}	3.6	**2.0**	-6.4	**2.0**	-6.7	**5.7**	**1.7**	-9.6	

Table 69: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of anti-CH_3CHOO + MeOH relative to different computational chemistry approaches both from this thesis and the literature (Δ_{SENSI}).

anti-CH_3CHOO + MeOH			Zero-point corrected energy (kJ mol^{-1})					Ref
Study	**Approach**		PRC 1	$TS_{AAAH}1$	AAAH 1	$TS_{AAAH}2$	AAAH 2	
This Thesis	*DF-LCCSD-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ*	ΔE	-35.1	-17.7	-187.1	-14.0	-186.4	-

Lin *et al.*	*QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)*	ΔE	-38.0	-20.4	-181.9	-16.1	-181.3	3
Overall Δ_{AGREE} ±3.6		Δ_{AGREE}	2.9	**2.6**	-5.3	**2.1**	-5.2	
Lin *et al.*	*QCISD(T)/CBS//M062X/aug-cc-pVTZ*	ΔE	-38.0	-28.8	-181.9	-23.7	-181.3	3
Overall Δ_{AGREE} ±6.8		Δ_{AGREE}	2.9	**11.0**	-5.3	**9.7**	-5.2	

Table 70: The zero-point corrected energy values and the error values for each stationary point on the potential energy surface of syn-CH_3CHOO + MeOH relative to different computational chemistry approaches both from this thesis and the literature (Δ_{SENSI}).

$(CH_3)_2COO$ + MeOH			Zero-point corrected energy (kJ mol^{-1})					Ref
Study	**Approach**		PRC 1	$TS_{AAAH}1$	AAAH 1	$TS_{AAAH}2$	AAAH 2	
This Thesis	*DF-LCCSD-F12a/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ*	ΔE	-34.4	1.2	-161.8	9.6	-152.4	-
Aroeira *et al.*	*QCISD(T)/CBS//CCSD(T)/ANO1*	ΔE	-37.4	2.3	-146.6	—	—	4
Overall Δ_{AGREE} ±6.4		Δ_{AGREE}	3.0	-1.0	-15.2	—	—	

Table 71: Sensitivity study of CI + alcohol reactions, comparing computationally generated results to that derived from other rate constants (k_{THEO} & k_{EXP}) by using the rate constant of dominant channel ($\mathbf{kTS_{AAAH}\ 1} = k_{EXP} \times \Gamma_{THEO}$), and the computationally-determined tunneling constant (**κ**), to determine the relative Gibbs free energy of the dominant channel (**ΔG (TS_{AAAH} 1)**) see equations above; and the difference between these computationally/experimentally-derived **ΔG (TS_{AAAH} 1)** values and the ΔG_{THEO} (TS_{AAAH} 1) from this thesis produces an "agreeability" factor (Δ_{SENSI}).

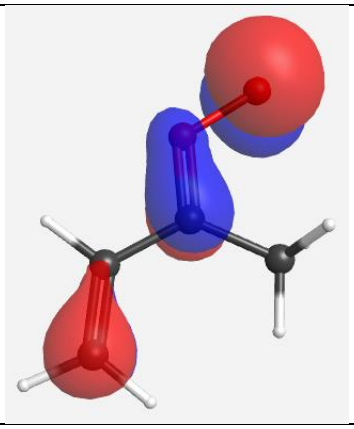
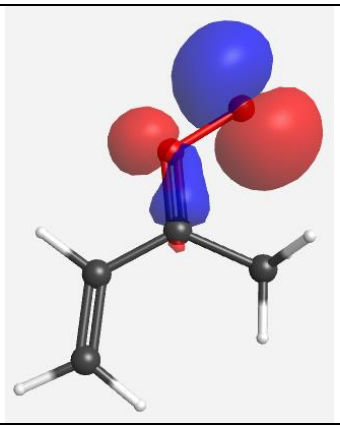
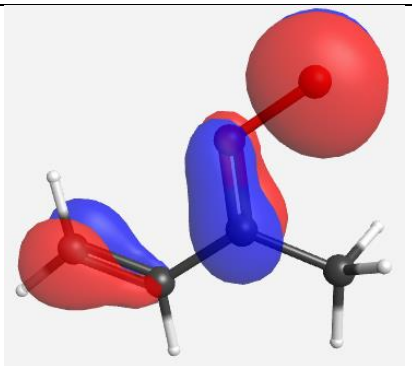
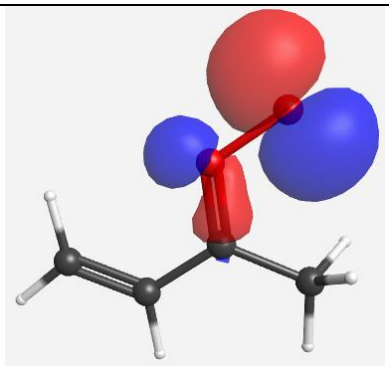
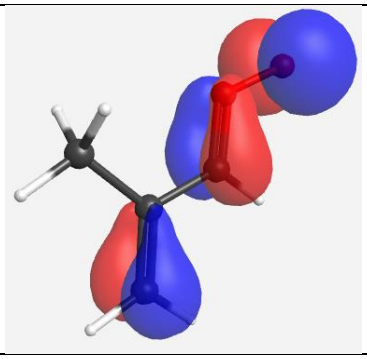
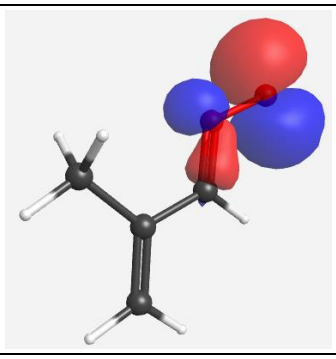
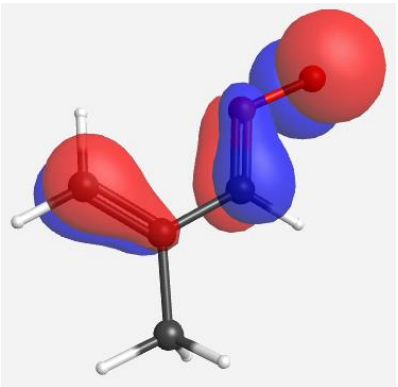
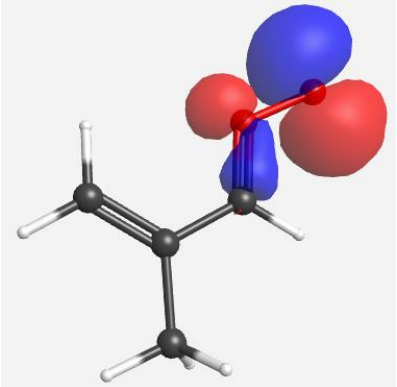
sCI	ROH	Method of Study	Overall k_{THEO} or k_{EXP} ($cm^3\ s^{-1}$)	Γ_{THEO} (TS_{AAAH} 1)	kTS_{AAAH} 1 ($cm^3\ s^{-1}$)	κ	ΔG (TS_{AAAH} 1) kJ mol^{-1}	Δ_{SENSI}	Ref
CH_2OO (**sCI 1**)	MeOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	1.19×10^{-14}	0.801	9.49×10^{-15}	1.10	42.6	—	This thesis
		DF-LCCSD(T)-F12a//M062X/aug-cc-pVTZ	4.19×10^{-14}		4.11×10^{-14}		39.0	-3.6	
		Experimental (298 K) * — McGillen *et al.*	~1.02×10^{-13}		7.46×10^{-14}		37.2	-5.3	[1]
		Experimental (295 K) — Tadayon *et al.*	~1.4×10^{-13}		1.02×10^{-13}		36.5	-6.1	[2]
		QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)	1.44×10^{-13}	0.777	1.12×10^{-13}		36.5	-6.1	[3]
		QCISD(T)/CBS//CCSD(T)/ANO1**	~3.0×10^{-14}	1	3.0×10^{-14}		39.7	-2.9	[4]
	EtOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	6.17×10^{-14}	0.472	2.92×10^{-14}	1.08	39.8	—	Thesis
		Experimental (298 K) * — McGillen *et al.*	1.19×10^{-13}		5.60×10^{-14}		38.2	-1.6	[1]
		Experimental (295 K) — Tadayon *et al.*	2.3×10^{-13}		1.09×10^{-13}		36.1	-3.6	[2]
	iPrOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	1.21×10^{-14}	0.539	6.54×10^{-15}	1.07	43.5	—	Thesis
		Experimental (295 K) — Tadayon *et al.*	1.9×10^{-13}		1.02×10^{-13}		36.3	-7.2	[2]
syn-CH_3CHOO (**sCI 2**)	MeOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	1.96×10^{-17}	0.917	1.77×10^{-17}	1.17	58.3	—	Thesis
		Experimental (298 K) — Lin *et al.* ***	$<2.0 \times 10^{-17}$		$<1.83 \times 10^{-17}$		>58.2	>-0.1	[5]
		QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)	9.18×10^{-17}	0.871	8.00×10^{-17}		54.6	-3.7	[3]
		QCISD(T)/CBS//B3LYP/aug-cc-pVTZ**	9.85×10^{-17}	0.98	9.65×10^{-17}		54.1	-4.2	[5]
anti-CH_3CHOO (**sCI 3**)	MeOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	2.12×10^{-12}	0.735	1.55×10^{-12}	1.16	30.1	—	Thesis
		Experimental (298 K) — Lin *et al.*	~4.8×10^{-12}		3.53×10^{-12}		28.1	-2.0	[5]
		QCISD(T)/CBS//B3LYP/6-311+G(2d,2p)	1.16×10^{-11}	0.731	9.14×10^{-12}		25.7	-4.4	[3]
		QCISD(T)/CBS//B3LYP/aug-cc-pVTZ	9.53×10^{-12}	0.806	7.68×10^{-12}		26.1	-4.0	[5]
$(CH_3)_2COO$ (**sCI 4**)	MeOH	DF-LCCSD(T)-F12a//B3LYP/aug-cc-pVTZ	5.76×10^{-16}	0.948	5.40×10^{-16}	1.35	50.2	—	Thesis
		Experimental (298 K) * — McGillen *et al.*	4.21×10^{-14}		3.99×10^{-14}		39.5	10.7	[1]
		QCISD(T)/CBS//CCSD(T)/ANO1**	~2.8×10^{-16}	1	2.8×10^{-16}		51.8	1.6	[4]

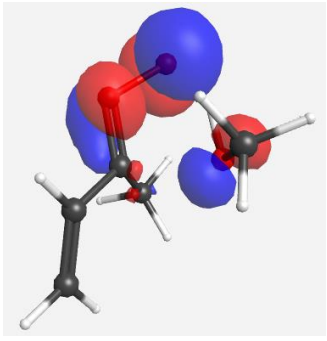
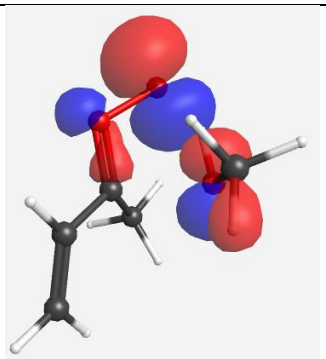
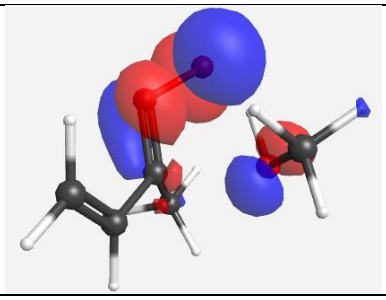
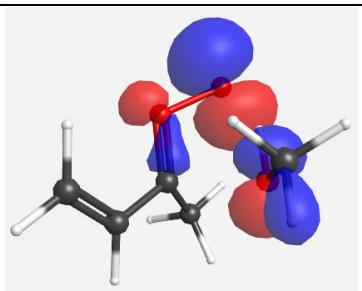
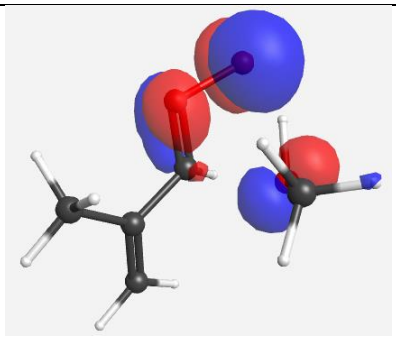
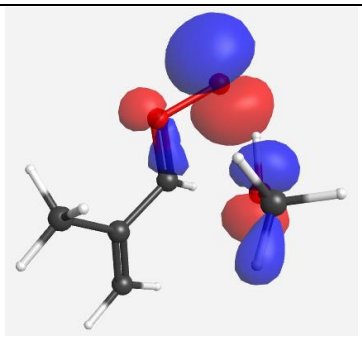
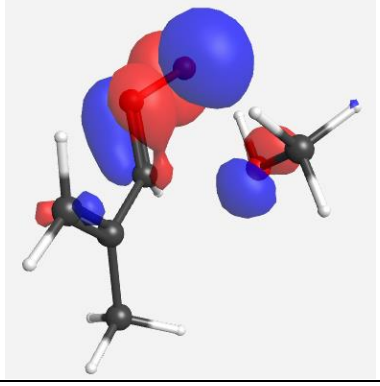
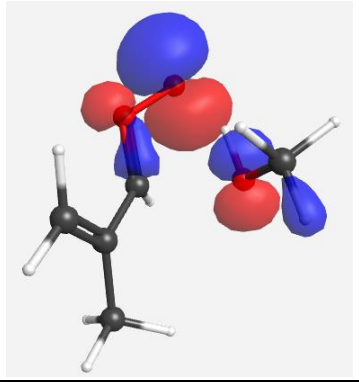
* The McGillen *et al.* experimental rate constants (k_{EXP}) given in this table are derived from the modified Arrhenius expressions for $CH_2OO + CH_3OH$ [$k(T) = 3.7 \times 10^{-21} \times T^2 \times e^{1710/T}$], CH_2OO + EtOH [$k(T) = 4.2 \times 10^{-14} \times T^2 \times e^{1717/T}$] & $(CH_3)_2COO + CH_3OH$ [$k(T) = 6.07 \times 10^{-33} \times T^{3.87} \times e^{5852/T} + 5.82 \times 10^{-16} \times T^{2.92} \times e^{3741/T}$].

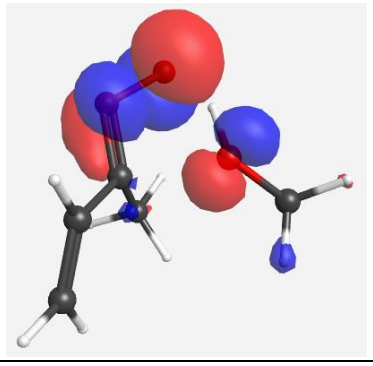
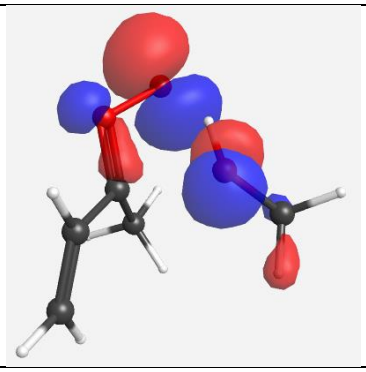
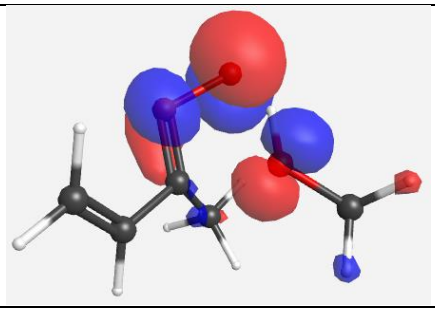
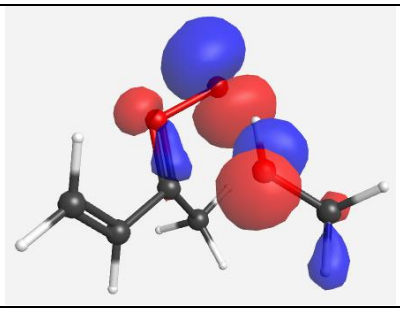
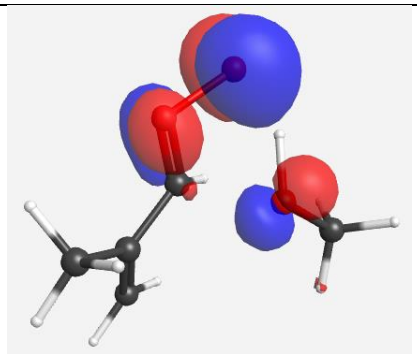
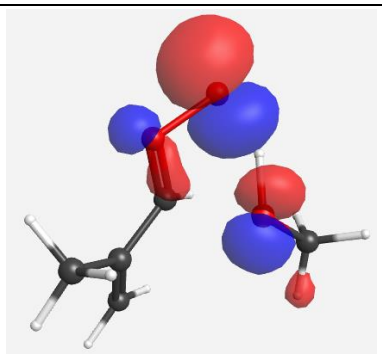
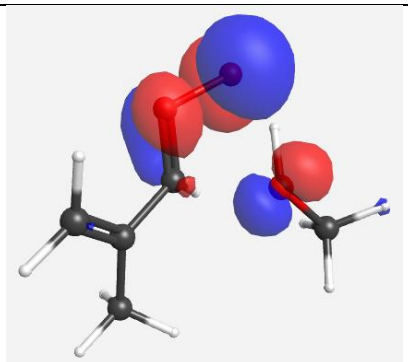
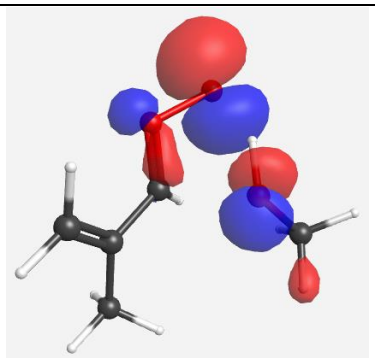
** This computational study derives the rate constant from only one reaction pathway and a rigid-rotor harmonic oscillator approximation.

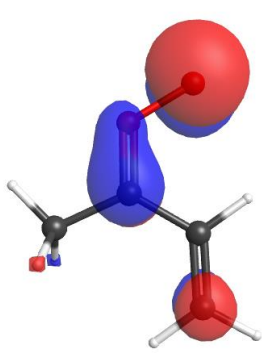
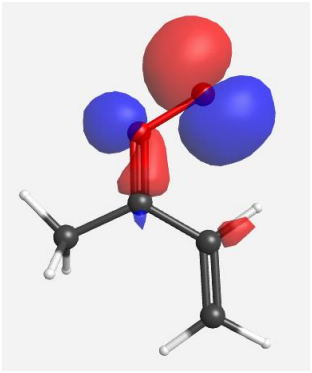
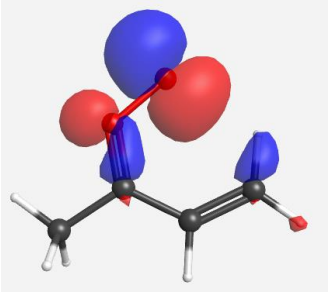
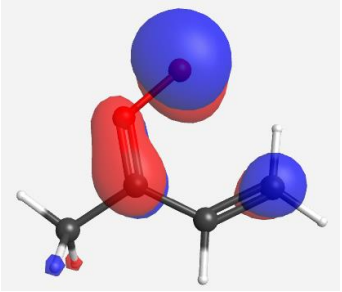
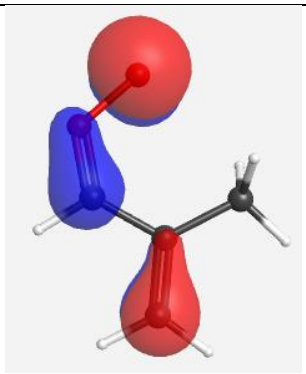
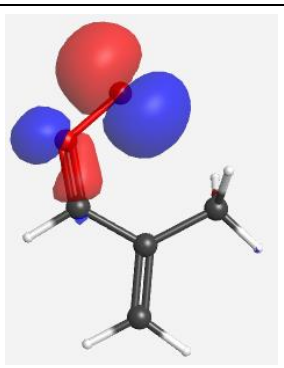
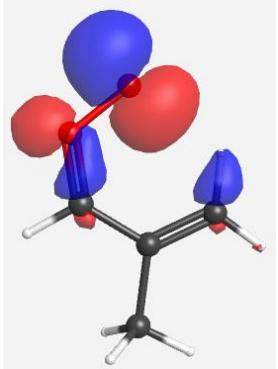
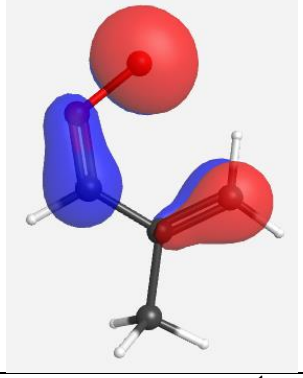
*** The rate constant for the *syn*-CH_3CHOO + MeOH reaction and so the ΔG_{EXP} and Δ_{SENSI} values calculated are simply the lower limit.

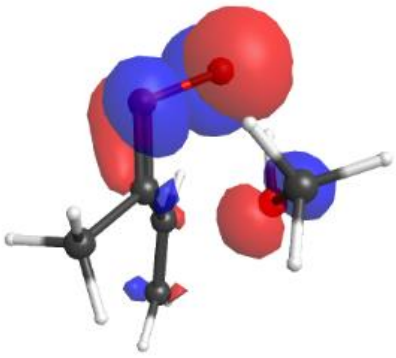
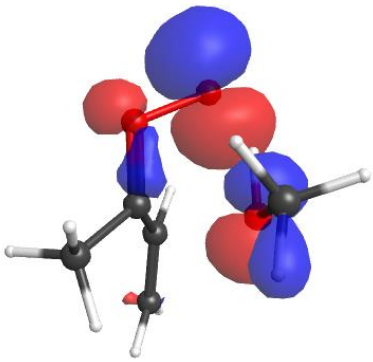
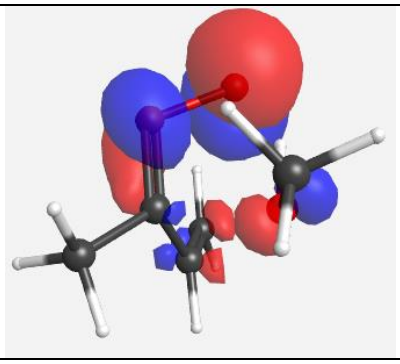
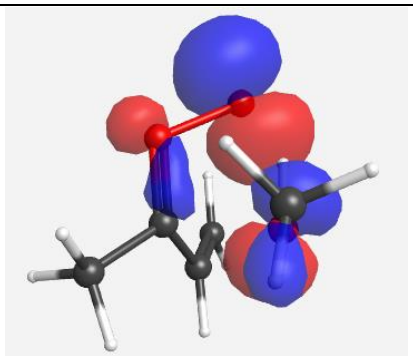
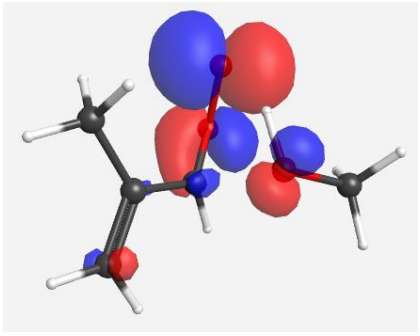
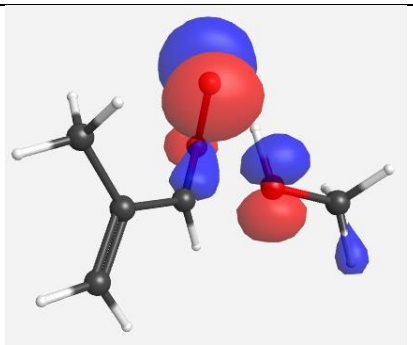
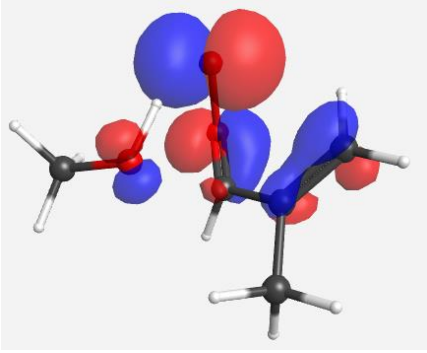
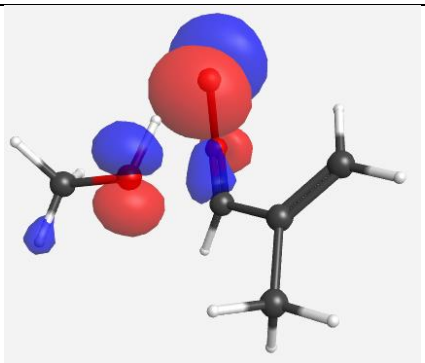
2.5 Molecular Orbital Diagrams of Isoprene derived sCIs

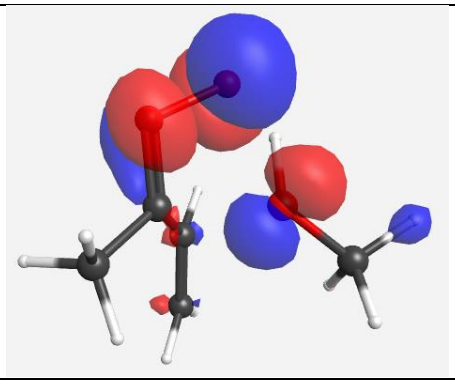
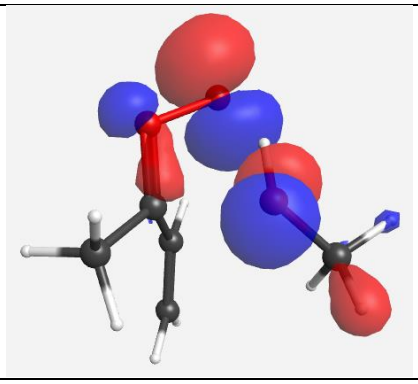
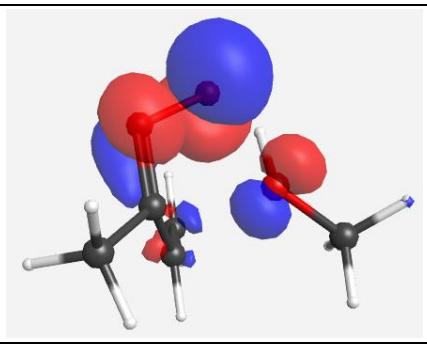
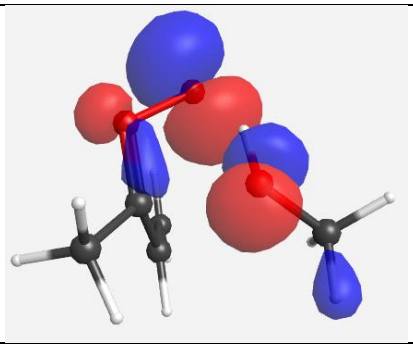
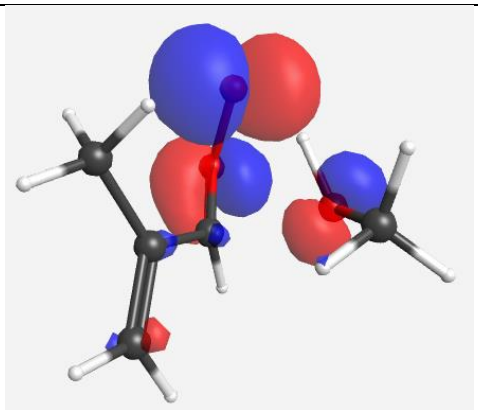
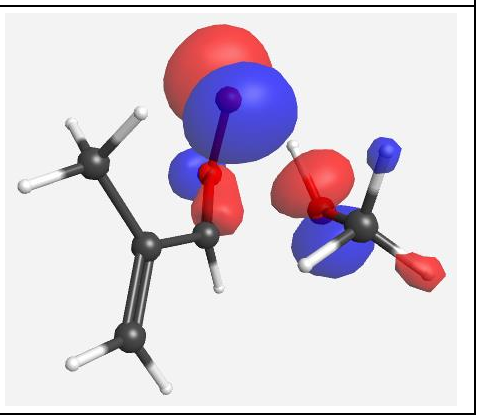
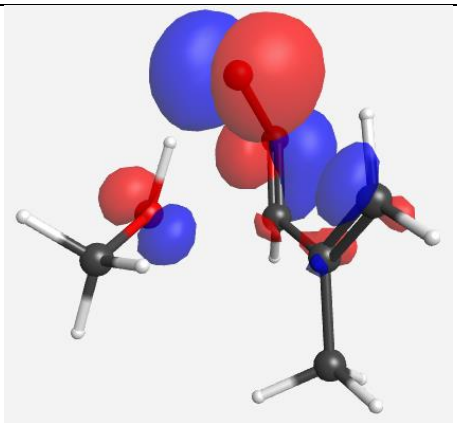
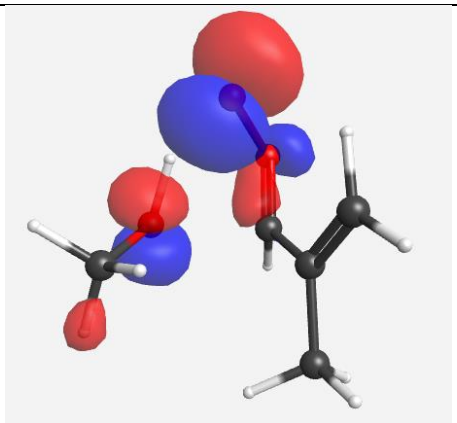
	HOMO	HOMO-1
sCI 13		
	-0.23819 Hartree	**-0.24439** Hartree
sCI 14		
	-0.23585 Hartree	**-0.24256** Hartree
sCI 15		
	-0.23984 Hartree	**-0.24689** Hartree
sCI 16		
	-0.24032 Hartree	**-0.24913** Hartree

	HOMO	HOMO-1
sCI 13 + MeOH TS_{AAAH} 1		
	-0.24096 Hartree	**-0.26026** Hartree
sCI 14 + MeOH TS_{AAAH} 1		
	-0.24024 Hartree	**-0.25866** Hartree
sCI 15 + MeOH TS_{AAAH} 1		
	-0.24679 Hartree	**-0.26300** Hartree
sCI 16 + MeOH TS_{AAAH} 1		
	-0.24381 Hartree	**-0.26076** Hartree

	HOMO	HOMO-1
sCI 13 + MeOH TS_{AAAH} 2		
	-0.24985 Hartree	**-0.25733** Hartree
sCI 14 + MeOH TS_{AAAH} 2		
	-0.23982 Hartree	**-0.25627** Hartree
sCI 15 + MeOH TS_{AAAH} 2		
	-0.24343 Hartree	**-0.25891** Hartree
sCI 16 + MeOH TS_{AAAH} 2		
	-0.24357 Hartree	**-0.25893** Hartree

	HOMO	HOMO-1	ΔE
sCI 17			
	-618.78 kJ mol^{-1}	**-628.78 kJ mol^{-1}**	**10.00 kJ mol^{-1}**
	-0.23568 Hartree	**-0.23949** Hartree	
sCI 18			
	-626.00 kJ mol^{-1}	**-628.96 kJ mol^{-1}**	**-2.96 kJ mol^{-1}**
	-0.23843 Hartree	**-0.23956** Hartree	
sCI 19			
	-629.78 kJ mol^{-1}	**-638.02 kJ mol^{-1}**	**8.24 kJ mol^{-1}**
	-0.23987 Hartree	**-0.24301** Hartree	
sCI 20			
	-647.66 kJ mol^{-1}	**-652.99 kJ mol^{-1}**	**-5.32 kJ mol^{-1}**
	-0.24668 Hartree	**-0.24871** Hartree	

	HOMO	HOMO-1
sCI 17 + MeOH TS_{AAAH} 1		
	-0.24246 Hartree	-0.26110 Hartree
sCI 18 + MeOH TS_{AAAH} 1		
	-0.23474 Hartree	**-0.25497** Hartree
sCI 19 + MeOH TS_{AAAH} 1		
	-0.23866 Hartree	**-0.25886** Hartree
sCI 20 + MeOH TS_{AAAH} 1		
	-0.23385 Hartree	**-0.25563** Hartree

	HOMO	HOMO-1
sCI 17 + MeOH TS_{AAAH} 2		
	-0.24261 Hartree	-0.25960 Hartree
sCI 18 + MeOH TS_{AAAH} 2		
	-0.23535 Hartree	**-0.25483** Hartree
sCI 19 + MeOH TS_{AAAH} 2		
	-0.23966 Hartree	**-0.25907** Hartree
sCI 20 + MeOH TS_{AAAH} 2		
	-0.23719 Hartree	**-0.25806** Hartree

2.6 Barrierless sCI + Alcohol Reactions

MeOH reaction with **sCI 7** (CF_2OO) has a barrierless TS_{AAAH} 1 channel but the TS_{AAAH} 2 channel has a barrier, as seen by the expansion and contraction of the H-O bond (in Figure 9). This does not matter too much as either way the k_{TST} from the TS_{AAAH} 2 pathway (1.96×10^{-8} cm^3 s^{-1}) exceeds both the $k_{d\text{-}d}$ & k_{COLL} values (7.07×10^{-10} & 1.63×10^{-10} cm^3 s^{-1}) confirming for CF_2OO + MeOH section effectively barrierless regardless of the inclusion of the barrierless TS_{AAAH} 1 channel.

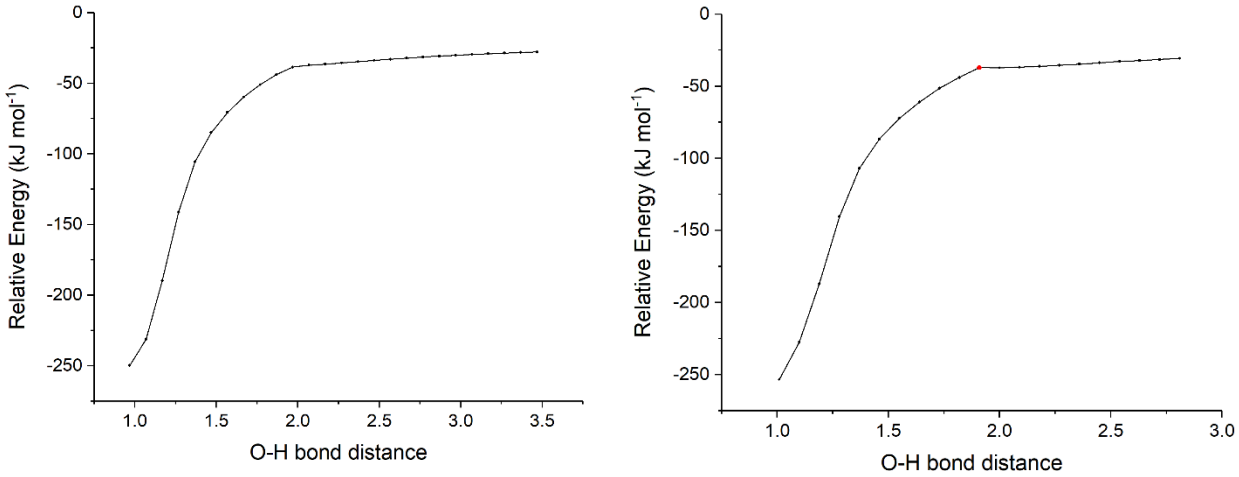


Figure 14: Potential Energy Profile MeOH + CF2OO TS_{AAAH} 1 & 2 (red dot is the TS_{AAAH} 2)

MeOH reaction with **sCI 25** (*syn*-CF_3CFOO) has a barrierless TS_{AAAH} 1 channel too but the TS_{AAAH} 2 channel has a barrier (Figure 10). However, the k_{TST} from the TS_{AAAH} 2 pathway is a lower (3.16×10^{-11} cm^3 s^{-1}) than the $k_{d\text{-}d}$ & k_{COLL} values (5.50×10^{-10} & 1.87×10^{-10} cm^3 s^{-1}).

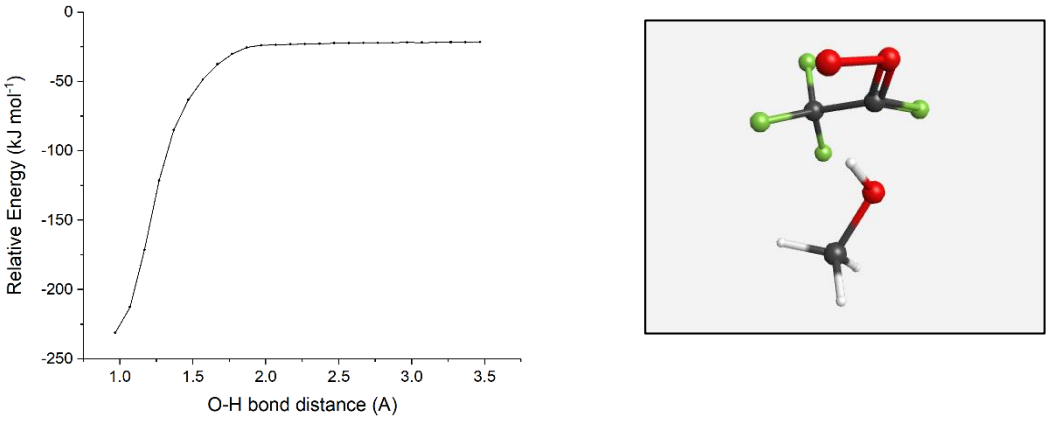


*Figure 15: Energy Profile of **sCI 25** + MeOH TS_{AAAH} 1 Channel (Left) & the TS_{AAAH} 2 structure (right)*

While there is a small risk a **sCI 25** + MeOH TS_{AAAH} 1 barrier may be identified at some point, the lack of this TS_{AAAH} 1 structure on the Channel on the energy profile, means the

author estimates that this is barrierless. Therefore, the $k_{d\text{-}d}$ value is employed as the rate constant of the **sCI 25** + MeOH reaction.

2.7 Concentrations of Atmospheric Species used in this Chapter

Table 72: Co-reactant concentrations used in this Chapter with locations and studies.

Co-reactant	Location	Abundance	Abundance (molec/cm^3)	Study	Ref
MeOH	São Paulo, Brazil	34.1 ppb	8.4×10^{11}	Nguyen *et al.*	[108]
EtOH	São Paulo, Brazil	176.3 ppb	4.3×10^{12}	Nguyen *et al.*	[108]
iPrOH	São Paulo, Brazil	44.2 ppb	1.1×10^{12}	Nguyen *et al.*	[108]
H_2O	São Paulo, Brazil	-	6.2×10^{17}	Bravo *et al.*	[109]
$(H_2O)_2$	São Paulo, Brazil	-	4.0×10^{14}	Bravo *et al.*	[109]
O_3	São Paulo, Brazil	-	7.3×10^{11}	Vereecken *et al.*	[55]
SO_2	São Paulo, Brazil	4.94 ppb	1.2×10^{11}	Bravo *et al.*	[109]
CO	São Paulo, Brazil	2.08	5.1×10^{13}	Bravo *et al.*	[109]
NO_2	São Paulo, Brazil	28.6	1.1×10^{11}	Bravo *et al.*	[109]
CO_2	Global	407.6 ppm	1.0×10^{16}	NASA	[110]
HNO_3	Houston, TX	4.5 ppb	1.1×10^{11}	Leong *et al.*	[111]
HCOOH	Urban		3.1×10^{11}	Lin *et al.*	[112]
CH_3COOH	Urban		3.9×10^{10}	Lin *et al.*	[112]
HCl	S. California	1.3	3.2×10^{10}	Crisp *et al.*	[113]

2.8 Application of Eckart Tunnelling Factors to TS_{VHP} Channels in MeOH + sCI reactions

The impact of κ_{ECKART} functions and the VHP channels change depending on three factors: the size of the TS_{VHP} barriers; the strength of the tunnelling; and the relative reactivity of the AAAH channels. For example, figure below shows that MeOH + **sCI 2** has an energy gap between TS_{VHP} 2 & TS_{AAAH} 1 barrier (16.3 kJ mol^{-1}), which produces a relatively low k_{VHP} ~4.19 × 10^{-20} cm^3 s^{-1}, and without an Eckart factor the Γ_{VHP} is < 0.01. However, the κ_{ECKART} correction of ~ 26 increases the k_{VHP} to 1.09 × 10^{-18} cm^3 s^{-1} and the Γ_{VHP} to a non-negligible ~0.06.

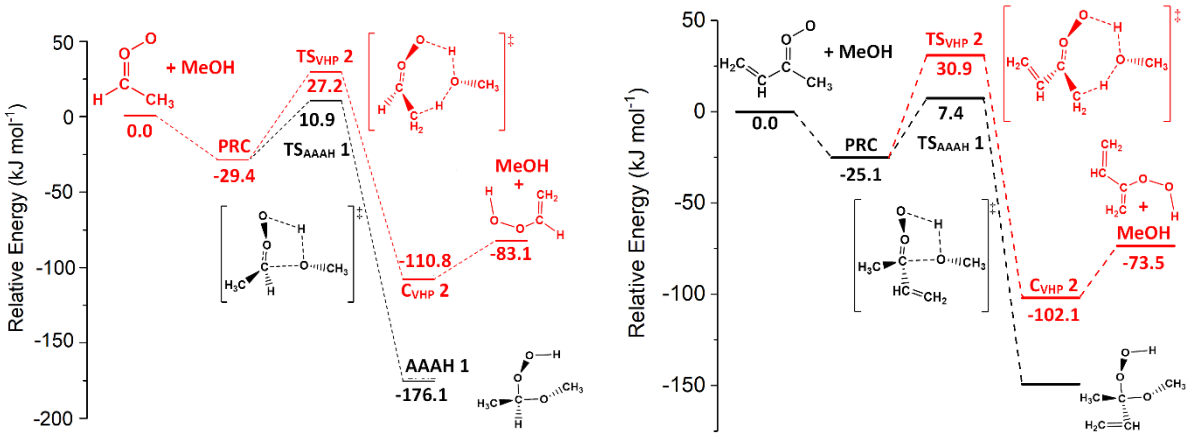


*Figure 4.16: Potential energy surfaces comparing lowest energy TS_{AAAH} and TS_{VHP} pathways for **sCI 2** + MeOH (left) and **sCI 14** + MeOH (right)*

Two of the three factors that contribute to the Γ_{VHP}, the relatively low TS_{VHP} barrier (25.3 kJ mol^{-1}) and a larger κ_{Eckart} contribution (~37), produce a high k_{VHP} for MeOH + **sCI 4** (5.81 × 10^{-18} cm^3 s^{-1}). However, the third factor, the low energy TS_{AAAH} barrier (1.21 kJ mol^{-1}) reduces the Γ_{VHP} to ~0.01. This small contribution of both the overall theoretical κ_{Eckart} values for the main pathway (1.36) and the small Γ_{VHP} is confirmed experimentally. In the study by Orr-Ewing and co-workers referenced earlier, the deuteration of the H atoms in the MeOH + **sCI 4** reaction has very little impact on the overall k_{EXP}.[102] Despite larger κ_{Eckart} corrections (~36.0 — 70.8), MeOH reactions with **sCIs 13** & **14** see similarly small Γ_{VHP} values (~0.01), due to a similarly larger difference (~20 — 23 kJ mol^{-1}) between TS_{AAAH} 1 & TS_{VHP} 2 barriers.

Whilst the Anglada *et* Sole study of sCI + H_2O reactions, do provide greater κ_{Eckart} contributions to the overall reactivity of these sCIs, the main observed change is that these reactions have much larger Γ_{VHP} values, with the Γ_{VHP} for **sCI 2** + H_2O exceeding 0.5.[114] However, throughout theoretical analysis of sCI reactions with both H_2O and $(H_2O)_2$, as well as with MeOH, that the Γ_{VHP} value are dictated mainly by the contribution of the

main reaction, as the k_{VHP} varies very little (~10^{-18} – 10^{-17} cm^3 s^{-1}) compared to the k_{HHP} or k_{AAAH} (~10^{-19} – 10^{-12} cm^3 s^{-1}). Whilst these are important trends, for the purposes of this study, the main contribution of the VHP channel is provided in small but non-negligible yields for side reactions, the biggest of which is for **sCl2** + MeOH with a Γ_{VHP} of 0.06.

3.0 Supplementary Information for Chapter 4: Bimolecular sinks of Criegee intermediates derived from Hydrofluoroolefins

3.1 Rate Constants

3.1.1 Master Equation Rate Constants calculated with MESMER

Rate constants for all non-barrierless reactions over a variety of temperatures:

Table 73: Master Equation rate constants for all non-barrierless reactions between 200—400K

Co-reactant	sCI	Grain size	k_{ME} (cm^3 s^{-1})				
			200 K	275 K	298.15 K	325 K	400 K
HCHO	1	10	2.77E-11	3.48E-12	2.79E-12	2.25E-12	1.40E-12
	2	10	2.02E-12	3.69E-13	2.69E-13	1.98E-13	1.11E-13
	3	10	2.27E-11	3.32E-12	2.49E-12	1.82E-12	8.59E-13
	5	5	4.59E-11	2.12E-11	1.66E-11	1.25E-11	5.86E-12
CF_3CFO	1	10	2.27E-10	2.92E-12	1.98E-12	1.32E-12	5.11E-13
SO_2	2	10	9.81E-12	2.52E-12	1.90E-12	1.41E-12	7.20E-13
HNO_3	1	15	3.89E-04	5.48E-08	8.22E-09	1.21E-09	3.95E-11
	2	15	5.47E-09	5.11E-11	2.06E-11	8.69E-12	1.70E-12
	3	15	1.99E-07	3.03E-10	8.87E-11	3.29E-11	8.53E-12
	4	15	4.03E-05	2.85E-07	9.51E-08	3.07E-08	2.44E-09
	5	15	2.97E-07	8.58E-11	7.57E-11	6.64E-11	4.30E-11
HF	1	10	2.24E-12	4.31E-13	3.32E-13	2.62E-13	1.71E-13
	2	10	2.51E-19	3.63E-18	6.67E-18	1.24E-17	4.79E-17
	3	10	2.44E-15	2.59E-15	2.86E-15	3.23E-15	4.48E-15
	4	10	5.35E-10	2.05E-11	1.19E-11	7.20E-12	2.73E-12
	5	10	2.41E-12	4.90E-13	3.66E-13	2.78E-13	1.64E-13
HCl	1	5	7.60E-08	8.37E-10	4.70E-10	3.21E-10	1.99E-10
	2	5	1.46E-14	3.34E-14	4.04E-14	4.93E-14	7.76E-14
	3	5	4.26E-10	9.05E-11	7.28E-11	5.72E-11	3.23E-11
	4	5	4.18E-10	2.05E-10	1.64E-10	1.28E-10	6.67E-11
	5	5	3.92E-09	1.42E-10	1.13E-10	8.66E-11	4.51E-11
H_2S	1	10	4.04E-15	6.31E-15	7.06E-15	8.00E-15	1.09E-14
	2	10	2.73E-17	1.37E-16	1.96E-16	2.84E-16	6.49E-16
	3	10	4.34E-15	5.36E-15	5.72E-15	6.18E-15	7.67E-15
	4	10	3.02E-12	7.91E-13	6.08E-13	4.74E-13	3.00E-13
	5	10	1.61E-14	1.26E-14	1.23E-14	1.21E-14	1.26E-14
H_2O	1	10	1.35E-17	8.04E-17	1.18E-16	1.73E-16	4.00E-16
	2	10	1.63E-20	6.27E-19	1.35E-18	2.90E-18	1.47E-17
	3	10	1.61E-17	7.99E-17	1.12E-16	1.59E-16	3.37E-16
	4	10	8.71E-11	8.15E-12	5.13E-12	3.23E-12	1.24E-12
	5	10	1.43E-12	3.06E-13	2.27E-13	1.69E-13	9.66E-14
$(H_2O)_2$	1	25	3.18E-09	9.88E-12	3.28E-12	1.22E-12	2.18E-13
	2	25	1.15E-09	7.04E-12	2.71E-12	1.09E-12	1.62E-13
	3	25	5.60E-09	7.50E-12	3.74E-12	1.96E-12	4.00E-13
	4	35	2.71E-06	2.21E-06	1.14E-06	4.91E-07	3.65E-08
	5	45	1.05E-07	8.51E-09	1.46E-09	1.30E-09	1.91E-10
MeOH	1	10	2.65E-14	1.34E-14	1.20E-14	1.09E-14	9.48E-15

	2	10	2.55E-17	7.34E-17	9.43E-17	1.23E-16	2.28E-16
	3	10	1.86E-13	4.32E-14	3.30E-14	2.57E-14	1.62E-14
	4	10	*1.10E-10*	*6.08E-11*	*5.17E-11*	*4.27E-11*	*2.52E-11*
	5	20	6.92E-09	7.91E-11	3.31E-11	1.04E-11	2.22E-12

3.1.2 Canonical Rate Constants calculated with MESMER

Rate constants for all non-barrierless reactions over a variety of temperatures:

*Table 74: Overall Canonical Rate Constants (k_{CAN}) of HCHO + **sCIs 1, 23, 24 & 26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	1.82E-09	9.99E-11	7.83E+10	1.43E+12
	275	5.66E-11	1.00E-10	2.44E+12	1.38E+12
	298	2.83E-11	1.00E-10	4.81E+12	1.36E+12
	325	1.45E-11	1.00E-10	9.29E+12	1.34E+12
	400	3.81E-12	1.00E-10	3.40E+13	1.29E+12
23	200	2.65E-12	1.01E-10	4.56E+10	1.20E+09
	275	4.17E-13	1.01E-10	9.49E+11	3.93E+09
	298	2.94E-13	1.01E-10	1.70E+12	4.98E+09
	325	2.11E-13	1.00E-10	2.99E+12	6.26E+09
	400	1.13E-13	1.00E-10	8.81E+12	9.95E+09
24	200	2.52E-10	1.01E-10	2.19E+10	5.48E+10
	275	1.15E-11	1.01E-10	9.49E+11	1.08E+11
	298	6.24E-12	1.01E-10	2.00E+12	1.24E+11
	325	3.45E-12	1.01E-10	4.11E+12	1.41E+11
	400	1.08E-12	1.00E-10	1.70E+13	1.83E+11
26	200	5.61E-08	1.01E-10	1.02E+09	5.71E+11
	275	5.31E-10	1.00E-10	9.80E+10	5.20E+11
	298	2.10E-10	1.00E-10	2.42E+11	5.07E+11
	325	8.46E-11	1.00E-10	5.83E+11	4.93E+11
	400	1.39E-11	1.00E-10	3.35E+12	4.63E+11

*Table 75: Overall Canonical Rate Constants (k_{CAN}) of CF_3CFO + **sCI 1** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4))*

sCI #	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	1.21E-09	1.01E-10	3.17E+09	3.50E+10	1.01E-10	9.36E+09	8.14E+09
	275	1.82E-11	1.01E-10	4.48E+11	7.03E+10	1.00E-10	1.13E+12	2.68E+10
	298	7.97E-12	1.01E-10	1.20E+12	8.08E+10	1.00E-10	2.92E+12	3.41E+10
	325	3.58E-12	1.01E-10	3.11E+12	9.26E+10	1.00E-10	7.37E+12	4.33E+10
	400	7.42E-13	1.01E-10	2.08E+13	1.22E+11	1.00E-10	4.63E+13	7.04E+10

*Table 76: Overall Canonical Rate Constants (k_{CAN}) of SO_2 + **sCI 23** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4)*

sCI #	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
23	200	7.06E-11	1.01E-10	1.78E+11	3.47E+10	1.01E-10	3.15E+11	1.59E+11
	275	5.20E-12	1.01E-10	3.95E+12	5.90E+10	1.01E-10	4.78E+12	1.76E+11
	298	3.16E-12	1.01E-10	7.18E+12	6.56E+10	1.01E-10	8.03E+12	1.79E+11
	325	1.97E-12	1.01E-10	1.28E+13	7.29E+10	1.00E-10	1.32E+13	1.82E+11
	400	7.94E-13	1.00E-10	3.87E+13	9.04E+10	1.00E-10	3.39E+13	1.89E+11

*Table 77: Overall Canonical Rate Constants (k_{CAN}) of HNO_3 + **sCIs 1, 23—26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	6.58E-03	1.01E-10	6.61E+02	4.30E+10
	275	2.66E-06	1.01E-10	3.96E+06	1.04E+11
	298	5.47E-07	1.01E-10	2.30E+07	1.25E+11
	325	1.15E-07	1.01E-10	1.30E+08	1.49E+11
	400	4.87E-09	1.00E-10	4.44E+09	2.15E+11
23	200	7.22E-09	1.00E-10	1.21E+07	8.73E+08
	275	7.72E-11	1.00E-10	2.52E+09	1.94E+09
	298	3.13E-11	1.00E-10	7.32E+09	2.28E+09
	325	1.29E-11	1.00E-10	2.08E+10	2.68E+09
	400	2.20E-12	1.00E-10	1.68E+11	3.70E+09
24	200	8.68E-07	1.01E-10	9.60E+05	8.29E+09
	275	2.95E-09	1.00E-10	7.70E+08	2.26E+10
	298	9.42E-10	1.00E-10	2.95E+09	2.77E+10
	325	3.08E-10	1.00E-10	1.11E+10	3.40E+10
	400	3.23E-11	1.00E-10	1.59E+11	5.14E+10
25	200	1.27E-01	1.00E-10	2.72E+02	3.45E+11
	275	1.42E-05	1.00E-10	1.91E+06	2.70E+11
	298	2.24E-06	1.00E-10	1.14E+07	2.56E+11
	325	3.63E-07	1.00E-10	6.68E+07	2.42E+11
	400	8.88E-09	1.00E-10	2.42E+09	2.14E+11
26	200	9.93E-03	1.01E-10	5.48E+02	5.39E+10
	275	2.13E-06	1.01E-10	3.72E+06	7.89E+10
	298	3.88E-07	1.01E-10	2.22E+07	8.56E+10
	325	7.25E-08	1.01E-10	1.29E+08	9.28E+10
	400	2.41E-09	1.00E-10	4.59E+09	1.10E+11

*Table 78: Overall Canonical Rate Constants (k_{CAN}) of HF + **sCIs 1, 23—26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	2.26E-12	1.01E-10	2.60E+04	5.81E+02
	275	4.37E-13	1.01E-10	2.29E+07	9.92E+04
	298	3.36E-13	1.01E-10	9.19E+07	3.07E+05
	325	2.65E-13	1.01E-10	3.64E+08	9.57E+05
	400	1.72E-13	1.01E-10	6.15E+09	1.05E+07
23	200	2.51E-19	1.01E-10	6.81E+07	1.70E-01
	275	3.63E-18	1.00E-10	5.17E+09	1.87E+02
	298	6.67E-18	1.00E-10	1.25E+10	8.28E+02
	325	1.24E-17	1.00E-10	2.96E+10	3.67E+03
	400	4.79E-17	1.00E-10	1.72E+11	8.23E+04
24	200	2.44E-15	1.01E-10	1.10E+07	2.67E+02
	275	2.59E-15	1.00E-10	2.07E+09	5.35E+04
	298	2.86E-15	1.00E-10	6.05E+09	1.72E+05
	325	3.23E-15	1.00E-10	1.74E+10	5.62E+05
	400	4.48E-15	1.00E-10	1.52E+11	6.79E+06
25	200	1.05E-09	1.01E-10	3.99E+07	4.17E+08
	275	4.61E-11	1.01E-10	5.39E+09	2.47E+09
	298	2.44E-11	1.01E-10	1.47E+10	3.57E+09
	325	1.31E-11	1.00E-10	3.94E+10	5.13E+09
	400	3.66E-12	1.00E-10	2.96E+11	1.08E+10
26	200	2.42E-12	1.01E-10	1.67E+06	4.02E+04
	275	4.93E-13	1.00E-10	4.61E+08	2.26E+06
	298	3.68E-13	1.00E-10	1.45E+09	5.31E+06
	325	2.79E-13	1.00E-10	4.50E+09	1.25E+07
	400	1.64E-13	1.00E-10	4.53E+10	7.42E+07

*Table 79: Overall Canonical Rate Constants (k_{CAN}) of HCl + **sCIs 1, 23—26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	6.60E-07	1.00E-10	2.16E+08	1.43E+12
	275	8.46E-09	1.00E-10	1.75E+10	1.48E+12
	298	3.48E-09	1.00E-10	4.29E+10	1.49E+12
	325	1.45E-09	1.00E-10	1.04E+11	1.51E+12
	400	2.46E-10	1.00E-10	6.22E+11	1.53E+12
23	200	1.46E-15	1.01E-10	1.28E+10	1.85E+05
	275	3.35E-15	1.01E-10	2.02E+11	6.70E+06
	298	4.05E-15	1.01E-10	3.49E+11	1.40E+07
	325	4.93E-15	1.01E-10	5.96E+11	2.92E+07
	400	7.76E-15	1.00E-10	1.72E+12	1.33E+08
24	200	2.80E-10	1.01E-10	1.62E+10	4.52E+10
	275	2.56E-11	1.00E-10	3.93E+11	1.00E+11
	298	1.59E-11	1.00E-10	7.46E+11	1.18E+11
	325	1.01E-11	1.00E-10	1.40E+12	1.40E+11
	400	4.05E-12	1.00E-10	4.93E+12	1.99E+11
25	200	3.30E-09	1.00E-10	9.27E+08	3.05E+10
	275	1.39E-10	1.00E-10	2.91E+10	4.03E+10
	298	7.32E-11	1.00E-10	5.81E+10	4.24E+10
	325	3.90E-11	1.00E-10	1.14E+11	4.45E+10
	400	1.10E-11	1.00E-10	4.44E+11	4.87E+10
26	200	1.38E-09	1.01E-10	1.18E+09	1.63E+10
	275	6.62E-11	1.00E-10	5.00E+10	3.30E+10
	298	3.64E-11	1.00E-10	1.06E+11	3.85E+10
	325	2.03E-11	1.00E-10	2.22E+11	4.50E+10
	400	6.41E-12	1.00E-10	9.77E+11	6.25E+10

*Table 80: Overall Canonical Rate Constants (k_{CAN}) of H_2S + **sCIs 1, 23—26**: based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	4.04E-15	1.01E-10	4.10E+11	9.05E+06	1.00E-10	4.62E+11	8.34E+06
	275	6.31E-15	1.01E-10	3.66E+12	1.24E+08	1.00E-10	3.99E+12	1.16E+08
	298	7.06E-15	1.01E-10	5.55E+12	2.09E+08	1.00E-10	6.01E+12	1.96E+08
	325	8.00E-15	1.01E-10	8.26E+12	3.51E+08	1.00E-10	8.88E+12	3.30E+08
	400	1.09E-14	1.01E-10	1.75E+13	1.01E+09	1.00E-10	1.86E+13	9.50E+08
2	200	2.73E-17	1.01E-10	5.05E+11	1.01E+05	1.00E-10	8.12E+11	5.66E+04
	275	1.37E-16	1.01E-10	1.67E+12	1.54E+06	1.00E-10	1.94E+12	8.56E+05
	298	1.96E-16	1.01E-10	2.05E+12	2.64E+06	1.00E-10	2.23E+12	1.48E+06
	325	2.84E-16	1.01E-10	2.47E+12	4.50E+06	1.00E-10	2.52E+12	2.52E+06
	400	6.49E-16	1.00E-10	3.35E+12	1.33E+07	1.00E-10	3.00E+12	7.50E+06
3	200	3.01E-10	1.01E-10	5.11E+13	1.52E+14	1.01E-10	1.52E+14	2.04E+09
	275	5.36E-15	1.01E-10	1.09E+14	3.72E+09	1.00E-10	2.42E+14	4.59E+09
	298	5.72E-15	1.01E-10	1.22E+14	4.40E+09	1.00E-10	2.56E+14	5.35E+09
	325	6.18E-15	1.01E-10	1.35E+14	5.18E+09	1.00E-10	2.67E+14	6.17E+09
	400	7.67E-15	1.01E-10	1.54E+14	7.10E+09	1.00E-10	2.69E+14	8.15E+09
4	200	2.99E-12	1.01E-10	7.85E+10	1.84E+09	1.00E-10	7.97E+10	4.96E+08
	275	7.39E-13	1.01E-10	6.78E+11	3.61E+09	1.00E-10	6.36E+11	1.29E+09
	298	5.71E-13	1.00E-10	1.02E+12	4.10E+09	1.00E-10	9.38E+11	1.56E+09
	325	4.49E-13	1.00E-10	1.50E+12	4.63E+09	1.00E-10	1.36E+12	1.87E+09
	400	2.92E-13	1.00E-10	3.07E+12	5.90E+09	1.00E-10	2.69E+12	2.68E+09
5	200	1.60E-14	1.01E-10	3.85E+10	3.70E+06	1.01E-10	3.97E+10	2.49E+06
	275	1.26E-14	1.00E-10	5.76E+11	4.19E+07	1.01E-10	5.97E+11	3.12E+07
	298	1.23E-14	1.00E-10	9.69E+11	6.82E+07	1.01E-10	1.00E+12	5.19E+07
	325	1.21E-14	1.00E-10	1.59E+12	1.10E+08	1.00E-10	1.65E+12	8.55E+07
	400	1.26E-14	1.00E-10	4.13E+12	2.92E+08	1.00E-10	4.29E+12	2.36E+08

*Table 81: Overall Canonical Rate Constants (k_{CAN}) of H_2O + **sCIs 1, 23—26**: based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	1.35E-17	1.00E-10	6.00E+07	7.04E+00	1.00E-10	6.00E+07	1.02E+00
	275	8.04E-17	1.00E-10	3.68E+09	2.38E+03	1.00E-10	3.68E+09	5.69E+02
	298	1.18E-16	1.00E-10	8.39E+09	7.79E+03	1.00E-10	8.39E+09	2.07E+03
	325	1.73E-16	1.00E-10	1.88E+10	2.51E+04	1.00E-10	1.88E+10	7.38E+03
	400	4.00E-16	1.00E-10	9.34E+10	2.73E+05	1.00E-10	9.34E+10	9.98E+04
2	200	1.63E-20	1.00E-10	1.54E+10	6.74E-01	1.00E-10	1.54E+10	1.83E+00
	275	6.27E-19	1.00E-10	1.15E+11	2.24E+02	1.00E-10	1.15E+11	4.98E+02
	298	1.35E-18	1.00E-10	1.69E+11	7.28E+02	1.00E-10	1.69E+11	1.55E+03
	325	2.90E-18	1.00E-10	2.44E+11	2.32E+03	1.00E-10	2.44E+11	4.74E+03
	400	1.47E-17	1.00E-10	4.86E+11	2.49E+04	1.00E-10	4.86E+11	4.65E+04
3	200	1.61E-17	1.01E-10	6.88E+08	9.27E+01	1.01E-10	6.88E+08	1.72E+01
	275	7.99E-17	1.00E-10	2.41E+10	1.52E+04	1.00E-10	2.41E+10	4.05E+03
	298	1.12E-16	1.00E-10	4.89E+10	4.25E+04	1.00E-10	4.89E+10	1.22E+04
	325	1.59E-16	1.00E-10	9.71E+10	1.17E+05	1.00E-10	9.71E+10	3.64E+04
	400	3.37E-16	1.00E-10	3.78E+11	9.31E+05	1.00E-10	3.78E+11	3.37E+05
4	200	1.12E-10	1.01E-10	1.29E+09	5.84E+08	1.01E-10	5.61E+08	3.69E+08
	275	8.88E-12	1.00E-10	4.52E+10	1.63E+09	1.01E-10	2.69E+10	1.40E+09
	298	5.33E-12	1.00E-10	9.11E+10	1.98E+09	1.01E-10	5.80E+10	1.81E+09
	325	3.23E-12	1.00E-10	1.80E+11	2.38E+09	1.01E-10	1.22E+11	2.31E+09
	400	1.19E-12	1.00E-10	6.89E+11	3.38E+09	1.01E-10	5.35E+11	3.71E+09
5	200	1.45E-12	1.01E-10	2.69E+08	1.25E+06	1.01E-10	2.69E+08	2.64E+06
	275	3.10E-13	1.00E-10	2.09E+10	2.46E+07	1.00E-10	2.09E+10	3.98E+07
	298	2.28E-13	1.00E-10	4.96E+10	4.46E+07	1.00E-10	4.96E+10	6.84E+07
	325	1.70E-13	1.00E-10	1.15E+11	7.99E+07	1.00E-10	1.15E+11	1.16E+08
	400	9.68E-14	1.00E-10	6.20E+11	2.60E+08	1.00E-10	6.20E+11	3.39E+08

*Table 82: Overall Canonical Rate Constants (k_{CAN}) of $(H_2O)_2$ + **sCIs 1, 23—26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	8.04E-09	1.01E-10	1.01E+07	1.99E+08	1.01E-10	7.06E+06	1.47E+07
			1.01E-10	5.45E+06	1.62E+08	1.01E-10	9.74E+06	2.71E+08
	275	4.28E-11	1.01E-10	8.14E+09	9.31E+08	1.01E-10	5.92E+09	1.25E+08
			1.01E-10	6.10E+09	8.84E+08	1.01E-10	9.04E+09	1.30E+09
	298	1.44E-11	1.00E-10	3.19E+10	1.24E+09	1.01E-10	2.33E+10	1.88E+08
			1.01E-10	2.56E+10	1.22E+09	1.01E-10	3.65E+10	1.75E+09
	325	4.85E-12	1.00E-10	1.23E+11	1.64E+09	1.01E-10	9.00E+10	2.79E+08
			1.01E-10	1.05E+11	1.66E+09	1.01E-10	1.45E+11	2.32E+09
	400	5.09E-13	1.00E-10	1.92E+12	2.75E+09	1.01E-10	1.41E+12	5.98E+08
			1.01E-10	1.89E+12	2.99E+09	1.00E-10	2.41E+12	3.96E+09
2	200	1.57E-09	1.01E-10	5.04E+07	2.28E+08	1.01E-10	4.92E+07	2.13E+07
			1.01E-10	1.52E+07	8.51E+07	1.01E-10	4.44E+07	2.24E+08
	275	1.01E-11	1.01E-10	3.58E+10	1.09E+09	1.00E-10	4.04E+10	2.22E+08
			1.01E-10	1.53E+10	5.13E+08	1.00E-10	3.58E+10	1.12E+09
	298	3.57E-12	1.00E-10	1.36E+11	1.46E+09	1.00E-10	1.59E+11	3.51E+08
			1.01E-10	6.24E+10	7.25E+08	1.00E-10	1.39E+11	1.52E+09
	325	1.26E-12	1.00E-10	5.05E+11	1.94E+09	1.00E-10	6.10E+11	5.48E+08
			1.00E-10	2.51E+11	1.01E+09	1.00E-10	5.33E+11	2.03E+09
	400	1.48E-13	1.00E-10	7.31E+12	3.30E+09	1.00E-10	9.49E+12	1.31E+09
			1.00E-10	4.27E+12	1.94E+09	1.00E-10	8.18E+12	3.55E+09
3	200	5.86E-08	1.01E-10	2.86E+08	7.70E+09	1.01E-10	2.59E+08	8.47E+10
			1.01E-10	1.69E+08	1.55E+10	1.01E-10	1.58E+08	2.14E+10
	275	1.33E-10	1.01E-10	1.32E+11	1.32E+10	1.01E-10	1.53E+11	9.42E+10
			1.01E-10	8.35E+10	2.19E+10	1.01E-10	8.85E+10	3.05E+10
	298	3.78E-11	1.01E-10	4.58E+11	1.44E+10	1.01E-10	5.63E+11	9.40E+10
			1.00E-10	2.96E+11	2.29E+10	1.01E-10	3.21E+11	3.21E+10
	325	1.08E-11	1.00E-10	1.57E+12	1.54E+10	1.01E-10	2.03E+12	9.29E+10
			1.00E-10	1.03E+12	2.36E+10	1.01E-10	1.15E+12	3.33E+10
	400	8.15E-13	1.00E-10	1.90E+13	1.70E+10	1.00E-10	2.79E+13	8.70E+10
			1.00E-10	1.30E+13	2.42E+10	1.00E-10	1.53E+13	3.44E+10
4	200	2.87E-01	1.00E-10	1.14E+04	2.95E+12	1.01E-10	5.96E+03	8.52E+12
			1.00E-10	2.78E+04	9.32E+12	1.00E-10	2.01E+04	1.66E+13
	275	1.04E-05	1.00E-10	1.26E+08	1.61E+12	1.00E-10	8.93E+07	3.99E+12
			1.00E-10	2.77E+08	4.25E+12	1.00E-10	2.31E+08	7.07E+12
	298	1.25E-06	1.00E-10	8.51E+08	1.39E+12	1.00E-10	6.41E+08	3.34E+12
			1.00E-10	1.83E+09	3.54E+12	1.00E-10	1.57E+09	5.81E+12
	325	1.53E-07	1.00E-10	5.62E+09	1.19E+12	1.00E-10	4.52E+09	2.78E+12
			1.00E-10	1.18E+10	2.93E+12	1.00E-10	1.05E+10	4.75E+12
	400	1.99E-09	1.00E-10	2.69E+11	8.39E+11	1.00E-10	2.49E+11	1.85E+12
			1.00E-10	5.47E+11	1.93E+12	1.00E-10	5.23E+11	3.05E+12
5	200	5.33E-03	1.01E-10	2.26E+04	1.59E+11	1.01E-10	1.04E+04	4.16E+11
			1.01E-10	2.17E+04	9.18E+10	1.01E-10	2.74E+04	4.16E+10
	275	4.80E-07	1.00E-10	1.69E+08	1.47E+11	1.01E-10	1.12E+08	3.39E+11
			1.01E-10	1.53E+08	9.17E+10	1.01E-10	1.60E+08	4.41E+10
	298	7.07E-08	1.00E-10	1.04E+09	1.41E+11	1.01E-10	7.48E+08	3.18E+11
			1.01E-10	9.33E+08	8.96E+10	1.01E-10	9.39E+08	4.35E+10
	325	1.06E-08	1.00E-10	6.31E+09	1.35E+11	1.01E-10	4.89E+09	2.96E+11
			1.01E-10	5.58E+09	8.66E+10	1.00E-10	5.40E+09	4.25E+10
	400	2.12E-10	1.00E-10	2.49E+11	1.17E+11	1.00E-10	2.29E+11	2.48E+11
			1.00E-10	2.16E+11	7.77E+10	1.00E-10	1.93E+11	3.88E+10

*Table 83: Overall Canonical Rate Constants (k_{CAN}) of MeOH + **sCIs 1, 23—26** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2 , k_3, k_{-3}, and k_4).*
*Note: **sCI 4** + MeOH has one barrierless step and one with a barrier so the dipole-dipole capture rate constant is used.*

sCI#	T (K)	k_{CAN} ($cm^3\ s^{-1}$)	k_1 ($cm^3\ s^{-1}$)	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 ($cm^3\ s^{-1}$)	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	2.65E-14	1.01E-10	2.89E+08	6.86E+04	1.01E-10	2.89E+08	7.70E+03
	275	1.34E-14	1.00E-10	2.21E+10	2.43E+06	1.00E-10	2.21E+10	5.23E+05
	298	1.20E-14	1.00E-10	5.21E+10	5.01E+06	1.00E-10	5.21E+10	1.24E+06
	325	1.09E-14	1.00E-10	1.21E+11	1.02E+07	1.00E-10	1.21E+11	2.89E+06
	400	9.48E-15	1.00E-10	6.41E+11	4.41E+07	1.00E-10	6.41E+11	1.64E+07
2	200	**2.55E-17**	1.01E-10	2.80E+10	6.90E+03	1.01E-10	2.80E+10	1.90E+02
	275	7.34E-17	1.01E-10	2.34E+11	1.59E+05	1.01E-10	2.34E+11	1.10E+04
	298	9.43E-17	1.01E-10	3.49E+11	3.02E+05	1.01E-10	3.49E+11	2.52E+04
	325	1.23E-16	1.01E-10	5.10E+11	5.67E+05	1.01E-10	5.10E+11	5.71E+04
	400	2.28E-16	1.00E-10	1.04E+12	2.06E+06	1.00E-10	1.04E+12	3.06E+05
3	200	**1.87E-13**	1.01E-10	2.70E+09	4.53E+06	1.01E-10	2.70E+09	4.97E+05
	275	4.34E-14	1.00E-10	1.30E+11	4.62E+07	1.00E-10	1.30E+11	1.00E+07
	298	3.31E-14	1.00E-10	2.80E+11	7.38E+07	1.00E-10	2.80E+11	1.85E+07
	325	2.57E-14	1.00E-10	5.88E+11	1.17E+08	1.00E-10	5.88E+11	3.37E+07
	400	1.62E-14	1.00E-10	2.55E+12	2.98E+08	1.00E-10	2.55E+12	1.15E+08
4	200	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	2.33E+08	1.41E+10
	275	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	2.32E+10	1.76E+10
	298	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	5.79E+10	1.82E+10
	325	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	1.41E+11	1.88E+10
	400	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	8.27E+11	1.98E+10
5	200	6.33E-09	1.01E-10	2.09E+08	5.93E+09	1.01E-10	1.20E+08	4.14E+09
	275	9.09E-11	1.00E-10	2.25E+10	9.23E+09	1.01E-10	1.53E+10	7.52E+09
	298	4.65E-11	1.00E-10	3.99E+10	1.00E+10	1.01E-10	3.99E+10	8.43E+09
	325	1.71E-11	1.00E-10	1.40E+11	1.09E+10	1.01E-10	1.02E+11	9.43E+09
	400	3.29E-12	1.00E-10	8.47E+11	1.26E+10	1.00E-10	6.59E+11	1.17E+10

3.1.3 MESMER Calculations of Non-standard Conditions

To validate the results in this thesis comparative calculations of the reactions of sCI + various co-reactant are undertaken here on non-standard conditions, to compare to already existing literature theoretical or experimental results of the same reaction:

*Table 84: **sCI 1** + co-reactants under experimental conditions, atmospheric pressure and temperature applied to MESMER method. Note: **sCI 25** + HCHO; **sCI 1** + CF_3CFO; **sCIs 1**, **24**, **25** and **26** with SO_2; and **sCIs 1, 23—26** with TFA are barrierless reactions (see IRCs in section S7) and so are not included in Table. The **sCI 25** + MeOH rate constant is only for TS2 as TS1 is barrierless.*

Reaction	p (Torr)	T (K)	Grain size	k_{CAN} ($cm^3\ s^{-1}$)				k_{ME}
				k_1	k_{-1}	k_2	k_{TS}	
				$cm^3\ s^{-1}$	s^{-1}	s^{-1}	$cm^3\ s^{-1}$	
sCI 1 + HNO_3	27	295	10	1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	31	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	35	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	760	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	1.04E-08
sCI 1 + H_2O	50	293	10	1.00E-10	7.10E+09	6.12E+03	8.64E-17	1.09E-16
				1.00E-10	7.10E+09	1.59E+03	2.24E-17	
	760	297	10	1.00E-10	8.12E+09	7.43E+03	9.17E-17	1.16E-16
				1.00E-10	8.12E+09	1.96E+03	2.42E-17	
sCI 1 + H_2S	100	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	250	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	500	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	100	278	10	1.01E-10	3.88E+12	1.33E+08	3.45E-15	6.40E-15
				1.00E-10	4.23E+12	1.24E+08	2.95E-15	
	100	318	10	1.01E-10	7.51E+12	3.10E+08	4.15E-15	7.75E-15
				1.00E-10	8.09E+12	2.91E+08	3.60E-15	
sCI 1 + MeOH	90	295	10	1.00E-10	4.70E+10	4.59E+06	9.81E-15	1.03E-13
				1.00E-10	4.70E+10	1.11E+06	2.38E-15	
	10	254.5	10	1.00E-10	8.86E+09	1.14E+06	1.29E-14	1.15E-12
				1.00E-10	8.86E+09	2.12E+05	2.41E-15	
	100	262.1	10	1.00E-10	1.27E+10	1.53E+06	1.21E-14	1.10E-13
				1.00E-10	1.27E+10	3.02E+05	2.40E-15	
	10	292.6	10	1.00E-10	4.32E+10	4.27E+06	9.94E-15	9.29E-13
				1.00E-10	4.32E+10	1.02E+06	2.38E-15	
	10	327.8	10	1.00E-10	1.30E+11	1.10E+07	8.43E-15	8.20E-13
				1.00E-10	1.30E+11	3.13E+06	2.41E-15	
sCI 1 + HCl	27	295	5	1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	31	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	35	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	760	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	4.98E-10

3.1.4 Conditions of MESMER Calculations

Table 85: The conditions applied to each reaction system calculated using MESMER: Including the grain sizes used for calculations; Transition States that do not apply an Eckart function; Reaction channels without TS minima referred to as "Barrierless"; and the Temperatures and Pressures applied to each system.

Reaction system	**Grain size** to determine k_{ME}	TSs without Eckart Functions	Barrierless channels and their $k_{d\text{-}d}$ value	**Grainsize** to determine Γ_{THEO}	**Temperatures (K) and Pressures (Torr)**
sCI 1 + HCHO	grainsize 10	N/A	N/A	grainsize 15	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 23 & **24** + HCHO, and **sCI 1** + CF_3CHO	grainsize 10 (grainsize 5 **sCI 24** + HCHO)	N/A	**sCI 1** + CF_3CHO TSc 1 & 2 ($k_{d\text{-}d}$ ~ 6.50×10^{-10} cm^3 s^{-1})	grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 25 & **26** + HCHO, and **sCI 1** + CF_3CFO	**sCI 26** + HCHO – grainsize 5 **sCI 1** + CF_3CFO – grainsize 10	**sCI 26** + HCHO TSc	**sCI 25** + HCHO TSc ($k_{d\text{-}d}$ ~ 7.20×10^{-10} cm^3 s^{-1})	grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + SO_2	N/A	N/A	**sCI 1** + SO_2 ($k_{d\text{-}d}$ ~ 7.25×10^{-10} cm^3 s^{-1})	grainsize 20	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 23 & **24** + SO_2	grainsize 10	**sCI 2** + SO_2	**sCI 24** + SO_2 ($k_{d\text{-}d}$ ~4.08×10^{-10} cm^3 s^{-1})	**sCI 2** + SO_2: grainsize 50 **sCI 3** + SO_2: grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 25 & **26** + SO_2	N/A	N/A	**sCIs 25** & **26** + SO_2 ($k_{d\text{-}d}$ ~ 4.51 & 4.42×10^{-10} cm^3 s^{-1})	grainsize 50	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + TFA	N/A	N/A	**sCI 1** + TFA TS ($k_{d\text{-}d}$ ~7.54×10^{-10} cm^3 s^{-1})	N/A	-295 K Pressures: 27, 31, 35 & 760 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + TFA	N/A	N/A	**sCI 23** + TFA TS ($k_{d\text{-}d}$ ~4.96×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K

sCI 24 + TFA	N/A	N/A	**sCI 24** + TFA TS ($k_{d\text{-}d}$ ~3.98×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + TFA	N/A	N/A	**sCI 25** + TFA TS ($k_{d\text{-}d}$ ~4.35×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + TFA	N/A	N/A	**sCI 26** + TFA TS ($k_{d\text{-}d}$ ~4.27×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + H_2O	grainsize 10	N/A	N/A	N/A	-At 293 K & 50 Torr; 297 K & 760 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + $(H_2O)_2$	grainsize 25	**sCI 25** + $(H_2O)_2$ $TS(H_2O)_2$ 1, 2, 3 & 4	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + MeOH	grainsize 10	N/A	N/A	N/A	-At 295 K & 90 Torr; 262.1 K & 100 Torr -At 10 Torr: 254.5, 292.6 & 327.8 K -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + MeOH	grainsize 15	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + MeOH	grainsize 15	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + MeOH	grainsize 25	N/A	**sCI 25** + MeOH $TS_{AAAH}1$ ($k_{d\text{-}d}$ ~ 5.50×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + MeOH	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + H_2S	grainsize 10	N/A	N/A	N/A	-At 100 Torr: 278, 299 & 318 K -At 299 K & 250 Torr; 299 K & 500 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HCl	grainsize 25	N/A	N/A	N/A	-At 295 K with 27, 31 & 35 Torr

					-At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 23 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 24 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 25 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 26 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K

3.1.5 Conventional Transition State Rate Constants

*Table 86: Breakdown of rate constant (k_{TST}) of sCI + atmospheric co-reactant using: equilibrium rate constant (K_{eq}); **Wignar** tunneling constant (k_{Wignar}); unimolecular rate constant (k_2); individual rate constant of transition state (k_{TS}); pathway breakdown (**Γ**); total rate constant (k_{total});*
*Note: **sCI 25** + HCHO; **sCI 1** + CF_3CFO; **sCIs 1**, **24**, **25** & **26** with SO_2; and **sCIs 1, 23-26** with TFA are barrierless reactions (see IRCs in section S7) and so are not included in Table X. The **sCI 25** + MeOH rate constant is only for TS2 as TS1 is barrierless.*

Co-reactant	CI	#TS	K_{eq}	k_{Wignar}	k_2	k_{TS}	**Γ**	k_{total}
			cm^3		s^{-1}	$cm^3\ s^{-1}$		$cm^3\ s^{-1}$
HCHO	1	TS_C	2.08E-23	1.01	1.37E+12	2.88E-11	1.00	2.88E-11
	2	TS_C	5.86E-23	1.00	5.00E+9	2.93E-13	1.00	2.93E-13
	3	TS_C	5.20E-23	1.00	1.21E+11	6.28E-12	1.00	6.28E-12
	5	TS_C	4.03E-22	1.00	5.15E+11	2.08E-10	1.00	2.08E-10
CF_3CFO	1	TS_{CYC} 1	5.73E-23	1.01	1.15E+11	6.69E-12	1.00	7.86E-12
		TS_{CYC} 2	4.95E-23	1.03	2.29E+10	1.17E-12	1.00	
SO_2	2	TS_{ENDO}	1.37E-23	1.00	6.73E+10	9.21E-13	1.00	3.21E-12
		TS_{EXO}	1.28E-23	1.00	1.79E+11	2.29E-12	1.00	
HNO_3	1	TS	4.30E-18	1.06	1.19E+11	5.40E-07	1.00	5.40E-7
	2	TS	1.42E-20	1.04	2.13E+9	3.15E-11	1.00	3.15E-11
	3	TS	3.32E-20	1.07	2.60E+10	9.19E-10	1.00	9.19E-10
	4	TS	8.73E-18	1.00	2.56E+11	2.24E-6	1.00	2.24E-6
	5	TS	4.41E-18	1.11	7.72E+10	3.79E-7	1.00	3.79E-7
HCl	1	TS	2.21E-21	1.01	1.66E+12	3.69E-9	1.00	3.69E-9
	2	TS	2.21E-21	1.00	6.34E+11	4.19E-15	1.00	4.19E-15
	3	TS	1.80E-21	1.13	2.05E+6	1.63E-11	1.00	1.63E-11
	4	TS	1.34E-22	1.17	1.04E+11	7.37E-11	1.00	7.37E-11
	5	TS	1.70E-21	1.01	4.31E+10	3.59E-11	1.00	3.59E-11
HF	1	TS	1.12E-18	1.67	1.46E+5	5.47E-13	1.00	5.47E-13
	2	TS	8.44E-21	1.54	4.51E+2	1.17E-17	1.00	1.17E-17
	3	TS	1.74E-20	1.70	7.82E+4	4.63E-15	1.00	4.63E-15
	4	TS	2.18E-19	1.14	1.02E+8	5.09E-11	1.00	5.09E-11
	5	TS	6.99E-20	1.43	3.38E+6	6.76E-13	1.00	6.76E-13
MeOH	1	$TS_{AAAH}1$	1.94E-21	1.09	4.51E+6	1.90E-14	0.80	1.19E-14
		$TS_{AAAH}2$	1.94E-21	1.10	1.11E+6	4.72E-15	0.20	
	2	$TS_{AAAH}1$	2.96E-22	1.06	2.79E+5	1.75E-16	0.92	9.47E-17
		$TS_{AAAH}2$	2.96E-22	1.07	2.30E+4	1.47E-17	0.08	
	3	$TS_{AAAH}1$	3.55E-22	1.06	7.11E+7	5.34E-14	0.80	3.34E-14
		$TS_{AAAH}2$	3.55E-22	1.05	1.78E+7	1.33E-14	0.20	
	4	$TS_{AAAH}1$	$>>k_{d\text{-}d}$	N/A	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$
		$TS_{AAAH}2$	1.79E-21	1.02	1.74E+10	6.33E-11	1.00	
	5	$TS_{AAAH}1$	1.72E-21	1.04	9.86E+9	3.53E-11	0.46	3.88E-11
		$TS_{AAAH}2$	2.50E-21	1.04	8.14E+9	4.22E-11	0.54	

*Table 87: Breakdown of rate constant (k_{TST}) of sCI + atmospheric co-reactant using: equilibrium rate constant (K_{eq}); **Wignar** tunneling constant (κ_{Wignar}); unimolecular rate constant (k_2); individual rate constant of transition state (k_{TS}); pathway breakdown (**Γ**); total rate constant (k_{total});*

Co-reactant	CI	#TS	K_{eq}	K_{Wignar}	k_2	k_{TS}	Γ	k_{total}
			cm^3		cm^3	$cm^3\ s^{-1}$		$cm^3\ s^{-1}$
H_2S	1	TS1	1.81E-23	1.08	1.95E+8	3.80E-15	0.54	1.41E-15
		TS2	1.68E-23	1.08	1.79E+8	3.25E-15	0.46	
	2	TS1	5.14E-23	1.03	2.48E+6	1.32E-16	0.66	3.98E-16
		TS2	4.80E-23	1.04	1.35E+6	6.75E-17	0.34	
	3	TS1	8.63E-25	1.04	4.11E+9	3.70E-15	0.63	1.17E-14
		TS2	4.08E-25	1.05	5.01E+9	2.14E-15	0.37	
	4	TS1	1.01E-22	1.01	4.03E+9	4.09E-13	0.71	5.75E-13
		TS2	1.06E-22	1.01	1.55E+9	1.65E-13	0.29	
	5	TS1	1.03E-22	1.04	6.59E+7	7.11E-15	0.58	2.47E-14
		TS2	1.02E-22	1.04	4.91E+7	5.23E-15	0.42	
H_2O	1	TSH_2O 1	1.22E-20	1.18	6.40E+3	1.85E-16	0.79	1.17E-16
		TSH_2O 2	1.22E-20	1.20	1.67E+3	4.89E-17	0.21	
	2	TSH_2O 1	6.07E-22	1.11	6.55E+2	4.41E-19	0.32	1.38E-18
		TSH_2O 2	6.07E-22	1.12	1.38E+3	9.40E-19	0.68	
	3	TSH_2O 1	2.07E-21	1.11	3.82E+4	8.82E-17	0.78	1.14E-16
		TSH_2O 2	2.07E-21	1.13	1.09E+4	2.54E-17	0.22	
	4	TSH_2O 1	1.12E-21	1.03	1.94E+9	2.23E-12	0.42	5.37E-12
		TSH_2O 2	1.74E-21	1.05	1.72E+9	3.13E-12	0.58	
	5	TSH_2O 1	2.06E-21	1.08	4.09E+7	9.11E-14	0.40	2.30E-13
		TSH_2O 2	2.06E-21	1.08	6.24E+7	1.39E-13	0.60	
$(H_2O)_2$	1	$TS(H_2O)_2$ 1	3.13E-21	1.11	1.12E+9	3.87E-12	0.27	1.41E-11
		$TS(H_2O)_2$ 2	4.28E-21	1.15	1.60E+8	7.87E-13	0.06	
		$TS(H_2O)_2$ 3	3.86E-21	1.12	1.08E+9	4.68E-12	0.33	
		$TS(H_2O)_2$ 4	2.71E-21	1.10	1.60E+9	4.78E-12	0.34	
	2	$TS(H_2O)_2$ 1	1.21E-22	1.08	3.65E+9	4.79E-13	0.20	2.41E-12
		$TS(H_2O)_2$ 2	1.17E-22	1.07	1.10E+10	1.38E-12	0.57	
		$TS(H_2O)_2$ 3	4.99E-23	1.06	2.62E+9	1.39E-13	0.06	
		$TS(H_2O)_2$ 4	5.39E-23	1.06	7.17E+9	4.09E-13	0.17	
	3	$TS(H_2O)_2$ 1	2.20E-22	1.07	1.35E+10	3.17E-12	0.08	3.84E-11
		$TS(H_2O)_2$ 2	1.83E-22	1.05	8.91E+10	1.72E-11	0.45	
		$TS(H_2O)_2$ 3	3.47E-22	1.05	2.18E+10	7.95E-12	0.21	
		$TS(H_2O)_2$ 4	3.17E-22	1.05	3.01E+10	1.00E-11	0.26	
	4	$TS(H_2O)_2$ 1	1.16E-19	1.04	1.58E+12	1.90E-7	0.14	1.36E-06
		$TS(H_2O)_2$ 2	1.53E-19	1.03	3.35E+12	5.28E-7	0.39	
		$TS(H_2O)_2$ 3	5.45E-20	1.02	3.96E+12	2.21E-7	0.16	
		$TS(H_2O)_2$ 4	6.28E-20	1.02	6.59E+12	4.21E-7	0.31	
	5	$TS(H_2O)_2$ 1	9.31E-20	1.05	1.39E+11	1.36E-8	0.19	7.22E-08
		$TS(H_2O)_2$ 2	1.32E-19	1.05	3.21E+11	4.44E-8	0.61	
		$TS(H_2O)_2$ 3	1.06E-19	1.06	8.56E+10	9.60E-9	0.13	
		$TS(H_2O)_2$ 4	1.00E-19	1.07	4.35E+10	4.68E-9	0.06	

3.2 MESMER Calculations of Product Branching Fractions

3.2.1 Potential Energy Surfaces of Complex Systems

The HFO-sCI (**sCIs 1, 23—26)** reactions of sCI with HCHO & SO_2 have lots of similar transition states and mainly only the lowest energy pathways are given in the main body of the text. The diagrams of the full potential energy surfaces are below.

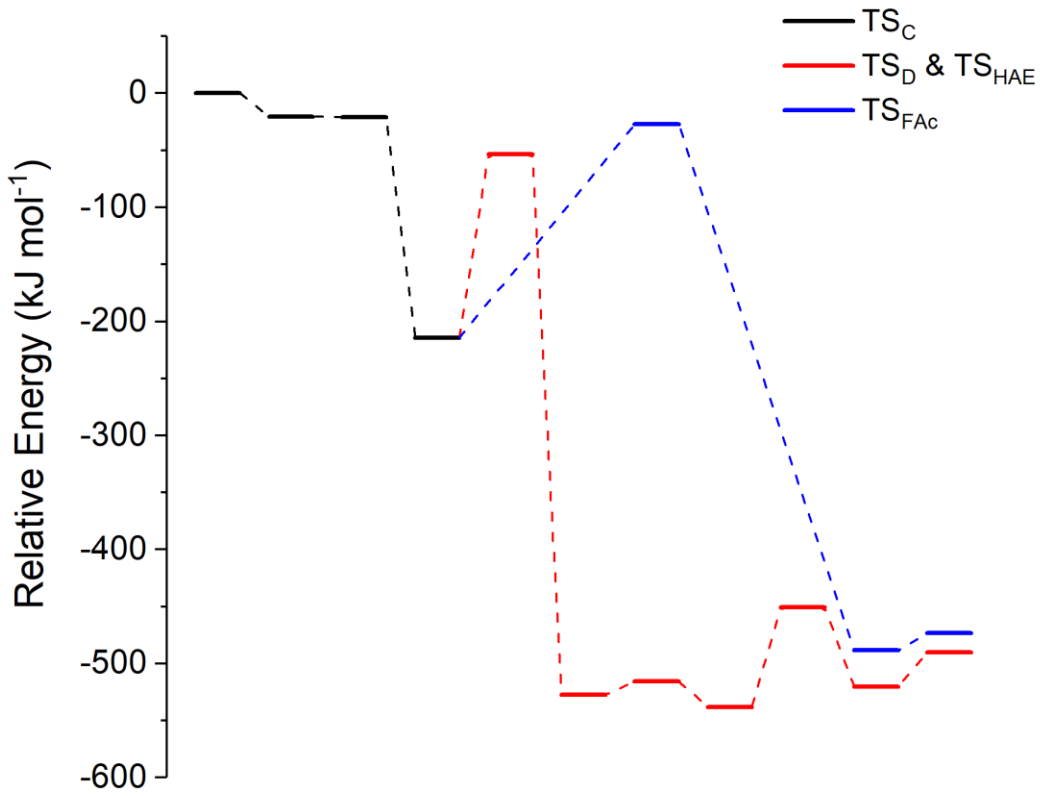


Figure 17: sCI1 + HCHO full PES with labels of channels in legend

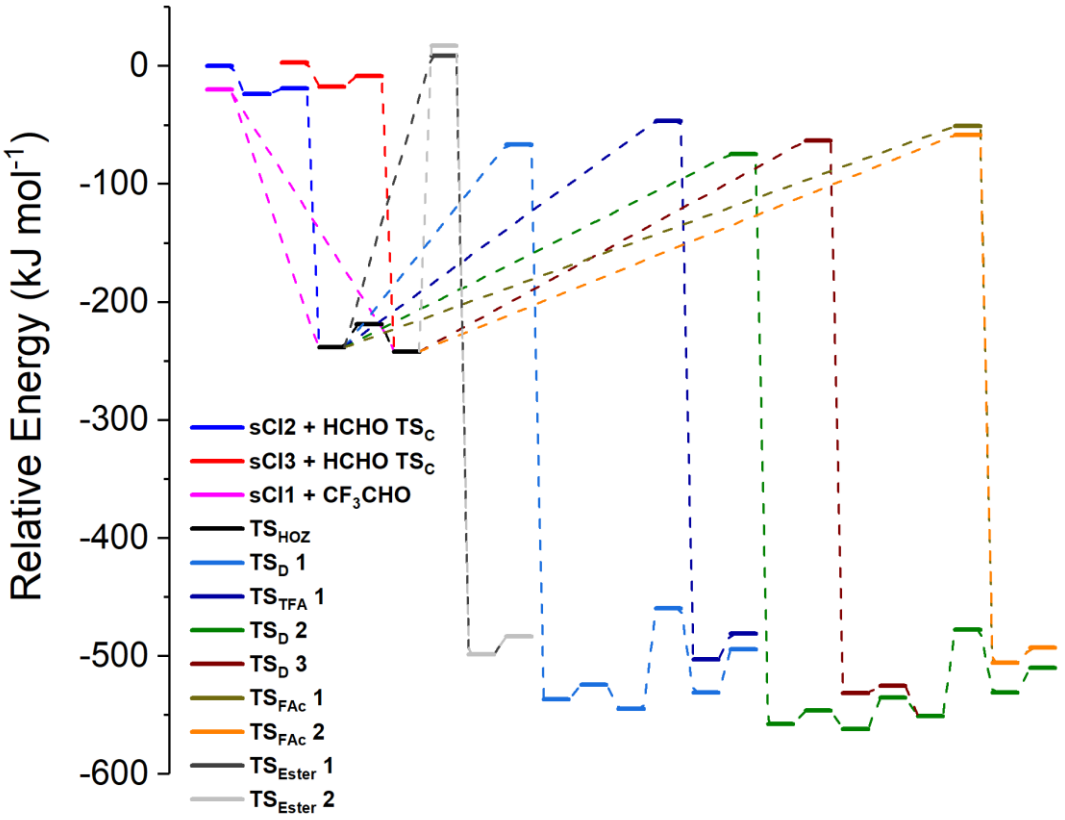


*Figure 18: PES which including reactions HCHO + **sCIs 23** & **24** & sCI1 + CF_3CHO*

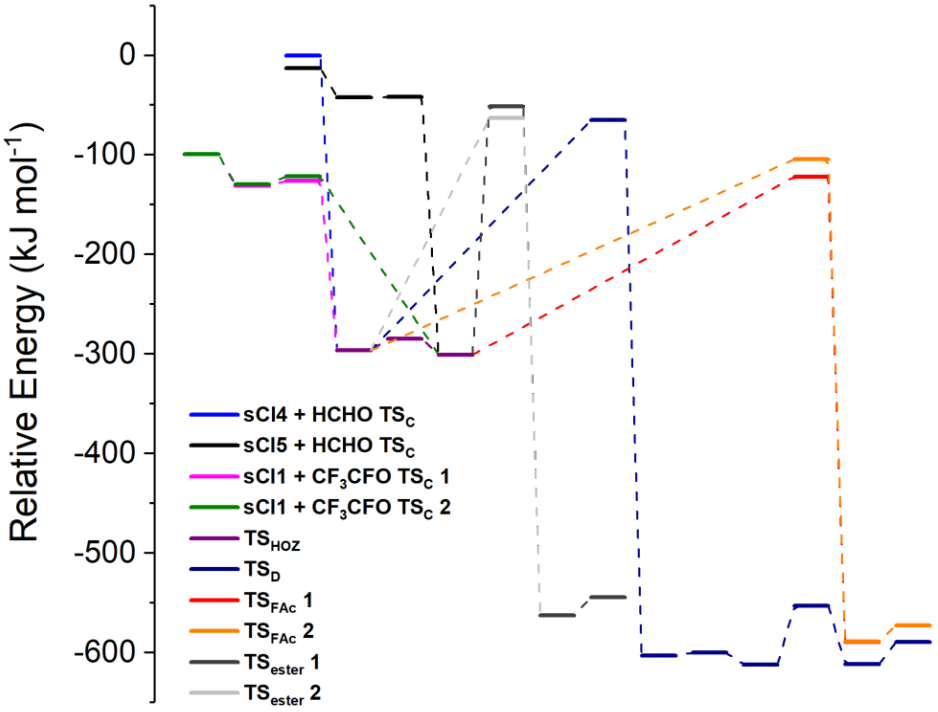


*Figure 19: PES which including reactions HCHO + **sCIs 25** & **26** & **sCI1** + CF_3CFO*

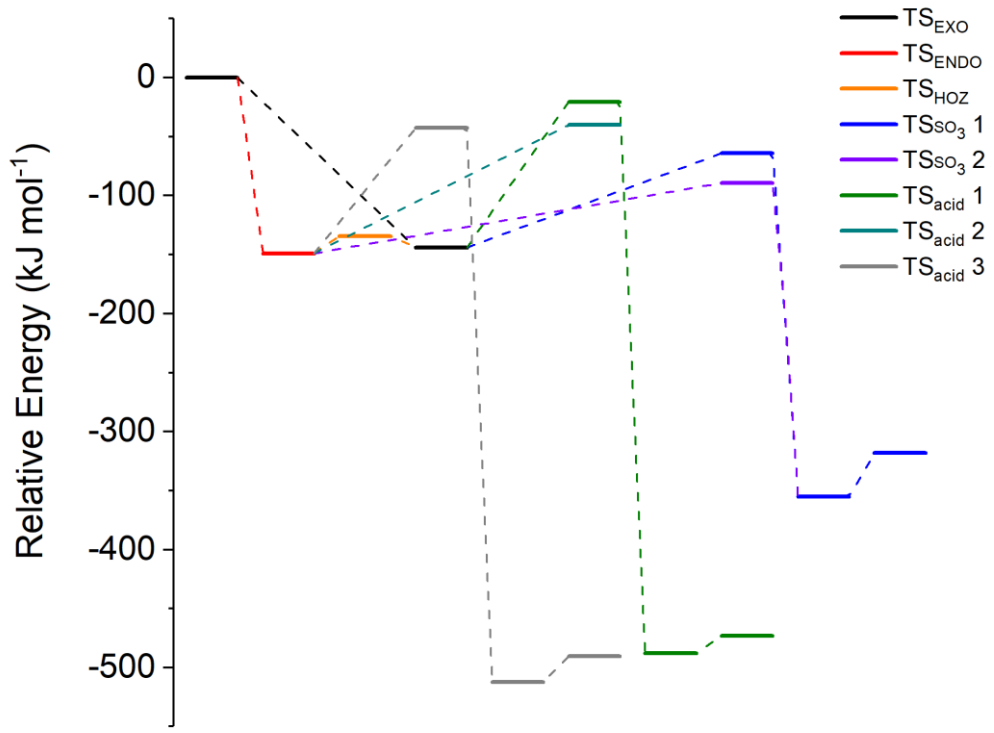


Figure S20: ***sCI 1*** *+ SO_2 PES with legend of channels attached.*

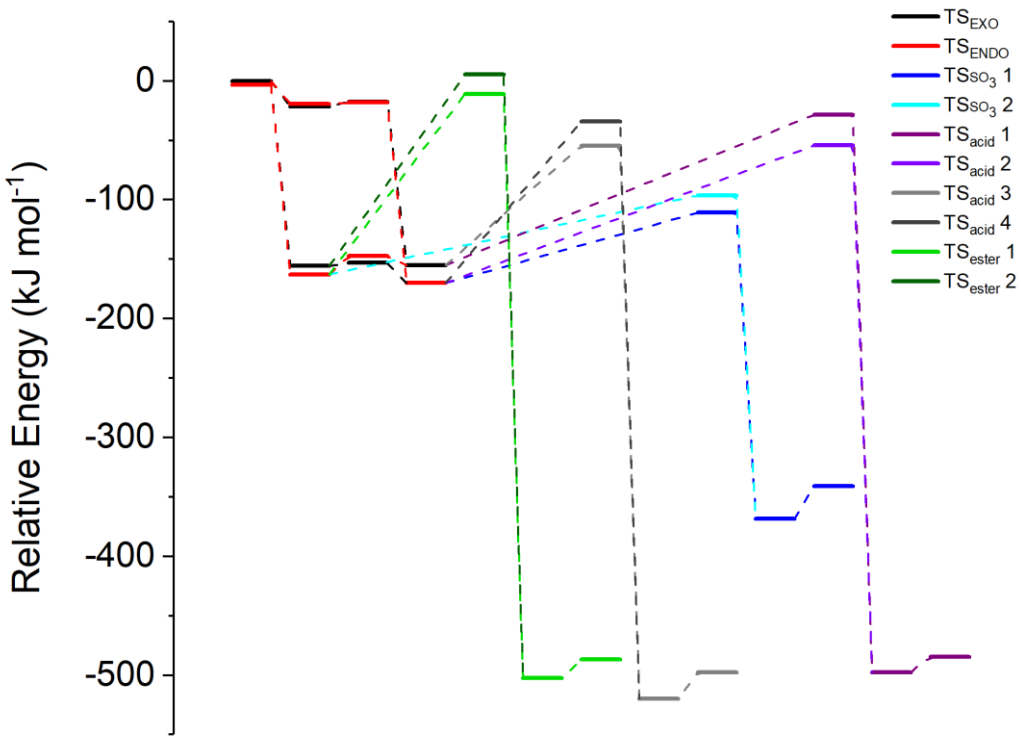


Figure S21: ***sCI 23*** *&* ***sCI 24*** *+ SO_2 PES with legend of channels attached.*

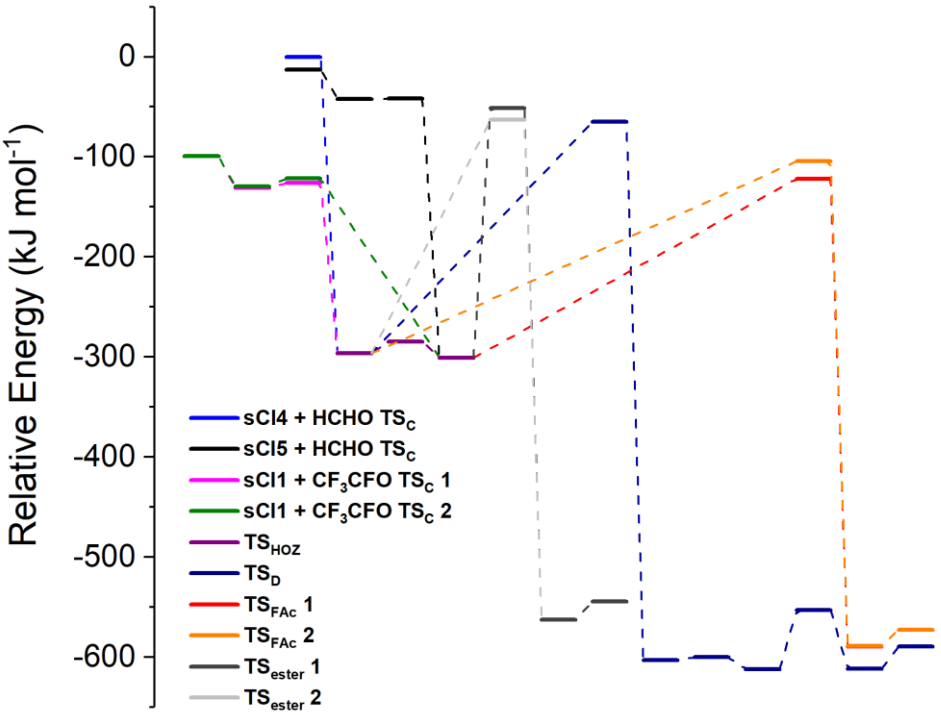


Figure S22: ***sCI 25*** *&* ***sCI 26*** *+ SO_2 PES with legend of channels attached.*

3.2.2 Product branching ratio of sCI 1 + HCHO, CF_3CHO and CF_3CFO

*Table 88: **sCI 1** + HCHO product distribution (Γ): (Γ_{HOZ}); (Γ_{CFa}); (Γ_{HAE})* grainsize=10

T (K)	Γ_{HOZ}	Γ_{CFa}	Γ_{HAE}
200	1.000	0.000	0.000
275	0.000	0.025	0.975
298.15	0.000	0.027	0.973
325	0.000	0.030	0.970
400	0.000	0.038	0.962

*Table 89: The product branching ratio of **sCI 1** + CF_3CHO with **CI 23 + HCHO** and **CI 24 + HCHO** as sinks (not barrierless) grainsize = 40.*

Product branching ratio (Γ)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
CI 23 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 24 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
HCOOH + CF_3CHO	0.8447	0.8282	0.8232	0.8176	0.8051
TS_{HAE} 2	0.0054	0.0094	0.0109	0.0128	0.0177
TS_{HAE} 3	0.6908	0.6479	0.6344	0.6195	0.5862
TS_{FAc} 1	0.0969	0.1084	0.1118	0.1155	0.1234
TS_{FAc} 2	0.0097	0.0142	0.0158	0.0177	0.0222
CF_3COOH + HCHO	0.0473	0.0578	0.0611	0.0648	0.0733
TS_{HAE} 1	0.1553	0.1717	0.1768	0.1824	0.1948
TS_{TFA} 1	0.1499	0.1624	0.1659	0.1696	0.1771
CF_3OCHO + HCHO	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 90: the product branching ratio of **sCI 1** + CF_3CFO with **CI 25 + HCHO** and **CI 26 + HCHO** as sinks for barrierless exit channel using the $k_{d\text{-}d}$ as pre-exponential factors (7.20×10^{-10} cm^3 $molec^{-1}$ s^{-1}). Grainsize = 40*

Product branching ratio (Γ)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
CI 25 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 26 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
HCOOH + CF_3CFO	1.0000	1.0000	1.0000	1.0000	1.0000
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.9940	0.9839	0.9784	0.9705	0.9419
TS_{FAc} 2	0.0060	0.0161	0.0216	0.0295	0.0581
CF_3OCFO + HCHO	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 91: The product branching ratio of **sCI 1** + CF_3CFO with **CI 25 + HCHO** and **CI 26 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.49×10^{-10} cm^3 s^{-1}) for barrierless exit channels. Grainsize = 40*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 25 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 26 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
HCOOH + CF_3CFO	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.9940	0.9839	0.9784	0.9705	0.9419
TS_{FAc} 2	0.0060	0.0161	0.0216	0.0295	0.0581
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

(Due to the very low yield of **CI 25 + HCHO** & **CI 26 + HCHO**, no models were ran excluding these pathways for **sCI 1** + CF_3CFO reactions, as they would yield the same results)

3.2.3 Product branching ratio of HCHO + sCIs 23 & 24

*Table 92: the product branching ratio of **sCI 23** + HCHO with **CI 1 + CF_3CHO** and **CI 24 + HCHO** as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (6.50×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – grainsize 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9809**	**0.9915**	**0.9931**	**0.9944**	**0.9965**
TS_{cyc} 3 (barrierless)	0.4914	0.4965	0.4973	0.4980	0.4998
TS_{cyc} 4 (barrierless)	0.4895	0.4950	0.4958	0.4963	0.4967
CI 24 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0158**	**0.0069**	**0.0056**	**0.0046**	**0.0028**
TS_{HAE} 2	0.0121	0.0052	0.0042	0.0033	0.0020
TS_{HAE} 3	0.0022	0.0010	0.0008	0.0007	0.0004
TS_{FAc} 1	0.0003	0.0002	0.0001	0.0001	0.0001
TS_{FAc} 2	0.0012	0.0006	0.0005	0.0004	0.0003
CF_3COOH + HCHO	**0.0034**	**0.0016**	**0.0013**	**0.0011**	**0.0007**
TS_{HAE} 1	0.0032	0.0015	0.0012	0.0010	0.0006
TS_{TFA} 1	0.0002	0.0001	0.0001	0.0001	0.0001
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 93: the product branching ratio of **sCI 23** + HCHO with **CI 1 + CF_3CHO** and **CI 24 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.52×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – grainsize 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9251**	**0.9695**	**0.9758**	**0.9809**	**0.9884**
TS_{cyc} 3 (barrierless)	0.4634	0.4853	0.4885	0.4910	0.4949
TS_{cyc} 4 (barrierless)	0.4617	0.4841	0.4873	0.4899	0.4935
CI 24 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0617**	**0.0248**	**0.0195**	**0.0153**	**0.0092**
TS_{HAE} 2	0.0475	0.0184	0.0144	0.0111	0.0065
TS_{HAE} 3	0.0084	0.0037	0.0029	0.0024	0.0015
TS_{FAc} 1	0.0012	0.0006	0.0005	0.0004	0.0003
TS_{FAc} 2	0.0046	0.0021	0.0017	0.0014	0.0009
CF_3COOH + HCHO	**0.0133**	**0.0058**	**0.0046**	**0.0037**	**0.0024**
TS_{HAE} 1	0.0125	0.0053	0.0042	0.0034	0.0021
TS_{TFA} 1	0.0008	0.0004	0.0004	0.0003	0.0003
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 94: the product branching ratio of **sCI 23** + HCHO with no reference to **CI 1 + CF_3CHO** and **CI 24 + HCHO** as sinks grainsize 30.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
HCOOH + CF_3CHO	**0.8227**	**0.8101**	**0.8054**	**0.7996**	**0.7836**
TS_{HAE} 2	0.6331	0.5992	0.5867	0.5712	0.5284
TS_{HAE} 3	0.1125	0.1206	0.1235	0.1269	0.1356
TS_{FAc} 1	0.0157	0.0202	0.0220	0.0244	0.0315
TS_{FAc} 2	0.0614	0.0700	0.0732	0.0771	0.0881
CF_3COOH + HCHO	**0.1773**	**0.1899**	**0.1946**	**0.2004**	**0.2164**
TS_{HAE} 1	0.1667	0.1745	0.1771	0.1801	0.1870
TS_{TFA} 1	0.0106	0.0154	0.0175	0.0203	0.0294
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 95: the product branching ratio of **sCI 24** + HCHO with **CI 1 + CF_3CHO** and **CI 23 + HCHO** as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (6.50×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – grainsize 40.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
CI 1 + CF_3CHO	**0.9749**	**0.9888**	**0.9910**	**0.9928**	**0.9956**
TS_{cyc} 3	0.4873	0.4943	0.4953	0.4961	0.4970
TS_{cyc} 4	0.4876	0.4945	0.4956	0.4966	0.4985
CI 23 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0207**	**0.0091**	**0.0074**	**0.0059**	**0.0036**
TS_{HAE} 2	0.0161	0.0069	0.0055	0.0044	0.0026
TS_{HAE} 3	0.0028	0.0013	0.0011	0.0009	0.0005
TS_{FAc} 1	0.0004	0.0002	0.0002	0.0001	0.0001
TS_{FAc} 2	0.0015	0.0007	0.0006	0.0005	0.0003
CF_3COOH + HCHO	**0.0044**	**0.0020**	**0.0017**	**0.0014**	**0.0009**
TS_{HAE} 1	0.0041	0.0019	0.0016	0.0013	0.0008
TS_{TFA} 1	0.0002	0.0001	0.0001	0.0001	0.0001
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 96: the product branching ratio of **sCI 24** + HCHO with **CI 1 + CF_3CHO** and **CI 23 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.52×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – grainsize 40.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
CI 1 + CF_3CHO	**0.9027**	**0.9593**	**0.9683**	**0.9756**	**0.9858**
TS_{cyc} 3 (barrierless)	0.4512	0.4796	0.4841	0.4877	0.4927
TS_{cyc} 4 (barrierless)	0.4515	0.4797	0.4842	0.4878	0.4931
CI 23 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0803**	**0.0332**	**0.0257**	**0.0197**	**0.0113**
TS_{HAE} 2	0.0624	0.0250	0.0192	0.0145	0.0081
TS_{HAE} 3	0.0107	0.0047	0.0038	0.0030	0.0018
TS_{FAc} 1	0.0014	0.0007	0.0006	0.0005	0.0003
TS_{FAc} 2	0.0058	0.0027	0.0022	0.0017	0.0011
CF_3COOH + HCHO	**0.0170**	**0.0075**	**0.0059**	**0.0047**	**0.0028**
TS_{HAE} 1	0.0160	0.0070	0.0055	0.0043	0.0026
TS_{TFA} 1	0.0009	0.0005	0.0005	0.0004	0.0003
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 97: the product branching ratio of **sCI 24** + HCHO **without** using **CI 1 + CF_3CHO** and **CI 23 + HCHO** as sinks – grainsize 40.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
HCOOH + CF_3CHO	**0.8250**	**0.8154**	**0.8116**	**0.8065**	**0.7907**
TS_{HAE} 2	0.6398	0.6142	0.6037	0.5901	0.5478
TS_{HAE} 3	0.1107	0.1170	0.1195	0.1226	0.1317
TS_{FAc} 1	0.0149	0.0182	0.0196	0.0216	0.0283
TS_{FAc} 2	0.0595	0.0660	0.0687	0.0722	0.0830
CF_3COOH + HCHO	**0.1750**	**0.1846**	**0.1884**	**0.1935**	**0.2093**
TS_{HAE} 1	0.1652	0.1714	0.1737	0.1765	0.1840
TS_{TFA} 1	0.0098	0.0132	0.0148	0.0170	0.0252
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

3.2.4 Product branching ratio of HCHO + sCIs 25 & 26

*Table 98: the product branching ratio of **sCI 25 + HCHO** with **CI 1** + CF_3CFO and **CI 26** + HCHO no barrierless exit channels.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
CI 1 + CF_3CFO	**0.8441**	**0.8437**	**0.8436**	**0.8435**	**0.8429**
TS_{CYC} 3	0.5708	0.5701	0.5698	0.5695	0.5683
TS_{CYC} 4	0.2732	0.2737	0.2738	0.2740	0.2746
CI 26 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CFO	**0.1559**	**0.1562**	**0.1564**	**0.1565**	**0.1570**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.1354	0.1353	0.1353	0.1353	0.1353
TS_{FAc} 2	0.0205	0.0209	0.0210	0.0212	0.0217
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table 99: the product branching ratio of **sCI 25 + HCHO** with no **CI 1** + CF_3CFO and **CI 26** + HCHO exit channels. Grainsize=20*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
HCOOH + CF_3CFO	**0.9996**	**0.9992**	**0.9990**	**0.9988**	**0.9978**
TS_{HAE} 2	0.0004	0.0006	0.0007	0.0009	0.0016
TS_{FAc} 1	0.8450	0.8271	0.8209	0.8133	0.7910
TS_{FAc} 2	0.1542	0.1715	0.1774	0.1845	0.2053
CF_3OCFO + HCHO	**0.0004**	**0.0008**	**0.0010**	**0.0012**	**0.0022**
TS_{ESTER} 1	<0.0001	0.0001	0.0001	0.0002	0.0004
TS_{ESTER} 2	0.0004	0.0007	0.0008	0.0011	0.0019

*Table 100: the product branching ratio of **sCI 26** + HCHO with **CI 1** + CF_3CFO and **CI 25** + HCHO as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (7.20×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels.*

Product branching ratio (Γ)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CFO	**0.8456**	**0.8432**	**0.8421**	**0.8406**	**0.8355**
TS_{CYC} 3	0.5750	0.5693	0.5669	0.5637	0.5541
TS_{CYC} 4	0.2705	0.2740	0.2753	0.2769	0.2813
CI 26 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0002**
HCOOH + CF_3CFO	**0.1544**	**0.1567**	**0.1578**	**0.1593**	**0.1641**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001
TS_{FAc} 1	0.1356	0.1354	0.1354	0.1354	0.1356
TS_{FAc} 2	0.0188	0.0213	0.0224	0.0238	0.0284
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**	**0.0002**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001

*Table 101: the product branching ratio of **sCI 26 + HCHO** with **CI 1** + CF_3CFO and **CI 25** + HCHO as sinks using the k_{COLL} as pre-exponential factor (1.49×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels.*

Product branching ratio (Γ)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CFO	**0.8455**	**0.8432**	**0.8422**	**0.8407**	**0.8356**
TS_{CYC} 3	0.5748	0.5693	0.5669	0.5637	0.5542
TS_{CYC} 4	0.2706	0.2740	0.2753	0.2769	0.2814
CI 26 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**
HCOOH + CF_3CFO	**0.1545**	**0.1567**	**0.1578**	**0.1593**	**0.1642**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001
TS_{FAc} 1	0.1357	0.1354	0.1354	0.1354	0.1356
TS_{FAc} 2	0.0188	0.0213	0.0224	0.0238	0.0285
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**	**0.0002**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001

*Table 102: the product branching ratio of **sCI 26 + HCHO** with no **CI 1** + CF_3CFO and **CI 25** + HCHO exit channels grainsize=30*

Product branching ratio (Γ)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
HCOOH + CF_3CFO	**0.9999**	**0.9998**	**0.9997**	**0.9996**	**0.9992**
TS_{HAE} 2	0.0001	0.0002	0.0003	0.0003	0.0006
TS_{FAc} 1	0.8735	0.8624	0.8581	0.8524	0.8324
TS_{FAc} 2	0.1263	0.1372	0.1414	0.1470	0.1662
CF_3OCFO + HCHO	**0.0001**	**0.0002**	**0.0003**	**0.0004**	**0.0008**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{ESTER} 2	0.0001	0.0002	0.0003	0.0003	0.0007

3.2.5 HFO-sCI + HCHO & SO_2 branching ratios of cycloaddition.

Where there are multiple cycloaddition pathways in these two step reactions (**sCI 1** reactions with CF_3CFO and **sCIs 1** & **23—26** reactions with SO_2) to determine what degree of preference of these cycloaddition pathways had in generating the rate constant.

*Table 103: intermediate product branching ratios (Γ) of **sCI** + CF_3CHO & SO_2 reaction*

Intermediate branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
sCI 1 + CF_3CFO					
TS_{cyc} 1	0.7486	0.7647	0.7663	0.7668	0.7609
TS_{cyc} 2	0.2514	0.2353	0.2337	0.2332	0.2391
sCI 2 + SO_2					
TS_{SO_3} 1	0.3278	0.3102	0.3070	0.3042	0.3001
TS_{SO_3} 2	0.6722	0.6898	0.6930	0.6958	0.6999
sCI 3 + SO_2					
TS_{SO_3} 1	0.4871	0.4991	0.4987	0.4975	0.4905
TS_{SO_3} 2	0.5129	0.5009	0.5013	0.5025	0.5095
sCI 4 + SO_2					
TS_{SO_3} 1	0.0027	0.4981	0.4990	0.4994	0.4998
TS_{SO_3} 2	0.9973	0.5019	0.5010	0.5006	0.5002
sCI 5 + SO_2					
TS_{SO_3} 1	0.4715	0.4905	0.4938	0.4962	0.4986
TS_{SO_3} 2	0.5285	0.5095	0.5062	0.5038	0.5014

(All other sCI + aldehyde/ketone and sCI + SO_2 reactions in this study produce one HOZ or SOZ conformer at 100% efficiency)

3.2.6 sCI 1 + SO_2 branching ratios.

*Table S104: SOZ fragmentation branching ratios (Γ) of **sCI 1** + SO_2 reaction all identified pathways included (grainsize=20)*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + HCHO	**0.9949**	**0.9936**	**0.9931**	**0.9926**	**0.9908**
TS_{SO_3} 1	0.0649	0.0694	0.0709	0.0725	0.0771
TS_{SO_3} 2	0.9106	0.9001	0.8966	0.8925	0.8803
SO_2 + HCOOH	**0.0051**	**0.0064**	**0.0069**	**0.0074**	**0.0092**
TS_{acid} 1	0.0001	0.0001	0.0002	0.0002	0.0003
TS_{acid} 2	0.0049	0.0061	0.0065	0.0070	0.0086
TS_{acid} 3	0.0196	0.0242	0.0258	0.0278	0.0337

*Table S105: SOZ decomposition branching ratios (Γ) of **sCI 1** + SO_2 reaction with some pathways included (grainsize=10)*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
SO_3 + HCHO	**0.9947**	**0.9933**	**0.9928**	**0.9922**	**0.9903**
TS_{SO_3} 1	0.0640	0.0686	0.0700	0.0717	0.0764
TS_{SO_3} 2	0.9307	0.9247	0.9227	0.9204	0.9138
SO_2 + HCOOH	**0.0053**	**0.0067**	**0.0072**	**0.0078**	**0.0097**
TS_{acid} 1	0.0001	0.0001	0.0002	0.0002	0.0003
TS_{acid} 2	0.0052	0.0066	0.0071	0.0076	0.0094

3.2.7 sCIs 23 & 24 + SO_2 branching ratios.

*Table S106: SOZ decomposition branching ratios (Γ) of **sCI 23** + SO_2 reaction all identified pathways included (grainsize=50), using the $k_{d\text{-}d}$ as pre-exponential factor (4.08×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for cyclo-reversion pathway.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
sCI 24 + SO_2	**0.0001**	**0.0012**	**0.0023**	**0.0046**	**0.0224**
TS_{EXO}	0.0001	0.0009	0.0017	0.0032	0.0148
TS_{ENDO}	<0.0001	0.0003	0.0007	0.0013	0.0076
SO_3 + CF_3CHO	**0.9988**	**0.9971**	**0.9958**	**0.9931**	**0.9733**
TS_{SO_3} 1	0.6907	0.6910	0.6909	0.6923	0.6883
TS_{SO_3} 2	0.3081	0.3061	0.3048	0.3008	0.2850
SO_2 + CF_3COOH	**0.0011**	**0.0016**	**0.0019**	**0.0024**	**0.0043**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0004	0.0008
TS_{acid} 3	0.0008	0.0013	0.0015	0.0018	0.0032
TS_{acid} 4	<0.0001	<0.0001	0.0001	0.0001	0.0002
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S107: SOZ decomposition branching ratios (Γ) of **sCI 23** + SO_2 reaction without cyclo-revision pathway to **CI 24** + SO_2 revision. Grainsize = 40.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
SO_3 + CF_3CHO	**0.9989**	**0.9984**	**0.9981**	**0.9976**	**0.9955**
TS_{SO_3} 1	0.6910	0.6901	0.6914	0.6936	0.6958
TS_{SO_3} 2	0.3080	0.3082	0.3067	0.3040	0.2997
SO_2 + CF_3COOH	**0.0011**	**0.0016**	**0.0019**	**0.0024**	**0.0045**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0005	0.0008
TS_{acid} 3	0.0008	0.0013	0.0015	0.0018	0.0034
TS_{acid} 4	<0.0001	<0.0001	0.0001	0.0001	0.0003
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S108: SOZ decomposition branching ratios (Γ) of **sCI 23** + SO_2 reaction without sCI pathways and with only pathways that lead directly to SOZs included. Grainsize = 30.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
SO_3 + CF_3CHO	**0.9998**	**0.9997**	**0.9996**	**0.9995**	**0.9992**
TS_{SO_3} 1	0.6921	0.6903	0.6928	0.6955	0.6992
TS_{SO_3} 2	0.3077	0.3094	0.3069	0.3041	0.3000
SO_2 + CF_3COOH	**0.0002**	**0.0003**	**0.0004**	**0.0005**	**0.0008**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0005	0.0008

*Table S109: **sCI 24** + SO_2 SOZ fragmentation branching ratios (Γ) with all identified pathways included. Grainsize = 50*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
sCI 23 + SO_2	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{EXO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ENDO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
SO_3 + CF_3CHO	**0.9987**	**0.9977**	**0.9973**	**0.9966**	**0.9941**
TS_{SO_3} 1	0.5088	0.4989	0.4989	0.4995	0.5045
TS_{SO_3} 2	0.4899	0.4989	0.4984	0.4971	0.4896
SO_2 + CF_3COOH	**0.0013**	**0.0023**	**0.0027**	**0.0033**	**0.0059**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010
TS_{acid} 3	0.0010	0.0016	0.0019	0.0024	0.0040
TS_{acid} 4	0.0001	0.0002	0.0003	0.0004	0.0008
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S110: **sCI 24** + SO_2 SOZ fragmentation branching ratios (Γ) with all identified pathways except cyclo-reversion pathways **CI 23** + SO_2. Grainsize = 40*

Product branching ratio (*Γ*)	Temperature (K)				
	200	275	298	325	400
SO_3 + CF_3CHO	**0.9987**	**0.9977**	**0.9973**	**0.9967**	**0.9941**
TS_{SO_3} 1	0.5117	0.4989	0.4989	0.4995	0.5045
TS_{SO_3} 2	0.4870	0.4989	0.4984	0.4971	0.4896
SO_2 + CF_3COOH	**0.0013**	**0.0023**	**0.0027**	**0.0033**	**0.0059**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010
TS_{acid} 3	0.0010	0.0016	0.0019	0.0024	0.0040
TS_{acid} 4	0.0001	0.0002	0.0003	0.0004	0.0008
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S111: SOZ decomposition branching ratios (Γ) of **sCI 24** + SO_2 reaction without sCI pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (Γ)	Temperature (K)				
	200	275	298	325	400
SO_3 + CF_3CHO	**0.9997**	**0.9996**	**0.9995**	**0.9994**	**0.9990**
TS_{SO_3} 1	0.5102	0.5005	0.5008	0.5019	0.5086
TS_{SO_3} 2	0.4895	0.4991	0.4987	0.4975	0.4904
SO_2 + CF_3COOH	**0.0003**	**0.0004**	**0.0005**	**0.0006**	**0.0010**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010

3.2.8 sCIs 25 & 26 + SO_2 branching ratios.

*Table S112: SOZ decomposition branching ratios (Γ) of **sCI 25** + SO_2 reaction with all identified pathways included. Grainsize = 50. The $k_{d\text{-}d}$ (4.42×10^{-10} cm^3 $molec^{-1}$ s^{-1}) used as pre-exponential factor for cyclo-reversion pathway.*

Product branching ratio (Γ)	Temperature (K)				
	200	275	298	325	400
sCI 26 + SO_2	**<0.0001**	**0.0010**	**0.0017**	**0.0029**	**0.0107**
TS_{EXO}	<0.0001	0.0002	0.0003	0.0005	0.0020
TS_{ENDO}	<0.0001	0.0009	0.0014	0.0024	0.0087
SO_3 + CF_3CHO	**1.0000**	**0.9913**	**0.9892**	**0.9861**	**0.9716**
TS_{SO_3} 1	<0.0001	0.1025	0.1052	0.1082	0.1147
TS_{SO_3} 2	1.0000	0.4995	0.4984	0.4972	0.4936
TS_{SO_3} 3	<0.0001	0.3892	0.3856	0.3807	0.3633
SO_2 + CF_3OCHO	**<0.0001**	**0.0077**	**0.0091**	**0.0110**	**0.0177**
TS_{ester} 1	<0.0001	0.0021	0.0024	0.0029	0.0045
TS_{ester} 2	<0.0001	0.0056	0.0067	0.0081	0.0132

*Table S113: SOZ decomposition branching ratios (Γ) of **sCI 25** + SO_2 reaction without cyclo-revision to **CI 26** + SO_2 revision. Grainsize = 50*

Product branching ratio (Γ)	Temperature (K)				
	200	275	298	325	400
SO_3 + CF_3CHO	**1.0000**	**0.9923**	**0.9909**	**0.9889**	**0.9818**
TS_{SO_3} 1	0.0005	0.1027	0.1056	0.1087	0.1169
TS_{SO_3} 2	0.9973	0.4998	0.4986	0.4977	0.4956
TS_{SO_3} 3	0.0022	0.3897	0.3867	0.3825	0.3693
SO_2 + CF_3OCHO	**<0.0001**	**0.0077**	**0.0091**	**0.0111**	**0.0182**
TS_{ester} 1	<0.0001	0.0021	0.0024	0.0029	0.0046
TS_{ester} 2	<0.0001	0.0057	0.0067	0.0082	0.0136

*Table S114: SOZ decomposition branching ratios (Γ) of **sCI 25** + SO_2 reaction without **CI 26** + SO_2 cyclo-revision pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**
TS_{SO_3} 1	0.0057	0.0886	0.0924	0.0965	0.1071
TS_{SO_3} 2	0.9643	0.5095	0.5062	0.5039	0.5014
TS_{SO_3} 3	0.0300	0.4019	0.4014	0.3996	0.3915

*Table S115: SOZ decomposition branching ratios (Γ) of **sCI 26** + SO_2 reaction with all identified pathways included. Grainsize = 50. The $k_{d\text{-}d}$ (4.51×10^{-10} cm^3 $molec^{-1}$ s^{-1}) used as pre-exponential factor for cyclo-reversion pathway.*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
sCI 25 + SO_2	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**
TS_{EXO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ENDO}	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
SO_3 + CF_3CHO	**0.9998**	**0.9963**	**0.9955**	**0.9943**	**0.9895**
TS_{SO_3} 1	0.0076	0.0881	0.0917	0.0957	0.1053
TS_{SO_3} 2	0.9523	0.5083	0.5049	0.5023	0.4987
TS_{SO_3} 3	0.0399	0.3999	0.3988	0.3963	0.3856
SO_2 + CF_3OCHO	**0.0002**	**0.0037**	**0.0045**	**0.0057**	**0.0103**
TS_{ester} 1	0.0001	0.0011	0.0013	0.0016	0.0027
TS_{ester} 2	0.0001	0.0026	0.0032	0.0041	0.0077

*Table S116: SOZ decomposition branching ratios (Γ) of **sCI 26** + SO_2 reaction without cyclo-revision to **CI 25** + SO_2 revision. Grainsize = 50*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9981**	**0.9963**	**0.9955**	**0.9943**	**0.9897**
TS_{SO_3} 1	0.0753	0.0881	0.0917	0.0957	0.1053
TS_{SO_3} 2	0.5279	0.5084	0.5049	0.5023	0.4987
TS_{SO_3} 3	0.3950	0.3998	0.3988	0.3964	0.3856
SO_2 + CF_3OCHO	**0.0019**	**0.0037**	**0.0045**	**0.0057**	**0.0103**
TS_{ester} 1	0.0007	0.0011	0.0013	0.0016	0.0027
TS_{ester} 2	0.0012	0.0026	0.0032	0.0041	0.0076

*Table S117: SOZ decomposition branching ratios (Γ) of **sCI 26** + SO_2 reaction without **CI 25** pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**
TS_{SO_3} 1	0.0042	0.0886	0.0924	0.0965	0.1071
TS_{SO_3} 2	0.9740	0.5096	0.5063	0.5039	0.5014
TS_{SO_3} 3	0.0219	0.4018	0.4014	0.3996	0.3915

3.2.9 HFO-sCI reactions with other co-reactants Pathway distribution.

*Table S118: Pathway Distribution (Γ) of **sCIs 1-5** reactions with H_2S, H_2O and MeOH.*

sCI	T (K)	H_2S		H_2O		MeOH	
		Γ_{TS1}	Γ_{TS2}	Γ_{TS1}	Γ_{TS2}	Γ_{TS1}	Γ_{TS2}
1	**200**	0.551	0.449	0.874	0.126	0.899	0.101
	275	0.539	0.461	0.807	0.193	0.823	0.177
	298.15	0.537	0.463	0.790	0.210	0.802	0.198
	325	0.534	0.466	0.773	0.227	0.780	0.220
	400	0.529	0.471	0.732	0.268	0.728	0.272
23	**200**	0.743	0.257	0.270	0.730	0.973	0.027
	275	0.677	0.323	0.311	0.689	0.935	0.065
	298.15	0.662	0.338	0.320	0.680	0.923	0.077
	325	0.647	0.353	0.329	0.671	0.908	0.092
	400	0.614	0.386	0.348	0.652	0.871	0.129
24	**200**	0.689	0.311	0.843	0.157	0.900	0.100
	275	0.644	0.356	0.789	0.211	0.821	0.179
	298.15	0.634	0.366	0.777	0.223	0.799	0.201
	325	0.624	0.376	0.763	0.237	0.776	0.224
	400	0.604	0.396	0.734	0.266	0.721	0.279
25	**200**	0.734	0.266	0.438	0.562	N/A	N/A
	275	0.710	0.290	0.424	0.576	N/A	N/A
	298.15	0.700	0.300	0.422	0.578	N/A	N/A
	325	0.688	0.312	0.420	0.580	N/A	N/A
	400	0.658	0.342	0.417	0.583	N/A	N/A
26	**200**	0.604	0.396	0.325	0.675	0.472	0.528
	275	0.581	0.419	0.383	0.617	0.465	0.535
	298.15	0.576	0.424	0.396	0.604	0.464	0.536
	325	0.571	0.429	0.408	0.592	0.462	0.538
	400	0.561	0.439	0.435	0.565	0.459	0.541

*Table S119: Branching Ratios (Γ) for $(H_2O)_2$ reaction with **sCIs 1-5***

sCI	T (K)	Γ_{TS1}	Γ_{TS2}	Γ_{TS3}	Γ_{TS4}
1	**200**	0.273	0.171	0.275	0.281
	275	0.279	0.143	0.283	0.295
	298.15	0.281	0.137	0.284	0.298
	325	0.282	0.133	0.286	0.300
	400	0.284	0.126	0.286	0.304
23	**200**	0.273	0.154	0.314	0.259
	275	0.289	0.122	0.315	0.274
	298.15	0.292	0.117	0.314	0.277
	325	0.296	0.113	0.311	0.280
	400	0.302	0.111	0.303	0.284
24	**200**	0.161	0.316	0.249	0.274
	275	0.144	0.333	0.246	0.277
	298.15	0.140	0.336	0.245	0.278
	325	0.138	0.339	0.245	0.279
	400	0.134	0.341	0.245	0.280
25	**200**	0.241	0.259	0.244	0.255
	275	0.228	0.273	0.235	0.264
	298.15	0.225	0.277	0.232	0.266
	325	0.220	0.282	0.229	0.269
	400	0.211	0.292	0.222	0.275
26	**200**	0.254	0.287	0.243	0.216
	275	0.256	0.324	0.233	0.188
	298.15	0.256	0.333	0.230	0.181
	325	0.256	0.344	0.227	0.174
	400	0.256	0.366	0.219	0.159

3.3 Effective Rate Constants (k_{EFF}) of HFO-sCI reactions.

3.3.1 Literature Co-reactant Abundances.

Table S120: Representative abundances of atmospheric co-reactants across different environments in the literature.

Co-reactant Environment	Abundance (Original units)	Study	Ref
Formaldehyde (HCHO)			
Mean of European homes	23.1 μg/m^3	Salthammer *et al.*	115
Range of European homes	20–30 μg/m^3	Salthammer *et al.*	115
Mean of Rural European sites	3.49 ppb	Salthammer *et al.*	115
Range of Rural European sites	0.4–5.5 ppb	Salthammer *et al.*	115
Homes with particle floorboards	32.0 μg/m^3	Raw *et al.*	116
Homes without particle floorboards	20.3 μg/m^3	Raw *et al.*	116
Homes with particle floorboards in main bedroom England	37.7 μg/m^3	Raw *et al.*	116
Homes without particle floorboards in main bedroom England	23.2 μg/m^3	Raw *et al.*	116
New homes	128 & 135 μg/m^3	Raw *et al.*	116
Average home	22.2 μg/m^3	Raw *et al.*	116
Minimum	1 μg/m^3	Raw *et al.*	116
Maximum	171 μg/m^3	Raw *et al.*	116
In buildings in the absent of ozone	<30 μg/m^3	Uhde *et al.*	117
Highest found with ozone present	148 μg/m^3	Uhde *et al.*	117
General	0.5 μg/m^3	WHO Regional Publications	118
Urban general	1—20 μg/m^3	WHO Regional Publications	118
Heavy traffic	100 μg/m^3	WHO Regional Publications	118
Mobile Home	490 μg/m^3	WHO Regional Publications	118
São Paulo, Brazil	5.0±2.8 ppbv	Nguyen *et al.*	108
Osaka, Japan	1.9±0.9 ppbv	Nguyen *et al.*	108
Acetaldehyde (CH_3CHO)			
São Paulo, Brazil	5.4±2.8 ppbv	Nguyen *et al.*	108
Osaka, Japan	1.5±0.8 ppbv	Nguyen *et al.*	108
General Aldehydes and Ketones (from Vereecken *et al.*)			
$R_1R_2C=O$ – Boreal Forest	1.2×10^{11}	Vereecken *et al.*	55
$R_1R_2C=O$ – Tropical Forest	1.9×10^{10}	Vereecken *et al.*	55
$R_1R_2C=O$ – Mega city	5.1×10^{11}	Vereecken *et al.*	55
$R_1R_2C=O$ – Rural Europe	6.6×10^{10}	Vereecken *et al.*	55

Sulphur Dioxide (SO_2)			
Beijing urban area, China	16.8 ± 13.1 ppb	Lin *et al.*	119
Gucheng rural area, China	14.8 ± 9.4 ppb	Lin *et al.*	119
Shangdianzi, China	7.5 ± 4.0 ppb	Lin *et al.*	119
London Bloomsbury, UK	2 μg/m^3	*defra*	120
London Marylebone Road, UK	7 μg/m^3	*defra*	120
London N. Kensington, UK	14 μg/m^3	*defra*	120
Grangemouth, Falkirk, UK	18 μg/m^3	*defra*	120
Londonderry Rosemount, NI, UK	18 μg/m^3	*defra*	120
0.1 km from Volcanic vents (Mount Etna)	~10,000 μg/m^3	Aiuppa *et al.*	121
10 km from Volcanic vents (Mount Etna)	7 μg/m^3	Aiuppa *et al.*	121
Sao Paulo citywide concentrations	4.94+2.99 ppb	Bravo *et al.*	109
Typical indoor	22.9 (≤50) ppb	Salthammer *et al.*	122
Typical urban concentrations	15 ppbv	Hunter *et al.*	123
SO_2 – Boreal Forest	1.7×10^{10}	Vereecken *et al.*	55
SO_2 – Tropical Forest	~0	Vereecken *et al.*	55
SO_2 – Mega city	9×10^{10}	Vereecken *et al.*	55
SO_2– Rural Europe	6.6×10^9	Vereecken *et al.*	55
Nitric Acid (HNO_3) 1.1×10^{11}			
Houston, TX	~4.5 ppb	Leong *et al.*	111
Los Angeles Southern California	20 ppbv	Foreman *et al.*	124
Southern California rural	0.1-8.0 ppb	Crisp *et al.*	113
Houston, TX	0.4-4.6 ppb	Leong *et al.*	111
HNO_3	*~10^{11}*	*Kumar and Fransisco*	125
Trifluoroacetic acid (CF_3COOH)			
Beijing (04/14-04/15)	1459 ± 223 pg/m^3	Zhang *et al.*	126
Beijing (04/14-04/15)	1162 ± 173 pg/m^3	Zhang *et al.*	126
lowest abundance of local TFA	283 pg/m^3	Zhang *et al.*	126
highest abundance of local TFA	6317 pg/m^3	Zhang *et al.*	126
Average Beijing (05/12-04/13)	1580 ± 558 pg/m^3	Wu *et al.*	127
Europe projected future abundance	0.06 — 0.94 ppt	Henne *et al.*	75
Carboxylic acid (RCOOH)			
RCOOH – Boreal Forest	1×10^{11}	Vereecken *et al.*	66
RCOOH – Tropical Forest	5×10^{10}	Vereecken *et al.*	66
RCOOH – Mega city	N/A	Vereecken *et al.*	66
RCOOH – Rural Europe	N/A	Vereecken *et al.*	66
Hydrofluoric acid (HF)			
Stratosphere	0.1-0.5 ppb	Mankin *et al.*	140
vicinity of volcano by ambient T (K)	up to 15 ppbv	Cheng *et al.*	141
At source of volcano	900 ug m^{-3}	Cheng *et al.*	141

Hydrochloric acid (HCl)			
Southern California (overall)	1.3 ppb	Crisp *et al.*	125
Southern California (halfway range)	8 ppb	Crisp *et al.*	125
Southern California (Mean)	2.2 ± 2.3 ppb	Crisp *et al.*	125
Southern California (lowest)	~0 ppb	Crisp *et al.*	125
Southern California (highest)	16 ppb	Crisp *et al.*	125
Los Angeles (Daytime)	5 ppb	Crisp *et al.*	125
Los Angeles (Nighttime)	3 ppb	Crisp *et al.*	125
San Francisco Bay	3.9 ppb	Crisp *et al.*	125
Standard tropospheric range	100 - 300 pptv	Sanhueza *et al.*	142
Industrial or marine environments	1.5 - 3 ppb	Graedel and Keene	143
Hydrogen sulphide (H_2S)			
Volcanoes	500 ppb	Kumar *et al.*	144
construction and demolition waste emissions - average	7 — 100 ppm	Kumar *et al.*	144
construction and demolition waste emissions- highest end	5,000–12,000 ppm	Kumar *et al.*	144
ambient air range	0.11–0.33 ppb	Abdollahi and Hosseini	145
industrial landfill, Terre Haute, Indiana, USA	2.0 – 300 ppb	Levels *et al.*	146
Dakota City 1999	≥ 90 ppb	Inserra *et al.*	147
Methanol (CH_3OH)			
Troposphere over Remote oceans	1 ppbv	Heikes *et al.*	148
Average Urban areas and forest	20 ppbv	Heikes *et al.*	148
São Paulo, Brazil	**34.1±9.2 ppb**	**Nguyen *et al.***	120
Osaka, Japan	5.8±3.8	Nguyen *et al.*	120
wooded North Carolina industrial area	78.5—297 ppbv	Kelly *et al.*	148,149

3.3.2 Effective Rate Constants Used in Manuscript.

*Table S121: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants ($k_{eff} = k_{THEO} \times$ **[co-reactant]**).*

[Co-reactant] (molec./cm^3)	sCI	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{exp} (cm^3 s^{-1})	k_{eff} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	5.60
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.54
2.0×10^{12}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	5.0
(Urban Heavy	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	1447
traffic) [130]	26	**1.66×10^{-11}**	7.07×10^{-10}	-	33.4
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	300
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.79
4.1×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	169
(Beijing urban	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	186
area) [131]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	183
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	94
	23	**2.06×10^{-11}**	5.93×10^{-10}	-	2.3
1.1×10^{11}	24	**8.87×10^{-11}**	4.76×10^{-10}	-	9.8
(Houston,	25	9.25×10^{-8}	**5.26×10^{-10}**	-	58
Texas) [123]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	8.4
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	2.5×10^{-2}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	1.7×10^{-2}
3.3×10^{7}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	1.3×10^{-2}
(Beijing higher	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	1.5×10^{-2}
emission areas)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	1.4×10^{-2}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	73
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.83
6.2×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	70
(~80% humidity	25	**5.13×10^{-12}**	7.54×10^{-10}	-	3.2×10^{6}
Sao Paulo) [121,150]	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.4×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	2.9×10^{3}
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	2.4×10^{3}
8.7×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	3.3×10^{3}
(~80% humidity	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.2×10^{5}
Sao Paulo) [121,150]	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.1×10^{5}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	0.010
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	7.9×10^{-5}
8.4×10^{11}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	0.028
(Sao Paulo,	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	462
Brazil) [120]	26	**3.31×10^{-11}**	5.39×10^{-10}	-	28
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	0.052
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	1.4×10^{-3}
1.2×10^{13}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	0.042
(Industrial	25	**6.08×10^{-13}**	3.81×10^{-10}	-	4.5
landfill) [146]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	0.091
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	58
	23	**4.04×10^{-15}**	4.51×10^{-10}	-	5.0×10^{-3}
1.2×10^{11}	24	**7.28×10^{-11}**	3.62×10^{-10}	-	8.96
(Daytime	25	**1.64×10^{-10}**	4.03×10^{-10}	-	20
Los Angeles) [125]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	14
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	0.12
3.7×10^{11}	23	**6.67×10^{-18}**	6.14×10^{-10}	-	2.5×10^{-6}
(near Volcano	24	**2.86×10^{-15}**	4.93×10^{-10}	-	1.1×10^{-3}
vicinity	25	**1.19×10^{-11}**	5.50×10^{-10}	-	4.4
ambient T) [141]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	0.14

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead*

3.3.3 Effective Rate Constants At Lower Range.

*Table S122: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants ($k_{eff} = k_{THEO} \times$ **[co-reactant]**).*

[Co-reactant] (molec./cm^3)	sCI	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{exp} (cm^3 s^{-1})	k_{eff} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	1.3

	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.12
4.6×10^{11}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	1.2
(European	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	334
Home average) [127]	26	**1.66×10^{-11}**	7.07×10^{-10}	-	7.7
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	88.3
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.23
1.2×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	49.7
(Sao Paulo,	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	54.8
Brazil) [121]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	53.8
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	60
9.9×10^{9}	23	**2.06×10^{-11}**	5.93×10^{-10}	-	9.8
(Houston,	24	**8.87×10^{-11}**	4.76×10^{-10}	-	53
Texas, lower	25	9.25×10^{-8}	**5.26×10^{-10}**	-	58
boundary) [123]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	57
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	1.7×10^{-3}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	1.1×10^{-3}
2.3×10^{6}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	9.2×10^{-4}
(Europe urban	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	1.0×10^{-3}
projected) [75]	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	9.9×10^{-4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	28
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.32
2.4×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	27
(Mega city) [66]	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.2×10^{6}
	26	**2.27×10^{-13}**	7.40×10^{-10}	-	5.44×10^{4}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	279
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	231
8.5×10^{13}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	318
(Mega city) [66]	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.1×10^{4}
	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.0×10^{4}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	1.7×10^{-3}
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	1.3×10^{-5}
1.4×10^{11}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	4.7×10^{-3}
(Osaka, Japan) [120]	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	79
	26	**3.31×10^{-11}**	5.39×10^{-10}	-	4.7
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	5.7×10^{-5}
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	1.6×10^{-6}
1.2×10^{9}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	4.6×10^{-5}
(ambient air	25	**6.08×10^{-13}**	3.81×10^{-10}	-	4.9×10^{-3}
range) [145]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	1.0×10^{-4}
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	3.5
	23	**4.04×10^{-15}**	4.51×10^{-10}	-	3.0×10^{-4}
7.4×10^{9}	24	**7.28×10^{-11}**	3.62×10^{-10}	-	0.54
(Standard	25	**1.64×10^{-10}**	4.03×10^{-10}	-	1.2
troposphere) [142]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	0.83
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	0.12
3.7×10^{11}	23	**6.67×10^{-18}**	6.14×10^{-10}	-	2.5×10^{-6}
(near Volcano	24	**2.86×10^{-15}**	4.93×10^{-10}	-	1.1×10^{-3}
vicinity	25	**1.19×10^{-11}**	5.50×10^{-10}	-	4.4
ambient T) [141]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	0.14

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

3.3.4 Effective Rate Constants At Medium Range.

*Table S123: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants ($k_{eff} = k_{THEO} \times$ **[co-reactant]**).*

[Co-reactant] (molec./cm^3)	sCI	k_{ME} ($cm^3\ s^{-1}$)	$k_{d\text{-}d}$ ($cm^3\ s^{-1}$)	k_{exp} ($cm^3\ s^{-1}$)	k_{eff} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	5.60
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.54
2.0×10^{12}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	5.0
(Heavy traffic) [130]	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	1447
	26	**1.66×10^{-11}**	7.07×10^{-10}	-	33.4
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	300
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.79
4.1×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	169
(Beijing urban	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	186

area) [131]	26	» $k_{d\text{-}d}$	**4.42 × 10^{-10}**	-	183
HNO_3	1	8.22 × 10^{-9}	**8.45 × 10^{-10}**	5.1 × 10^{-10}	60
	23	**2.06 × 10^{-11}**	5.93 × 10^{-10}	-	9.8
1.1 × 10^{11}	24	**8.87 × 10^{-11}**	4.76 × 10^{-10}	-	53
(Houston,	25	9.25 × 10^{-8}	**5.26 × 10^{-10}**	-	58
Texas) [123]	26	**7.53 × 10^{-11}**	5.16 × 10^{-10}	-	8.4
TFA	1	» $k_{d\text{-}d}$	**7.54 × 10^{-10}**	3.50 × 10^{-10}	4.6 × 10^{-3}
	23	» $k_{d\text{-}d}$	**4.96 × 10^{-10}**	-	3.0 × 10^{-3}
6.1 × 10^{6}	24	» $k_{d\text{-}d}$	**3.98 × 10^{-10}**	-	2.4 × 10^{-3}
(Beijing average	25	» $k_{d\text{-}d}$	**4.35 × 10^{-10}**	-	2.7 × 10^{-3}
emission areas) [138]	26	» $k_{d\text{-}d}$	**4.27 × 10^{-10}**	-	2.6 × 10^{-3}
H_2O	1	**1.18 × 10^{-16}**	1.06 × 10^{-9}	*2.4 × 10^{-16}*	73
6.2 × 10^{17}	23	**1.35 × 10^{-18}**	8.38 × 10^{-10}	-	0.83
(~80%	24	**1.12 × 10^{-16}**	6.73 × 10^{-10}	-	70
humidity,	25	**5.13 × 10^{-12}**	7.54 × 10^{-10}	-	3.2 × 10^{6}
Sao Paulo) [121,150]	26	**2.27 × 10^{-13}**	7.40 × 10^{-10}	-	1.4 × 10^{5}
$(H_2O)_2$	1	**3.28 × 10^{-12}**	1.07 × 10^{-9}	7.50 × 10^{-12}	2.9 × 10^{3}
8.7 × 10^{14}	23	**2.71 × 10^{-12}**	7.99 × 10^{-10}	-	2.4 × 10^{3}
(~80%	24	**3.74 × 10^{-12}**	6.42 × 10^{-10}	-	3.3 × 10^{3}
humidity,	25	1.14 × 10^{-6}	**7.14 × 10^{-10}**	-	6.2 × 10^{5}
Sao Paulo) [121,150]	26	1.46 × 10^{-9}	**7.01 × 10^{-10}**	-	6.1 × 10^{5}
MeOH	1	**1.20 × 10^{-14}**	8.15 × 10^{-10}	1.1 × 10^{-13}	0.010
	23	**9.43 × 10^{-17}**	6.14 × 10^{-10}	-	7.9 × 10^{-5}
8.4 × 10^{11}	24	**3.30 × 10^{-14}**	4.93 × 10^{-10}	-	0.028
(Sao Paulo,	25	» $k_{d\text{-}d}$	**5.50 × 10^{-10}**	-	462
Brazil) [120]	26	**3.31 × 10^{-11}**	5.39 × 10^{-10}	-	28
H_2S	1	**7.06 × 10^{-15}**	5.68 × 10^{-10}	1.7 × 10^{-13}	0.052
	23	**1.96 × 10^{-16}**	4.26 × 10^{-10}	-	1.4 × 10^{-3}
1.2 × 10^{13}	24	**5.72 × 10^{-15}**	3.42 × 10^{-10}	-	0.042
(Industrial	25	**6.08 × 10^{-13}**	3.81 × 10^{-10}	-	4.5
landfill) [146]	26	**1.23 × 10^{-14}**	3.74 × 10^{-10}	-	0.091
HCl	1	**4.70 × 10^{-10}**	6.06 × 10^{-10}	4.1 × 10^{-11}	19
3.2 × 10^{10}	23	**4.04 × 10^{-15}**	4.51 × 10^{-10}	-	1.3 × 10^{-4}
(Southern	24	**7.28 × 10^{-11}**	3.62 × 10^{-10}	-	0.24
California	25	**1.64 × 10^{-10}**	4.03 × 10^{-10}	-	0.53
Overall) [125]	26	**1.13 × 10^{-10}**	3.96 × 10^{-10}	-	0.36
HF	1	**3.32 × 10^{-13}**	8.15 × 10^{-10}	-	9.0
	23	**6.67 × 10^{-18}**	6.14 × 10^{-10}	-	1.8 × 10^{-4}
2.7 × 10^{13}	24	**2.86 × 10^{-15}**	4.93 × 10^{-10}	-	0.076
(At Volcanic	25	**1.19 × 10^{-11}**	5.50 × 10^{-10}	-	320
source)	26	**3.66 × 10^{-13}**	5.39 × 10^{-10}	-	9.9

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

3.3.5 Effective Rate Constants At Higher Range.

*Table S124: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants (k_{eff} = k_{THEO} × **[co-reactant]**).*

[Co-reactant] (molec./cm^3)	sCI	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{exp} (cm^3 s^{-1})	k_{eff} (s^{-1})
HCHO	1	**2.79 × 10^{-12}**	1.06 × 10^{-9}	-	27.4
	23	**2.69 × 10^{-13}**	8.04 × 10^{-10}	-	2.64
9.8 × 10^{12}	24	**2.49 × 10^{-12}**	6.46 × 10^{-10}	-	24.5
(Caravan/	25	» $k_{d\text{-}d}$	**7.20 × 10^{-10}**	-	7088
mobile home) [130]	26	**1.66 × 10^{-11}**	7.07 × 10^{-10}	-	164
CF_3CHO	1	» $k_{d\text{-}d}$	6.50 × 10^{-10}	-	-
CF_3CFO	1	**1.98 × 10^{-12}**	3.34 × 10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25 × 10^{-10}**	3.80 × 10^{-11}	68217
	23	**1.90 × 10^{-12}**	5.08 × 10^{-10}	-	178
9.4 × 10^{13}	24	» $k_{d\text{-}d}$	**4.08 × 10^{-10}**	-	38398
(0.1 km from	25	» $k_{d\text{-}d}$	**4.51 × 10^{-10}**	-	42373
Mt. Etna) [133]	26	» $k_{d\text{-}d}$	**4.42 × 10^{-10}**	-	41563
HNO_3	1	8.22 × 10^{-9}	**8.45 × 10^{-10}**	5.1 × 10^{-10}	416
	23	**2.06 × 10^{-11}**	5.93 × 10^{-10}	-	10.1
4.9 × 10^{11}	24	**8.87 × 10^{-11}**	4.76 × 10^{-10}	-	43.7
(Southern	25	9.25 × 10^{-8}	**5.26 × 10^{-10}**	-	259
California rural) [125]	26	**7.53 × 10^{-11}**	5.16 × 10^{-10}	-	37.3
TFA	1	» $k_{d\text{-}d}$	**7.54 × 10^{-10}**	3.50 × 10^{-10}	2.5 × 10^{-2}
	23	» $k_{d\text{-}d}$	**4.96 × 10^{-10}**	-	1.7 × 10^{-2}
3.3 × 10^{7}	24	» $k_{d\text{-}d}$	**3.98 × 10^{-10}**	-	1.3 × 10^{-2}
(Beijing higher	25	» $k_{d\text{-}d}$	**4.35 × 10^{-10}**	-	1.5 × 10^{-2}

emission areas) [131]	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	1.4×10^{-2}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	91
7.7×10^{17}	23	**1.35×10^{-18}**	8.38×10^{-10}	-	1.0
(~100%	24	**1.12×10^{-16}**	6.73×10^{-10}	-	87
Sao Paulo	25	**5.13×10^{-12}**	7.54×10^{-10}	-	4.0×10^{6}
outside) [121,150]	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.8×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	4.5×10^{3}
1.4×10^{15}	23	**2.71×10^{-12}**	7.99×10^{-10}	-	3.7×10^{3}
(~100%	24	**3.74×10^{-12}**	6.42×10^{-10}	-	5.1×10^{3}
Sao Paulo	25	1.14×10^{-6}	**7.14×10^{-10}**	-	9.7×10^{5}
outside) [121,150]	26	1.46×10^{-9}	**7.01×10^{-10}**	-	9.5×10^{5}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	0.088
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	6.9×10^{-4}
7.3×10^{12}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	0.24
(North Carolina	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	4.0×10^{3}
Industrial zone) [149]	26	**3.31×10^{-11}**	5.39×10^{-10}	-	242
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	2100
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	58
3.0×10^{17}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	1700
(construction	25	**6.08×10^{-13}**	3.81×10^{-10}	-	1.8×10^{5}
Waste- peak) [144]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	1500
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	190
3.9×10^{11}	23	**4.04×10^{-15}**	4.51×10^{-10}	-	0.016
(Southern	24	**7.28×10^{-11}**	3.62×10^{-10}	-	29
California	25	**1.64×10^{-10}**	4.03×10^{-10}	-	65
Highest) [125]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	44
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	9.0
	23	**6.67×10^{-18}**	6.14×10^{-10}	-	1.8×10^{-4}
2.7×10^{13}	24	**2.86×10^{-15}**	4.93×10^{-10}	-	0.076
(At Volcanic	25	**1.19×10^{-11}**	5.50×10^{-10}	-	320
source) [141]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	9.9

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

3.3.6 Effective Rate Constants At Higher Range.

*Table S125: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants ($k_{eff} = k_{THEO} \times$ [**co-reactant**]). Abundance obtained from study by Vereecken et al..* [66]

[Co-reactant] (molec./cm^3)	sCI	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{exp} (cm^3 s^{-1})	k_{eff} (s^{-1})
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	46
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.53
3.9×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	44
(Boreal	25	**5.13×10^{-12}**	7.54×10^{-10}	-	2.0×10^{6}
Forest)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	8.8×10^{4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	72
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.82
6.1×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	69
(Tropical	25	**5.13×10^{-12}**	7.54×10^{-10}	-	3.1×10^{6}
Forest)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.4×10^{5}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	28
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.32
2.4×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	27
(Mega city)	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.2×10^{6}
	26	**2.27×10^{-13}**	7.40×10^{-10}	-	5.44×10^{4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	45
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.51
3.8×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	43
(Rural	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.9×10^{6}
Europe)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	8.6×10^{4}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	754
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	624
2.3×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	861
(Boreal	25	1.14×10^{-6}	**7.14×10^{-10}**	-	1.6×10^{5}
Forest)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	1.6×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	1.8×10^{3}
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	1.5×10^{3}
5.5×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	2.1×10^{3}
(Tropical	25	1.14×10^{-6}	**7.14×10^{-10}**	-	3.9×10^{5}
Forest)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	3.9×10^{5}

$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	279
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	231
8.5×10^{13}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	318
(Mega city)	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.1×10^{4}
	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.0×10^{4}
$(H_2O)_2$	1	**3.11×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	688
	23	**2.25×10^{-12}**	7.99×10^{-10}	-	570
2.1×10^{14}	24	**6.64×10^{-10}**	6.42×10^{-10}	-	786
(Rural	25	1.14×10^{-6}	**7.14×10^{-10}**	-	1.5×10^{5}
Europe)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	1.5×10^{5}

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

*Table S126: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{exp}); and effective rate constants ($k_{eff} = k_{THEO} \times$ [**co-reactant**]). Abundance obtained from study by Vereecken et al.. [66]*

[Co-reactant] (molec./cm^3)	sCI	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{exp} (cm^3 s^{-1})	k_{eff} (s^{-1})
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	12
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.032
1.7×10^{10}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	6.9
(Boreal	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	7.7
Forest)	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	7.5
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	65
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.17
9.0×10^{10}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	37
(Mega city)	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	41
	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	40
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	4.8
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.013
6.6×10^{9}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	2.7
(Rural	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	3.0
Europe)	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	2.9
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.33
1.2×10^{11}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.032
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.30
(R_1R_2CO: Boreal	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	86
Forest)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	2.0
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.053
1.9×10^{10}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	5.1×10^{-3}
(R_1R_2CO:	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.047
Tropical	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	14
Forest)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	0.32
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	1.4
5.1×10^{11}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.14
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	1.3
(R_1R_2CO: Mega	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	367
city)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	8.5
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.18
6.6×10^{10}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.018
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.16
(R_1R_2CO: Rural	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	48
Europe)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	1.1
RCOOH	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	75
1.0×10^{11}	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	50
(RCOOH:	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	40
Boreal	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	43
Forest)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	43
RCOOH	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	38
5.0×10^{10}	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	25
(RCOOH:	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	20
Tropical	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	22
Forest)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	21

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

3.4 Relative Energies, Enthalpies and Gibbs Free Energies.

*Table 127: **sCI 1** + HCHO relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	**sCI 1 + HCHO Cycloaddition**				
	PRC	-30.01	-20.697	-22.37	18.78
	TS_C	-31.24	-20.771	-25.26	22.54
	HOZ	-240.60	-214.398	-221.72	-167.46
	HOZ to FAc pathway instant				
	HOZ	-240.60	-214.398	-221.72	-167.46
	TS_{FAc} 1	-31.27	-27.221	-32.64	18.22
	C_{FAc} 2	-499.21	-488.439	-487.37	-455.44
	HCHO + HCOOH con 2	-479.10	-473.302	-473.41	-473.31
	HOZ to FAc pathway via HAE				
	HOZ	-240.60	-214.398	-221.72	-167.46
	TS_d	-55.03	-53.629	-60.17	-7.28
	HAE con 1	-552.41	-527.558	-532.15	-484.81
	TS_{iso}	-538.07	-515.748	-521.06	-473.82
	HAE con 2	-564.24	-537.972	-543.27	-493.49
	TS_{HAE}	-461.21	-450.820	-456.96	-405.34
	C_{FAc} 1	-534.87	-520.548	-521.48	-483.02
	HCHO + HCOOH con 1	-496.94	-490.251	-490.54	-490.25

*Table 128: **sCIs 23** & **24**-HCHO relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
23 & 24	**sCI 23 + HCHO Cycloaddition**				
	sCI 23 + HCHO PRC	-25.46	-20.762	-19.54	16.22
	sCI 23 + HCHO TS_c1	-19.91	-11.620	-15.07	33.88
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	sCI 24 + HCHO Cycloaddition				
	sCI 24 + HCHO	-2.54	-3.384	-2.84	-5.13
	sCI 24 + HCHO PRC2	-33.92	-26.983	-27.12	11.38
	sCI 24 + HCHO TS_c2	-30.86	-22.337	-25.61	21.15
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	sCI 1 + CF_3CHO Cycloaddition (barrierless to both HOZ 1 and HOZ 2)				
	sCI 1 + CF_3CHO	-25.58	-23.031	-23.88	-28.29
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	HOZ interconversion				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{HOZ}	-244.72	-222.160	-229.91	-172.06
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	HOZ to TFA pathway via HAE				
	HOZ 2	-69.21	-69.80	-75.28	-21.27
	TS_d 1	-563.17	-540.11	-543.46	-497.71
	HAE1	-563.17	-540.11	-543.46	-497.71

	TS_{iso} 1	-548.18	-527.55	-531.87	-484.43
	HAE2	-572.00	-547.90	-551.77	-504.07
	TS_{HAE} 2	-470.55	-462.94	-467.47	-419.42
	C_{TFA} 1	-546.45	-534.10	-534.02	-497.41
	HCHO + TFA con 1	-503.26	-497.58	-497.56	-499.29
	HOZ to TFA pathway instant				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{acid} 1	-51.64	-49.669	-53.97	-2.98
	C_{TFA} 2	-515.99	-506.127	-504.67	-470.12
	HCHO + TFA con 2	-490.02	-484.350	-484.35	-486.57
	HOZ to FAc pathway via HAE 1				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TS_{d} 2	-78.75	-77.785	-83.39	-29.16
	HAE3	-583.13	-561.064	-564.90	-516.69
	TS_{iso} 2	-569.16	-549.560	-554.18	-505.61
	HAE5	-587.81	-565.054	-569.35	-518.55
	TS_{iso} 3	-559.56	-538.677	-544.96	-489.08
	HAE6	-577.33	-554.290	-558.81	-507.64
	TS_{HAE} 2	-490.71	-481.145	-486.71	-433.25
	C_{FAc} 1	-547.63	-534.425	-533.65	-501.21
	CF_3CHO + HCOOH con 1	-522.52	-513.282	-514.42	-518.54
	HOZ to FAc pathway via HAE 2				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{d} 3	-66.82	-66.612	-72.08	-18.28
	HAE4	-556.17	-534.737	-538.48	-488.78
	TS_{iso} 4	-547.52	-528.525	-533.16	-482.92
	HAE6	-577.33	-554.290	-558.81	-507.64
	TS_{HAE} 2	-490.71	-481.145	-486.71	-433.25
	C_{FAc} 1	-547.63	-534.425	-533.65	-501.21
	CF_3CHO + HCOOH con 1	-522.52	-513.282	-514.42	-518.54
	HOZ to FAc pathway instant 1				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TS_{FAc} 2	-57.38	-54.01	-58.84	-6.25
	C_{FAc} 2	-519.30	-508.906	-506.27	-489.77
	CF_3CHO + HCOOH con 2	-504.68	-496.333	-497.29	-501.59
	HOZ to FAc pathway instant 2				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{FAc} 3	-64.58	-61.516	-66.49	-13.52
	C_{FAc} 1	-519.30	-508.906	-506.27	-489.77
	CF_3CHO + HCOOH con 2	-504.68	-496.333	-497.29	-501.59
	HOZ to Ester pathway 1				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TSester 2	8.61	14.232	10.93	59.39
	Cester 1	-509.42	-501.720	-499.59	-471.59
	SO_2 + CF_3OCHO	-491.39	-486.849	-487.23	-486.48
	HOZ to Ester pathway 2				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TSester 1	-1.75	5.375	2.10	49.25
	Cester 1	-509.42	-501.720	-499.59	-471.59

*Table S129: **sCIs 25** & **26** +HCHO relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
25 & 26	**sCI 25 + HCHO Cycloaddition**				
	sCI 25 + HCHO	0.00	0.00	0.00	0.00
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	sCI 26 + HCHO Cycloaddition				
	sCI 26 + HCHO	-13.71	-13.00	-12.94	-14.17
	sCI 26 + HCHO PRC2	-49.26	-42.03	-41.98	-2.73
	sCI 26 + HCHO TSc2	-50.58	-41.87	-45.21	3.44
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	sCI 1 + CF_3CFO Cycloaddition (barrierless) and interconversion				
	sCI 1 + CF_3CFO	-104.69	-99.204	-100.88	-104.39
	sCI 1 + CF_3CFO PRC 1	-142.02	-130.881	-132.56	-88.12
	sCI 1 + CF_3CFO TSc 3	-137.70	-125.889	-130.53	-78.24
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	sCI 1 + CF_3CFO PRC 2	-140.32	-129.582	-130.88	-87.76
	sCI 1 + CF_3CFO TSc 4	-133.79	-121.601	-126.45	-73.87
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	HOZ interconversion				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_{HOZ}	-306.38	-284.60	-292.77	-233.16
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	HOZ to FAc pathway via HAE				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_d 3	-62.48	-64.96	-69.63	-17.20
	HAE4	-623.96	-603.09	-608.14	-554.75
	TS_{iso} 4	-620.09	-600.04	-607.14	-548.57
	HAE6	-633.12	-611.96	-616.94	-563.57
	TS_{HAE} 2	-562.48	-552.91	-558.75	-505.22
	C_{FAc} 1	-627.18	-611.53	-611.33	-578.03
	CF_3CFO + HCOOH con 1	-601.63	-589.46	-591.42	-594.65
	HOZ to FAc pathway instant 1				
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	TS_{FAc} 1	-125.35	-121.86	-127.32	-72.20
	C_{FAc} 2	-602.46	-589.07	-587.71	-562.25
	CF_3CFO + HCOOH con 2	-583.79	-572.51	-574.29	-577.70
	HOZ to FAc pathway instant 2				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_{FAc} 2	-107.18	-104.33	-109.25	-56.05
	C_{FAc} 3	-602.30	-588.97	-587.54	-563.31
	HOZ to Ester pathway 1				
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	TSester 1	-58.73	-51.48	-55.19	-5.01
	Cester 1	-572.76	-562.29	-561.57	-527.35
	SO_2 + CF_3OCHO	-550.95	-544.10	-545.28	-543.71
	HOZ to Ester pathway 2				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TSester 1	-70.99	-62.91	-66.83	-16.40
	Cester 1	-572.76	-562.29	-561.57	-527.35

Table S130:sCI-SO_2 relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	**SOZ interconversion**				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{SOZ}	-148.79	-134.22	-140.76	-83.16
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	SOZ to C_{SO_3} pathway 1				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{SO_3} 1	-71.81	-63.96	-68.44	-15.15
	C_{SO_3}	-364.76	-355.00	-355.80	-311.56
	HCHO + SO_3	-319.41	-317.93	-317.75	-315.70
	SOZ to C_{SO_3} pathway 2				
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	TS_{SO_3} 2	-96.60	-89.19	-93.94	-39.79
	C_{SO_3}	-364.76	-355.00	-355.80	-311.56
	SOZ to C_{acid} pathway 1				
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	TS_{acid} 1	-18.91	-20.42	-23.58	27.15
	C_{acid} 2	-496.42	-488.05	-485.39	-459.81
	SO_2 + FA con 2	-479.10	-473.30	-473.41	-473.31
	SOZ to C_{acid} pathway 2				
	SOZ 1	-164.58	-148.85	-154.01	-98.88
	TS_{acid} 2	-38.71	-39.84	-43.17	8.09
	C_{acid} 2	-496.42	-488.05	-485.39	-459.81
	SOZ to C_{acid} pathway 3				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{acid} 3	-38.10	-42.54	-44.69	3.51
	C_{acid} 1	-523.27	-512.07	-511.27	-474.88
	SO_2 + FA con 1	-447.56	-444.39	-448.56	-397.19
23 & 24	**sCI 23 + SO_2 Cycloaddition 1**				
	PRC 1	-25.32	-21.41	-19.94	19.83
	TS_{cyc}1	-22.24	-17.56	-19.25	31.05
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	sCI 23 + SO_2 Cycloaddition 2				
	PRC 2	-22.93	-19.35	-17.58	19.99
	TS_{cyc} 2	-22.44	-18.26	-19.50	28.79
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	SOZ interconversion 1				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{SOZ} 1	-158.48	-147.23	-152.55	-93.32
	SOZ3	-175.58	-162.78	-166.61	-110.95
	SOZ interconversion 2				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{SOZ} 2	-164.88	-153.08	-158.54	-99.10
	SOZ4	-168.13	-155.49	-159.08	-103.90
	SOZ to C_{SO_3} pathway 1				
	SOZ3	-175.58	-162.78	-166.61	-110.95
	TS_{SO_3} 1	-102.70	-96.16	-99.88	-44.28
	C_{SO_3} 1	-376.65	-368.24	-367.24	-328.61
	CF_3CHO + SO_3	-345.00	-340.98	-341.64	-343.99
	SOZ to C_{SO_3} pathway 2				

	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{SO_3} 2	-102.70	-96.16	-99.88	-44.28
	C_{SO_3} 1	-376.65	-368.24	-367.24	-328.61
	SOZ to C_{acid} pathway 1				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{acid} 1	-24.22	-28.27	-29.89	20.72
	C_{acid} 2	-503.48	-496.08	-492.63	-472.03
	SO_2 + TFA con 2	-490.02	-484.35	-484.35	-486.57
	SOZ to C_{acid} pathway 2				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{acid} 2	-51.12	-54.28	-56.40	-4.50
	C_{acid} 3	-504.21	-496.76	-493.37	-472.07
	SOZ to C_{acid} pathway 3				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{acid} 3	-48.54	-54.58	-55.50	-7.46
	C_{acid} 3	-504.21	-496.76	-493.37	-472.07
	SOZ to C_{acid} pathway 4				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{acid} 4	-27.66	-33.91	-34.58	12.63
	C_{acid} 1	-528.65	-520.00	-517.52	-488.76
	SO_2 + TFA con 1	-503.26	-497.58	-497.56	-499.29
	SOZ to C_{ester} pathway 1				
	SOZ3	-175.58	-162.78	-166.61	-110.95
	TS_{ester} 1	-11.45	-11.06	-11.57	35.51
	C_{ester} 1	-509.50	-502.18	-499.90	-467.54
	SO_2 + CF_3OCFO	-491.39	-486.85	-487.23	-486.48
	SOZ to C_{ester} pathway 2				
	SOZ4	-168.13	-155.49	-159.08	-103.90
	TS_{ester} 2	5.96	5.63	5.37	48.87
	C_{ester} 1	-509.50	-502.18	-499.90	-467.54
25 & 26	**SOZ interconversion 1**				
	SOZ 1	-203.93	-193.02	-196.79	-140.53
	TS_{SOZ} 1	-196.71	-187.24	-192.42	-134.96
	SOZ3	-226.47	-215.04	-219.25	-161.44
	SOZ interconversion 2				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{SOZ} 2	-210.99	-200.86	-206.57	-145.35
	SOZ4	-211.13	-200.27	-203.99	-147.93
	SOZ to C_{SO_3} pathway 1				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{SO_3} 1	-117.49	-112.23	-115.98	-60.87
	C_{SO_3} 1	-443.42	-434.24	-432.59	-402.54
	CF_3CHO + SO_3	-424.10	-417.15	-418.64	-420.10
	SOZ to C_{SO_3} pathway 2				
	SOZ3	-226.47	-215.04	-219.25	-161.44
	TS_{SO_3} 2	-157.94	-152.16	-156.41	-98.42
	C_{SO_3} 2	-443.42	-434.24	-432.59	-402.54
	SOZ to C_{SO_3} pathway 3				
	SOZ4	-211.13	-200.27	-203.99	-147.93
	TS_{SO_3} 3	-134.70	-129.54	-133.57	-76.21

	C_{SO_3} 3	-443.42	-434.24	-432.59	-402.54
	SOZ to C_{ester} pathway 1				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{ester} 1	-85.28	-83.91	-85.02	-35.78
	C_{ester} 1	-561.50	-553.32	-550.70	-531.54
	$SO_2 + CF_3OCHO$	-550.95	-544.10	-545.28	-543.71
	SOZ to C_{ester} pathway 2				
	SOZ 1	-203.93	-193.02	-196.79	-140.53
	TS_{ester} 2	-69.69	-69.29	-69.92	-24.46
	C_{ester} 2	-561.72	-553.43	-550.90	-529.31

Table S131: sCI-HNO_3 relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-58.97	-54.38	-54.44	-11.56
	TS	-48.34	-48.32	-51.29	-1.74
	Pr	-192.76	-179.86	-181.93	-132.29
23	PRC	-39.46	-35.47	-33.82	2.60
	TS	-28.94	-29.05	-31.33	22.38
	Pr	-205.61	-196.26	-196.60	-147.26
24	PRC	-47.09	-42.96	-42.10	0.50
	TS	-34.54	-35.92	-38.21	14.08
	Pr	-200.32	-190.26	-191.08	-139.84
25	PRC	-60.66	-56.31	-55.35	-13.31
	TS	-59.30	-57.16	-59.45	-5.41
	Pr	-220.67	-213.94	-214.08	-164.68
26	PRC	-60.27	-56.03	-55.16	-11.62
	TS	-49.84	-52.49	-54.68	-0.74
	Pr	-209.83	-203.44	-203.90	-152.16

Table S132: sCI-TFA relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-45.19	-41.91	-40.16	-5.73
	Pr	-194.67	-180.21	-182.57	-130.73
23	PRC	-33.09	-30.30	-27.81	5.36
	Pr	-195.66	-184.09	-185.55	-130.37
24	PRC	-34.83	-31.94	-29.55	173.58
	Pr	-204.27	-192.57	-193.93	-138.83
25	PRC	-41.65	-38.73	-36.27	-2.79
	Pr	-224.07	-214.23	-215.92	-158.97
26	PRC	-40.48	-37.60	-35.19	0.04
	Pr	-216.16	-207.43	-208.82	-153.23

Table S133:sCI-HF relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-49.75	-39.94	-43.70	-8.23

	TS	-5.74	-1.52	-8.35	35.32
	Pr	-198.52	-178.46	-183.89	-142.94
23	PRC	-34.78	-26.13	-28.54	3.90
	TS	20.19	22.62	16.53	61.77
	Pr	-209.51	-192.00	-196.73	-154.41
24	PRC	-40.17	-30.95	-34.22	2.10
	TS	5.75	8.86	2.69	47.20
	Pr	-211.14	-192.83	-197.92	-153.99
25	PRC	-37.88	-29.10	-32.14	4.34
	TS	-21.37	-16.75	-23.08	23.14
	Pr	-251.93	-235.33	-240.46	-197.01
26	PRC	-42.30	-33.68	-36.44	-1.35
	TS	-7.91	-4.96	-11.10	34.41
	Pr	-244.40	-228.59	-233.72	-188.66

Table S134:sCI-HCl relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-31.56	-25.70	-28.93	7.08
	TS	-30.45	-25.83	-31.26	10.50
	Pr	-202.76	-180.51	-185.15	-144.07
23	PRC	-23.31	-17.26	-18.64	12.23
	TS	3.34	6.03	1.41	44.79
	Pr	-213.79	-194.13	-197.86	-154.89
24	PRC	-25.24	-19.12	-21.40	14.04
	TS	-15.75	-13.43	-18.13	24.28
	Pr	-213.84	-193.33	-197.47	-152.83
25	PRC	-27.68	-21.39	-22.89	7.87
	TS	-24.08	-19.06	-23.84	20.19
	Pr	-231.78	-213.42	-217.41	-172.92
26	PRC	-28.93	-22.96	-24.70	9.23
	TS	-18.59	-16.50	-21.07	22.66
	Pr	-225.22	-207.62	-211.63	-165.72

Table S135:sCI-H_2S relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	PRC1	-20.13	-13.92	-14.65	19.13
	TS1	-2.57	4.26	-1.18	44.84
	Pr 1	-210.81	-188.36	-192.97	-148.26
	PRC2	-19.88	-13.71	-14.42	19.32
	TS2	-2.20	4.61	-0.87	45.24
	Pr 2	-209.59	-187.39	-191.75	-147.66
23	PRC1	-13.67	-9.89	-8.34	16.54
	TS1	2.81	9.95	5.34	53.07
	Pr 1	-226.11	-205.92	-209.55	-163.12
	PRC2	-11.88	-7.98	-6.42	16.71
	TS2	5.08	11.86	7.37	54.74
	Pr 2	-229.42	-209.23	-212.81	-166.63
24	PRC1	-11.12	-6.04	-5.77	26.67
	TS1	-5.20	1.73	-3.10	44.82
	Pr 1	-228.05	-207.02	-211.14	-162.81
	PRC2	-9.33	-4.25	-3.99	28.53
	TS2	-3.89	3.00	-1.86	46.19
	Pr 2	-222.85	-202.41	-206.02	-159.23
25	PRC1	-19.79	-15.27	-14.27	14.87
	TS1	-15.76	-9.16	-12.98	33.07
	Pr1	-240.02	-221.25	-225.09	-177.10
	PRC2	-19.28	-14.83	-13.77	14.75
	TS2	-13.31	-6.89	-10.74	35.32
	Pr2	-238.68	-220.07	-223.56	-177.03
26	PRC1	-23.07	-18.27	-17.64	14.81
	TS1	-7.06	-1.01	-5.53	43.20
	Pr1	-236.10	-218.41	-222.02	-173.29
	PRC2	-23.07	-18.31	-17.65	14.84
	TS2	-6.51	-0.41	-4.94	43.97
	Pr2	-235.98	-218.50	-221.90	-174.09

Table S136:sCI-H_2O relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-33.45	-25.23	-26.71	2.98
	TS1	3.66	14.28	6.75	54.28
	Pr 1	-198.40	-177.58	-183.33	-139.24
	TS2	7.30	17.54	9.95	57.61
	Pr 2	-197.78	-177.21	-182.69	-139.24
23	PRC	-20.02	-13.83	-13.66	10.42
	TS1	16.17	25.70	19.17	67.37
	Pr 1	-216.28	-198.27	-203.24	-157.68
	TS2	14.94	24.60	18.00	65.52
	Pr 2	-210.94	-194.29	-198.52	-155.45
24	PRC	-29.63	-22.29	-23.22	7.38
	TS1	1.92	12.20	5.33	54.25
	Pr 1	-220.98	-201.72	-207.21	-159.98
	TS2	4.56	14.62	7.62	57.37
	Pr 2	-216.01	-197.85	-202.59	-157.32
25	PRC1	-29.54	-22.47	-23.08	8.91
	TS1	-23.47	-13.40	-19.82	28.92
	Pr1	-262.27	-245.71	-250.98	-204.25
	PRC2	-31.47	-24.20	-25.02	7.81
	TS2	-23.25	-13.34	-19.86	28.12
	Pr2	-262.26	-245.48	-250.81	-204.05
26	PRC	-34.39	-26.80	-27.95	7.40
	TS1	-15.50	-5.89	-12.48	36.97
	Pr1	-248.73	-233.05	-238.13	-190.76
	TS2	-17.18	-7.47	-14.07	35.93
	Pr2	-257.20	-241.56	-246.67	-198.96

Table S137:sCI-$(H_2O)_2$ relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	PRC1.1	-49.94	-39.05	-42.86	6.35
	TS1.1	-37.08	-26.33	-36.42	27.73
	Pr1.1	-209.63	-187.13	-193.79	-136.65
	AAAH- con 1 + H_2O	-178.18	-166.33	-170.00	-151.72
	PRC1.2	-49.71	-39.63	-42.97	5.58
	TS1.2	-31.89	-22.56	-32.71	31.77
	Pr1.2	-212.35	-190.79	-196.74	-140.82
	AAAH- con 2 + H_2O	-177.56	-165.96	-169.36	-151.71
	PRC1.3	-52.02	-40.84	-44.84	5.83
	TS1.3	-37.47	-27.17	-37.34	27.30
	Pr1.3	-215.73	-193.17	-199.71	-142.41
	AAAH- con 2 + H_2O	-177.56	-165.96	-169.36	-151.71
	PRC1.4	-50.89	-39.70	-43.73	6.71
	TS1.4	-38.06	-27.03	-37.10	27.20
	Pr1.4	-211.93	-189.14	-195.99	-138.25
	AAAH- con 1 + H_2O	-178.18	-166.33	-170.00	-151.72
23	PRC1.1	-44.07	-34.62	-37.44	14.41
	TS1.1	-33.71	-24.33	-33.38	32.85
	Pr1.1	-225.49	-207.53	-212.46	-155.75
	AAAH- con 2 + H_2O	-190.73	-183.04	-185.19	-167.93
	PRC1.2	-45.59	-35.42	-38.62	14.50
	TS1.2	-37.16	-27.10	-36.10	30.21
	Pr1.2	-227.04	-208.90	-213.81	-157.22
	AAAH- con 2 + H_2O	-190.73	-183.04	-185.19	-167.93
	PRC1.3	-41.52	-32.45	-34.99	16.62
	TS1.3	-32.06	-21.91	-30.89	35.88
	Pr1.3	-225.79	-207.51	-212.36	-155.73
	AAAH- con 1 + H_2O	-196.06	-187.02	-189.91	-170.15
	PRC1.4	-42.99	-33.27	-36.24	16.42
	TS1.4	-35.14	-24.60	-33.56	33.19
	Pr1.4	-230.34	-211.42	-216.72	-158.84
	AAAH- con 1 + H_2O	-196.06	-187.02	-189.91	-170.15
24	PRC1.1	-45.80	-36.24	-39.29	12.94
	TS1.1	-39.81	-29.91	-39.16	28.14
	Pr1.1	-230.20	-211.29	-216.65	-157.80
	AAAH con 2 + H_2O	-195.79	-186.60	-189.25	-169.79
	PRC1.2	-47.90	-37.15	-40.95	13.39
	TS1.2	-44.92	-34.20	-43.41	23.91
	Pr1.2	-234.30	-214.87	-220.32	-162.09
	AAAH con 2 + H_2O	-195.79	-186.60	-189.25	-169.79
	PRC1.3	-46.58	-36.49	-39.81	11.81
	TS1.3	-42.62	-31.73	-40.88	25.82
	Pr1.3	-232.92	-212.74	-218.65	-158.95
	AAAH con 2 + H_2O	-200.76	-190.47	-193.88	-172.45
	PRC1.4	-47.44	-37.11	-40.58	12.03
	TS1.4	-43.44	-32.44	-41.56	25.24
	Pr1.4	-234.79	-214.44	-220.45	-160.33
	AAAH con 2 + H_2O	-200.76	-190.47	-193.88	-172.45

25	PRC1.1	-65.71	-54.79	-58.92	-2.60
	TS1.1	-67.51	-57.30	-66.16	0.80
	Pr1.1	-278.44	-261.06	-266.52	-208.19
	AAAH- con 2 + H_2O	-242.05	-234.23	-237.48	-216.53
	PRC1.2	-67.94	-56.28	-60.84	-3.29
	TS1.2	-70.81	-59.93	-68.72	-1.75
	Pr1.2	-278.44	-261.06	-266.52	-208.19
	AAAH- con 2 + H_2O	-242.05	-234.23	-237.48	-216.53
	PRC1.3	-65.12	-53.83	-58.33	-0.73
	TS1.3	-69.10	-58.00	-66.66	0.38
	Pr1.3	-283.44	-266.55	-271.62	-214.61
	AAAH- con 1 + H_2O	-242.05	-234.46	-237.64	-216.72
	PRC1.4	-66.14	-54.49	-59.28	-1.08
	TS1.4	-70.78	-59.46	-68.03	-1.22
	Pr1.4	-283.44	-266.55	-271.62	-214.61
	AAAH- con 1 + H_2O	-242.05	-234.46	-237.64	-216.72
26	PRC1.1	-62.87	-53.00	-56.31	-2.06
	TS1.1	-60.67	-51.06	-59.89	7.37
	Pr1.1	-271.27	-255.42	-260.48	-201.38
	AAAH con 2 + H_2O	-236.98	-230.31	-233.34	-211.43
	PRC1.2	-65.55	-54.87	-58.65	-2.92
	TS1.2	-64.48	-54.26	-63.06	4.42
	Pr1.2	-273.87	-257.64	-262.87	-203.30
	AAAH con 2 + H_2O	-236.98	-230.31	-233.34	-211.43
	PRC1.3	-62.79	-52.60	-55.99	-2.37
	TS1.3	-59.52	-50.09	-59.06	8.25
	Pr1.3	-271.91	-255.94	-260.97	-202.54
	AAAH con 1 + H_2O	-228.51	-221.80	-224.80	-203.23
	PRC1.4	-61.51	-51.64	-54.83	-2.24
	TS1.4	-57.37	-48.45	-57.53	10.05
	Pr1.3	-271.91	-255.94	-260.97	-202.54
	AAAH con 1 + H_2O	-228.51	-221.80	-224.80	-203.23

Table 138: sCI-MeOH relative energies (ΔE), zero-point corrected energy(ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-34.19	-28.02	-27.75	7.54
	TS1	-12.01	-3.82	-8.37	42.59
	Con 1	-214.74	-199.05	-202.39	-153.88
	TS2	-7.16	0.10	-4.34	46.06
	Con 2	-205.71	-190.64	-193.87	-146.25
23	PRC 1	-20.14	-16.11	-14.10	12.20
	TS1	-0.87	5.80	2.56	54.13
	Pr1	-234.32	-221.49	-223.71	-173.78
	TS2	6.00	11.67	8.27	60.32
24	PRC	-31.11	-25.71	-24.89	11.75
	TS1	-16.83	-9.41	-13.27	39.95
	Pr1	-229.68	-215.37	-218.26	-165.47
	TS2	-12.45	-5.49	-9.13	43.38
	Pr2	-230.78	-216.98	-219.65	-168.36
25	PRC1	-30.26	-25.74	-24.07	8.00
	TS1	N/A	N/A	N/A	N/A
	Pr1	-278.79	-266.92	-269.31	-218.19
	PRC2	-35.73	-30.11	-29.29	7.75
	TS2	-33.98	-27.30	-30.75	22.32
	Pr2	-274.66	-262.01	-264.94	-212.13
26	PRC	-35.99	-30.77	-29.72	7.83
	TS1	-32.60	-26.18	-29.59	23.81
	Pr1	-258.18	-247.21	-249.63	-197.29
	PRC2	-36.93	-31.82	-30.73	6.91
	TS2	-32.73	-26.39	-29.66	23.37
	Pr2	-267.52	-256.12	-258.66	-206.58

3.5 Dipole-Dipole Capture ($k_{d\text{-}d}$) and Collision Limit (k_{COLL}) Values

To calculate to dipole-dipole capture ($k_{d\text{-}d}$) and collision limit (k_{COLL}) values the following details on each reactant is required:

Table 139: Reactants Dipole moments (μ_D, Debye), mass (m, amu), radii (r, Å) and C-O-O bond ratios

Reactant	Dipole Moment (μ_D, Debye)	Mass (m, amu)	radii (r, Å)	C=O-O Bond Ratio
sCI 1	4.3104	46.005	3.209	1.078
sCI 23	3.4822	113.993	4.082	1.064
sCI 24	2.5055	113.993	4.418	1.071
sCI 25	3.016	131.983	4.099	1.114
sCI 26	2.9299	131.983	4.447	1.101
HCHO	2.3887	30.011	2.017	N/A
HNO_3	2.2588	62.996	2.938	N/A
SO_2	1.8065	63.962	2.491	N/A
CF_3COOH	2.2289	113.993	4.237	N/A
HCl	1.1157	35.977	1.284	N/A
H_2O	1.8472	18.011	1.536	N/A
$(H_2O)_2$	2.631	36.021	3.911	N/A
H_2S	0.9902	33.988	1.944	N/A
HF	1.8124	20.006	0.924	N/A
MeOH	1.6556	32.026	2.829	N/A

3.5.1 Gas-collision limit (k_{COLL})

Table 140: The Gas-Collision Limits for all HFO-sCI reactions in this thesis at a variety of temperatures.

Reaction	Collision Limit (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + HCHO	1.04	1.21	1.26	1.32	1.46
sCI 1 + HNO_3	1.18	1.39	1.45	1.51	1.67
sCI 1 + SO_2	1.02	1.19	1.24	1.29	1.44
sCI 1 + CF_3COOH	1.57	1.84	1.91	2.00	2.21
sCI 1 + HCl	0.73	0.85	0.89	0.93	1.03
sCI 1 + H_2O	1.01	1.19	1.23	1.29	1.43
sCI 1 + $(H_2O)_2$	1.82	2.14	2.23	2.32	2.58
sCI 1 + H_2S	0.97	1.14	1.19	1.24	1.37
sCI 1 + HF	0.74	0.87	0.90	0.94	1.05
sCI 1 + MeOH	1.36	1.59	1.66	1.73	1.92
sCI 1 + CF_3CHO	1.24	1.46	1.52	1.58	1.76
sCI 1 + CF_3CFO	1.27	1.49	1.55	1.62	1.80
sCI 23 + HCHO	1.23	1.45	1.51	1.57	1.74
sCI 23 + HNO_3	1.25	1.47	1.53	1.59	1.77
sCI 23 + SO_2	1.09	1.28	1.33	1.39	1.54
sCI 23 + CF_3COOH	1.48	1.74	1.81	1.89	2.10
sCI 23 + HCl	0.89	1.04	1.09	1.13	1.26
sCI 23 + H_2O	1.29	1.52	1.58	1.65	1.83
sCI 23 + $(H_2O)_2$	1.97	2.31	2.41	2.52	2.79
sCI 23 + H_2S	1.15	1.34	1.40	1.46	1.62
sCI 23 + HF	0.98	1.15	1.20	1.25	1.39
sCI 23 + MeOH	1.54	1.81	1.88	1.97	2.18
sCI 24 + HCHO	1.37	1.61	1.68	1.75	1.94
sCI 24 + HNO_3	1.37	1.61	1.68	1.75	1.94
sCI 24 + SO_2	1.21	1.41	1.47	1.54	1.70
sCI 24 + CF_3COOH	1.60	1.88	1.96	2.04	2.27
sCI 24 + HCl	1.00	1.18	1.23	1.28	1.42
sCI 24 + H_2O	1.45	1.70	1.77	1.85	2.05
sCI 24 + $(H_2O)_2$	2.14	2.51	2.62	2.73	3.03
sCI 24 + H_2S	1.28	1.50	1.56	1.63	1.81
sCI 24 + HF	1.12	1.31	1.36	1.43	1.58
sCI 24 + MeOH	1.70	1.99	2.07	2.16	2.40
sCI 25 + HCHO	1.22	1.43	1.49	1.56	1.73
sCI 25 + HNO_3	1.23	1.44	1.50	1.56	1.73
sCI 25 + SO_2	1.07	1.25	1.31	1.36	1.51
sCI 25 + CF_3COOH	1.44	1.68	1.75	1.83	2.03
sCI 25 + HCl	0.88	1.03	1.08	1.12	1.25
sCI 25 + H_2O	1.29	1.51	1.57	1.64	1.82
sCI 25 + $(H_2O)_2$	1.95	2.29	2.38	2.48	2.76
sCI 25 + H_2S	1.14	1.33	1.39	1.45	1.61
sCI 25 + HF	0.98	1.15	1.19	1.25	1.38
sCI 25 + MeOH	1.53	1.79	1.87	1.95	2.16
sCI 26 + HCHO	1.37	1.60	1.67	1.74	1.93
sCI 26 + HNO_3	1.35	1.58	1.65	1.72	1.91
sCI 26 + SO_2	1.19	1.39	1.45	1.51	1.68
sCI 26 + CF_3COOH	1.56	1.83	1.90	1.99	2.20
sCI 26 + HCl	1.00	1.17	1.22	1.27	1.41
sCI 26 + H_2O	1.45	1.70	1.77	1.85	2.06
sCI 26 + $(H_2O)_2$	2.12	2.49	2.59	2.71	3.00
sCI 26 + H_2S	1.27	1.49	1.55	1.62	1.80
sCI 26 + HF	1.12	1.31	1.37	1.43	1.58
sCI 26 + MeOH	1.69	1.98	2.06	2.15	2.38

3.5.2 Isotropic Dipole-Dipole Capture Limit

Table 141: The Isotropic Dipole-Dipole Capture Limit for all sCI + alcohol reactions in this thesis at a variety of temperatures.

Reaction	Isotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + HCHO	11.34	10.75	10.61	10.45	10.10
sCI 1 + HNO_3	9.03	8.56	8.45	8.32	8.04
sCI 1 + SO_2	7.75	7.35	7.25	7.15	6.91
sCI 1 + CF_3COOH	8.06	7.64	7.54	7.43	7.18
sCI 1 + HCl	6.47	6.14	6.06	5.97	5.77
sCI 1 + H_2O	11.31	10.73	10.58	10.43	10.08
sCI 1 + $(H_2O)_2$	11.46	10.87	10.73	10.57	10.21
sCI 1 + H_2S	6.07	5.76	5.68	5.60	5.41
sCI 1 + HF	10.76	10.21	10.07	9.93	9.59
sCI 1 + MeOH	8.71	8.26	8.15	8.03	7.76
sCI 1 + CF_3CHO	6.95	6.59	6.50	6.41	6.19
sCI 1 + CF_3CFO	3.57	3.38	3.34	3.29	3.18
sCI 23 + HCHO	8.60	8.15	8.04	7.93	7.66
sCI 23 + HNO_3	6.34	6.01	5.93	5.85	5.65
sCI 23 + SO_2	5.43	5.15	5.08	5.01	4.84
sCI 23 + CF_3COOH	5.30	5.03	4.96	4.89	4.72
sCI 23 + HCl	4.82	4.57	4.51	4.45	4.30
sCI 23 + H_2O	8.95	8.49	8.38	8.26	7.98
sCI 23 + $(H_2O)_2$	8.54	8.10	7.99	7.88	7.61
sCI 23 + H_2S	4.55	4.32	4.26	4.20	4.06
sCI 23 + HF	8.45	8.01	7.91	7.79	7.53
sCI 23 + MeOH	6.56	6.22	6.14	6.05	5.85
sCI 24 + HCHO	6.90	6.55	6.46	6.37	6.15
sCI 24 + HNO_3	5.09	4.83	4.76	4.69	4.53
sCI 24 + SO_2	4.36	4.14	4.08	4.02	3.89
sCI 24 + CF_3COOH	4.26	4.04	3.98	3.93	3.79
sCI 24 + HCl	3.87	3.67	3.62	3.57	3.45
sCI 24 + H_2O	7.19	6.82	6.73	6.63	6.40
sCI 24 + $(H_2O)_2$	6.86	6.50	6.42	6.33	6.11
sCI 24 + H_2S	3.66	3.47	3.42	3.37	3.26
sCI 24 + HF	6.79	6.43	6.35	6.26	6.04
sCI 24 + MeOH	5.27	5.00	4.93	4.86	4.70
sCI 25 + HCHO	7.70	7.30	7.20	7.10	6.86
sCI 25 + HNO_3	5.62	5.33	5.26	5.18	5.00
sCI 25 + SO_2	4.82	4.57	4.51	4.44	4.29
sCI 25 + CF_3COOH	4.65	4.41	4.35	4.29	4.14
sCI 25 + HCl	4.31	4.09	4.03	3.98	3.84
sCI 25 + H_2O	8.06	7.64	7.54	7.43	7.18
sCI 25 + $(H_2O)_2$	7.63	7.24	7.14	7.04	6.80
sCI 25 + H_2S	4.07	3.86	3.81	3.76	3.63
sCI 25 + HF	7.60	7.21	7.11	7.01	6.77
sCI 25 + MeOH	5.87	5.57	5.50	5.42	5.23
sCI 26 + HCHO	7.55	7.16	7.07	6.97	6.73
sCI 26 + HNO_3	5.51	5.23	5.16	5.08	4.91
sCI 26 + SO_2	4.72	4.48	4.42	4.36	4.21
sCI 26 + CF_3COOH	4.56	4.32	4.27	4.21	4.06
sCI 26 + HCl	4.23	4.01	3.96	3.90	3.77
sCI 26 + H_2O	7.90	7.50	7.40	7.29	7.04
sCI 26 + $(H_2O)_2$	7.49	7.10	7.01	6.91	6.67
sCI 26 + H_2S	3.99	3.79	3.74	3.68	3.56
sCI 26 + HF	7.45	7.07	6.97	6.87	6.64
sCI 26 + MeOH	5.76	5.46	5.39	5.31	5.13

3.5.3 Adiabatic Anisotropic Dipole-Dipole Capture Limit

Table 142: The Adiabatic Anisotropic Dipole-Dipole Capture Limit for all sCI + alcohol reactions in this thesis at a variety of temperatures.

Reaction	Adiabatic anisotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + HCHO	7.45	7.06	6.97	6.87	6.63
sCI 1 + HNO_3	5.93	5.62	5.55	5.47	5.28
sCI 1 + SO_2	5.09	4.83	4.76	4.70	4.54
sCI 1 + CF_3COOH	5.29	5.02	4.95	4.88	4.72
sCI 1 + HCl	4.25	4.03	3.98	3.92	3.79
sCI 1 + H_2O	7.43	7.05	6.95	6.85	6.62
sCI 1 + $(H_2O)_2$	7.53	7.14	7.05	6.94	6.71
sCI 1 + H_2S	3.99	3.78	3.73	3.68	3.56
sCI 1 + HF	7.07	6.70	6.61	6.52	6.30
sCI 1 + MeOH	5.72	5.42	5.35	5.27	5.10
sCI 1 + CF_3CHO	4.57	4.33	4.27	4.21	4.07
sCI 1 + CF_3CFO	2.34	2.22	2.19	2.16	2.09
sCI 23 + HCHO	5.65	5.36	5.28	5.21	5.03
sCI 23 + HNO_3	4.16	3.95	3.90	3.84	3.71
sCI 23 + SO_2	3.57	3.39	3.34	3.29	3.18
sCI 23 + CF_3COOH	3.48	3.30	3.26	3.21	3.10
sCI 23 + HCl	3.17	3.00	2.96	2.92	2.82
sCI 23 + H_2O	5.88	5.58	5.50	5.42	5.24
sCI 23 + $(H_2O)_2$	5.61	5.32	5.25	5.18	5.00
sCI 23 + H_2S	2.99	2.84	2.80	2.76	2.66
sCI 23 + HF	5.55	5.26	5.19	5.12	4.94
sCI 23 + MeOH	4.31	4.09	4.03	3.98	3.84
sCI 24 + HCHO	4.53	4.30	4.24	4.18	4.04
sCI 24 + HNO_3	3.34	3.17	3.13	3.08	2.98
sCI 24 + SO_2	2.87	2.72	2.68	2.64	2.55
sCI 24 + CF_3COOH	2.80	2.65	2.62	2.58	2.49
sCI 24 + HCl	2.54	2.41	2.38	2.35	2.27
sCI 24 + H_2O	4.72	4.48	4.42	4.35	4.21
sCI 24 + $(H_2O)_2$	4.51	4.27	4.22	4.16	4.01
sCI 24 + H_2S	2.40	2.28	2.25	2.21	2.14
sCI 24 + HF	4.46	4.23	4.17	4.11	3.97
sCI 24 + MeOH	3.46	3.28	3.24	3.19	3.08
sCI 25 + HCHO	5.06	4.80	4.73	4.66	4.51
sCI 25 + HNO_3	3.69	3.50	3.45	3.40	3.29
sCI 25 + SO_2	3.16	3.00	2.96	2.92	2.82
sCI 25 + CF_3COOH	3.05	2.90	2.86	2.82	2.72
sCI 25 + HCl	2.83	2.69	2.65	2.61	2.52
sCI 25 + H_2O	5.29	5.02	4.95	4.88	4.72
sCI 25 + $(H_2O)_2$	5.01	4.76	4.69	4.62	4.47
sCI 25 + H_2S	2.67	2.54	2.50	2.47	2.38
sCI 25 + HF	4.99	4.73	4.67	4.60	4.45
sCI 25 + MeOH	3.86	3.66	3.61	3.56	3.44
sCI 26 + HCHO	4.96	4.70	4.64	4.58	4.42
sCI 26 + HNO_3	3.62	3.43	3.39	3.34	3.22
sCI 26 + SO_2	3.10	2.94	2.90	2.86	2.76
sCI 26 + CF_3COOH	3.00	2.84	2.80	2.76	2.67
sCI 26 + HCl	2.78	2.63	2.60	2.56	2.47
sCI 26 + H_2O	5.19	4.92	4.86	4.79	4.63
sCI 26 + $(H_2O)_2$	4.92	4.66	4.60	4.54	4.38
sCI 26 + H_2S	2.62	2.49	2.45	2.42	2.34
sCI 26 + HF	4.90	4.64	4.58	4.52	4.36
sCI 26 + MeOH	3.78	3.59	3.54	3.49	3.37

3.5.3 Non-Adiabatic Anisotropic Dipole-Dipole Capture Limit

Table 143: The Non-Adiabatic Anisotropic Dipole-Dipole Capture Limit for all sCI + alcohol reactions in this thesis at a variety of temperatures.

Reaction	Non-adiabatic anisotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + HCHO	5.43	5.15	5.08	5.00	4.83
sCI 1 + HNO_3	4.32	4.10	4.04	3.98	3.85
sCI 1 + SO_2	3.71	3.52	3.47	3.42	3.31
sCI 1 + CF_3COOH	3.86	3.66	3.61	3.56	3.44
sCI 1 + HCl	3.10	2.94	2.90	2.86	2.76
sCI 1 + H_2O	5.42	5.14	5.07	4.99	4.82
sCI 1 + $(H_2O)_2$	5.49	5.20	5.13	5.06	4.89
sCI 1 + H_2S	2.91	2.76	2.72	2.68	2.59
sCI 1 + HF	5.15	4.89	4.82	4.75	4.59
sCI 1 + MeOH	4.17	3.95	3.90	3.84	3.71
sCI 1 + CF_3CHO	3.33	3.16	3.11	3.07	2.96
sCI 1 + CF_3CFO	1.71	1.62	1.60	1.57	1.52
sCI 23 + HCHO	4.12	3.90	3.85	3.80	3.67
sCI 23 + HNO_3	3.03	2.88	2.84	2.80	2.70
sCI 23 + SO_2	2.60	2.47	2.43	2.40	2.32
sCI 23 + CF_3COOH	2.54	2.41	2.37	2.34	2.26
sCI 23 + HCl	2.31	2.19	2.16	2.13	2.06
sCI 23 + H_2O	4.29	4.06	4.01	3.95	3.82
sCI 23 + $(H_2O)_2$	4.09	3.88	3.83	3.77	3.64
sCI 23 + H_2S	2.18	2.07	2.04	2.01	1.94
sCI 23 + HF	4.04	3.84	3.78	3.73	3.60
sCI 23 + MeOH	3.14	2.98	2.94	2.90	2.80
sCI 24 + HCHO	3.30	3.13	3.09	3.05	2.94
sCI 24 + HNO_3	2.44	2.31	2.28	2.25	2.17
sCI 24 + SO_2	2.09	1.98	1.95	1.93	1.86
sCI 24 + CF_3COOH	2.04	1.93	1.91	1.88	1.81
sCI 24 + HCl	1.85	1.76	1.73	1.71	1.65
sCI 24 + H_2O	3.44	3.26	3.22	3.17	3.07
sCI 24 + $(H_2O)_2$	3.28	3.11	3.07	3.03	2.93
sCI 24 + H_2S	1.75	1.66	1.64	1.61	1.56
sCI 24 + HF	3.25	3.08	3.04	3.00	2.89
sCI 24 + MeOH	2.52	2.39	2.36	2.33	2.25
sCI 25 + HCHO	3.69	3.50	3.45	3.40	3.28
sCI 25 + HNO_3	2.69	2.55	2.52	2.48	2.40
sCI 25 + SO_2	2.30	2.19	2.16	2.13	2.05
sCI 25 + CF_3COOH	2.23	2.11	2.08	2.05	1.98
sCI 25 + HCl	2.06	1.96	1.93	1.90	1.84
sCI 25 + H_2O	3.86	3.66	3.61	3.56	3.44
sCI 25 + $(H_2O)_2$	3.65	3.47	3.42	3.37	3.26
sCI 25 + H_2S	1.95	1.85	1.82	1.80	1.74
sCI 25 + HF	3.64	3.45	3.40	3.35	3.24
sCI 25 + MeOH	2.81	2.67	2.63	2.59	2.51
sCI 26 + HCHO	3.62	3.43	3.38	3.33	3.22
sCI 26 + HNO_3	2.64	2.50	2.47	2.43	2.35
sCI 26 + SO_2	2.26	2.14	2.12	2.09	2.01
sCI 26 + CF_3COOH	2.18	2.07	2.04	2.01	1.94
sCI 26 + HCl	2.02	1.92	1.89	1.87	1.80
sCI 26 + H_2O	3.78	3.59	3.54	3.49	3.37
sCI 26 + $(H_2O)_2$	3.58	3.40	3.35	3.31	3.19
sCI 26 + H_2S	1.91	1.81	1.79	1.76	1.70
sCI 26 + HF	3.57	3.38	3.34	3.29	3.18
sCI 26 + MeOH	2.76	2.62	2.58	2.54	2.46

3.6 sCI 23 & 24 + HCl Comparative Literature Analysis.

In a Cabezas *et* Endo study, a computational analysis of the potential energy surface of the *syn*- & *anti*-CH_3CHOO + HCl reactions, which is the closest analogous reaction to **sCIs 23** & **24** + HCl (*syn*- & *anti*-CF_3CHOO + HCl). The lack of hyperconjugation usually provided by the α-H atoms in a -CH_3 group means that **sCI 24** + HCl produced a higher TS barrier (-13.4 kJ mol^{-1}) than the barrierless that *anti*-CH_3CHOO + HCl reaction. The *syn*-CH_3CHOO + HCl, following trends in the literature is less reactive than produces its *anti* equivalent, producing a barrier (-39.1 kJ mol^{-1}). Contrary to the usual trend in this chapter, the **sCI 23** + HCl reaction in this chapter has a higher energy barrier (6.0 kJ mol^{-1}) than that of *syn*-CH_3CHOO + HCl energy barrier. But the Cabezas *et* Endo study uses a different less exhaustive approach (CCSD/aug-cc-pVTZ) compared to the work in this chapter, so it would require a more intense comparative analysis of these methods or may require experimental analysis to determine the true reactivity order. To the author's knowledge there are no other experimental or theoretical data to this work on **sCIs 23—26** with HF or HCl.

4.0 Supplementary Information for Chapter 6: Modelling the Ozonolysis of Alkenes With Lengthy Alkyl Substituents

4.1 Background Previous Literature Information

The general structures of the alkenes used in this section are outlined below. These are propene, 1-butene, 2-methyl-2-butene, 2-methyl-2-pentene, *E*-2-pentene, *Z*-2-pentene, *E*-2-butene, *Z*-2-butene and *Z*-2-hexene (Alkenes **1**, **2**, **6**, **7** & **15**—**19**):

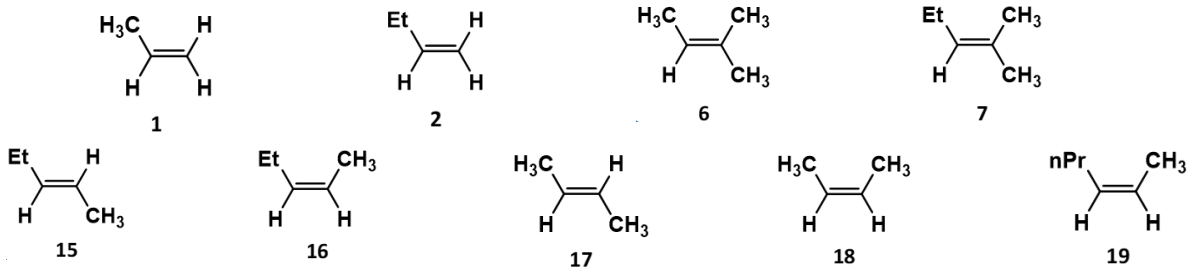


*Figure 6.23: Chemical Structures of Alkenes **1**, **2**, **6**, **7** & **15—19***

The section here contains some data from the literature that was used to validate that the ozonolysis of Alkenes with lengthy alkyl substituents were worth exploring.

4.1.1 Previous Atmospheric Levels of Lengthy Alkenes

Table 144: The abundance of lengthy alkenes in various environments.

Co-reactant Environment	Abundance (Original units)	Study	Ref
1-Pentene			
- Mega city	9.0×10^9 cm^3 s^{-1}	Vereecken *et al.*	66
- Rural Europe	1.5×10^8 cm^3 s^{-1}	Vereecken *et al.*	66
Taipei Urban - Summer Daytime	0.06 ppbv	Wang *et al.*	69
Taipei Urban - Summer Night-time	0.08 ppbv	Wang *et al.*	69
Taipei Urban - Autumn Daytime	0.03 ppbv	Wang *et al.*	69
Taipei Urban - Autumn Night-time	0.04 ppbv	Wang *et al.*	69
1-pentene in Los Angeles	0.14 — 2.75 ppb	North *et al.*	77
1-Hexene			
- Mega city	3.0×10^9 cm^3 s^{-1}	Vereecken *et al.*	66
- Rural Europe	8.4×10^7 cm^3 s^{-1}	Vereecken *et al.*	66
(*E*)-2-hexene			
Taipei Urban - Summer Daytime	0.05 ppbv	Wang *et al.*	69
Taipei Urban - Summer Night-time	0.06 ppbv	Wang *et al.*	69
Taipei Urban - Autumn Daytime	0.03 ppbv	Wang *et al.*	69
Taipei Urban - Autumn Night-time	0.04 ppbv	Wang *et al.*	69
E-2-hexene in Los Angeles	0.13 — 2.31 ppb	North *et al.*	77
Alkene 19 (*Z*-2-hexene)			

Taipei Urban - Summer Daytime	0.02 ppbv	Wang *et al.*	[69]
Taipei Urban - Summer Night-time	0.03 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Daytime	0.01 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Night-time	0.01 ppbv	Wang *et al.*	[69]
Z-2-hexene in Los Angeles	0.05 — 1.04 ppb	North *et al.*	[77]
Boston	0.02 ppbv	Percival *et al.*	[70]
Porto Alegre	1.6 ppbv	Percival *et al.*	[70]
4-Methyl-1-pentene			
Taipei Urban - Summer Daytime	0.05 ppbv	Wang *et al.*	[69]
Taipei Urban - Summer Night-time	0.04 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Daytime	0.02 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Night-time	0.02 ppbv	Wang *et al.*	[69]
2-Methyl-1-pentene			
Taipei Urban - Summer Daytime	0.05 ppbv	Wang *et al.*	[69]
Taipei Urban - Summer Night-time	0.04 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Daytime	0.02 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Night-time	0.02 ppbv	Wang *et al.*	[69]
α-pinene			
Taipei Urban - Summer Daytime	0.21 ppbv	Wang *et al.*	[69]
Taipei Urban - Summer Night-time	0.12 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Daytime	0.08 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Night-time	0.06 ppbv	Wang *et al.*	[69]
β-pinene			
Taipei Urban - Summer Daytime	0.01 ppbv	Wang *et al.*	[69]
Taipei Urban - Summer Night-time	0.01 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Daytime	0.01 ppbv	Wang *et al.*	[69]
Taipei Urban - Autumn Night-time	0.01 ppbv	Wang *et al.*	[69]
Ozone (O_3)			
summertime conditions - Houston	40–60 ppbv	Ryerson *et al.*	[65]
Can exceed	200 ppbv	Ryerson *et al.*	[65]
O_3 – Boreal Forest	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	[66]
O_3 – Tropical Forest/Rainforest	7.3×10^{11} cm^3 s^{-1}	Vereecken *et al.*	[66]
O_3 – Mega city	1.9×10^{12} cm^3 s^{-1}	Vereecken *et al.*	[66]
O_3 – Rural Europe	1.4×10^{12} cm^3 s^{-1}	Vereecken *et al.*	[66]

4.1.2 Experimental Literature on the Ozonolysis of Lengthy Alkenes

The Rate constants given here are simply to show that prior to work being undertaken in the main thesis, the ozonolysis of these alkenes shows that determining the k_{EXP} values is valuable.

Table 145: Experimental Rate Constants (k_{EXP}) of the Ozonolysis of Various Example Lengthy Alkenes.

Alkene	k_{EXP} ($\times 10^{-17}$ cm^3 s^{-1})	Study	Ref
1-pentene	1.06 ± 0.32	Calvert *et al.*	[12]
	0.87 ± 0.02	Avzianova and Ariya	[14]
	1.09	Grosjean and Grosjean	[151]
	0.92 ± 0.05	Treacy *et al.*	[21]
1-Hexene	1.13 ± 0.28	Calvert *et al.*	[12]
	0.96 ± 0.02	Avzianova and Ariya	[14]
	0.97	Grosjean and Grosjean	[151]
	1.02 ± 0.06	Treacy *et al.*	[21]
	1.17 ± 0.35	Atkinson and Carter	[26]
1-Heptene	1.2 ± 0.15	Calvert *et al.*	[12]
	0.92 ± 0.03	Avzianova and Ariya	[14]
	0.94	Grosjean and Grosjean	[151]
	1.73	Atkinson *et al.*	[36]
	0.81	Cadle *et al.*	[152]
trans-2-Hexene	1.57 ± 0.47	Calvert *et al.*	[12]
	15.5 ± 0.06	Avzianova and Ariya	[14]
Alkene **19** (*cis*-2-Hexene)	14.4 ± 4.3	Calvert *et al.*	[12]
	10.9 ± 0.04	Avzianova and Ariya	[14]
2-Methyl-1-pentene	1.6 ± 0.5	Calvert *et al.*	[12]
4-Methyl-1-pentene	1.0 ± 0.3	Calvert *et al.*	[12]

*Table 146: Yield of OH radicals (OH yield) of the Ozonolysis of similar alkenes to Alkene **19**. (Degree of uncertainty in parentheses)*

Alkene	OH yield	Study	Ref
1-pentene	0.24—0.37 (0.19—0.55)	Calvert *et al.*	[12]
1-Hexene	0.18—0.32 (0.14—0.48)	Calvert *et al.*	[12]
1-Heptene	0.27 (± 0.13)	Calvert *et al.*	[12]
1-Octene	0.10—0.18 (0.07—0.27)	Calvert *et al.*	[12]
trans-2-pentene	0.27—0.29 (0.20—0.35)	Calvert *et al.*	[12]
Alkene **19** (*cis*-2-pentene)	0.46 (0.38—0.54)	Calvert *et al.*	[12]
trans-3-Hexene	0.53 (± 0.08)	Calvert *et al.*	[12]
cis-3-Hexene	0.36 (± 0.08)	Calvert *et al.*	[12]

Similar product distribution results are found in the main body of Chapter 6 in Section 6.8.

4.1.3 Previous Methods of Modelling Complex Reaction Systems

Whilst a full study using either *ab initio* or DFT methods would have too high a computational cost, there are some other approaches that are potentially useful when analysing O_3 + Alkene **19**, including using molecular dynamics methods or Monte-Carlo simulations. Molecular dynamics explores the interactions and trajectories of a reaction using Newton's laws of motion and the known forces acting upon individual atoms within the molecule.[153] It does not allow the identification of specific transition states or minima using quantum chemistry. Therefore molecular dynamics calculations would have much reduced accuracy, and is usually only applied in much larger reaction systems than the ozonolysis of Z-2-hexene, such as how pharmaceutical drugs fit into active sites.[154-156]

On the other hand, Monte-Carlo simulation methods can be employed to manage reactions involving flexible structures by running vast numbers of randomly generated reaction trajectories, often ~10^6, on the two reactants.[157] Due to the huge numbers of random simulations, there is a high probability that all TSs would be identified and therefore the total reaction chemical analysis can be derived. These reaction trajectories can be generated using normal DFT, or can be undertaken using MD which can be subsequently refined by *ab initio* methods. No knowledge is required of either TSs or products to use this method.[158] This has previously been applied to the decomposition of sCIs from the ozonolysis of *trans*-2-butene and 2,3-dimethyl-2-butene; *β*-pinene-derived-sCI + $H_2O/(H_2O)_2$; and SO_2 + $HCHOO/(CH_3)_2COO$.[157-159] Whilst it often provides accurate analysis for a specific system, the vast number of simulations still require very large amounts of computational cost and therefore is not necessarily any more useful in exploring a broad range of alkenes.

Some computational studies, for example the investigation of the reaction between H_2O and the *anti*-sCI derived from Sabinene, choose to disregard any computational complexity and investigate only the alleged lowest energy pathways to determine the reaction chemistry.[160-164] This is a hugely imperfect solution because, even assuming that the lowest energy pathways calculated are correct, the contributions of sub-pathways can alter both the k_{THEO} and Γ_{THEO} values significantly, as shown for both O_3 reactions with Alkenes **2** & **8**, in Chapter 3.

McGillen and co-workers produced a straightforward model to determine the alkene ozonolysis rate constant based on alkenes geometric structure, referred to as a *Structure-Activity Relationship* (SAR).[48] This model is generates a numerical "χ" value that incorporates the structural factors of a mono-alkene (deemed important by McGillen and

co-workers), and fits these χ values derived from a range of alkenes to their respective ozonolysis k_{EXP} values. The subsequent correlation between the χ value and the $\log_{10}(k_{EXP})$ value is used as the "SAR equation" to estimate the rate constant (k_{SAR}) of other alkenes using their structural features. (An extended background of the SAR model is found in Section 1.8.5 and the method is found in Section 2.7)

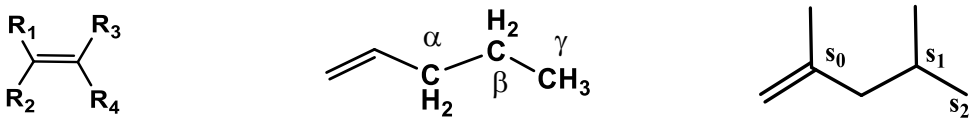


Figure 6.24: Alkenes R_1—R_4 substituent positions and the positions of hydrogen analogues on a substituent carbon chain labelled using Greek letters (α, β, γ …), and the structure of 2,4-dimethyl-1-pentene labelled s_0, s_1 & s_2 according to which alkyl segment(s) causes the s_0, s_1 & s_2 steric effect in the SAR model.

The two structural concepts used to generate this χ value include: that a larger number of the alkyl groups in the R_1—R_4 positions induces greater alkene reactivity, and that the spatial arrangement and steric bulk of those alkyl groups can obstruct the >C=C< reaction site. These two factors are shown to influence alkene ozonolysis in Chapter 3. The specific spatial arrangement of having two alkyl substituents in the R_1 & R_2 positions, such as for 2,4-dimethyl-1-pentene, increases steric bulk around the >C=C< bond and hampers reactivity (referred to as the s_0 effect in Figure 6.9). Alkene substituents with additional β- or γ-alkyl groups (on s_1 or s_2) inhibit reactivity more substantially.

This SAR model developed by McGillen and co-workers shows several advantages most notably that it is a very simple model that can determine relatively accurate k_{SAR} values for alkene ozonolysis compared to literature k_{EXP} values.[48] However, the SAR model does not determine SAR product branching ratios (Γ_{SAR}) for CIs or even for the aldehyde/ketone products.[14] Also, this model does not distinguish between *E*- & *Z*-alkenes, despite there being a significant difference in both k_{EXP} and Γ_{EXP} values for these different conformeric forms.[14] Analysis of the O_3 + Alkene **19** requires both Γ_{THEO} values and different chemistry for *E* & *Z*-alkenes, so this SAR method is not comprehensive enough to be used for O_3 + Alkene **19**.[101–105] For these reasons, the k_{SAR} values for O_3 + Alkene **19** (2.89×10^{-16} cm^3 s^{-1}) is used here only as a comparison to the results of the authors new methodologies.

4.1.4 Existing Literature Studies on the Ozonolysis of Lengthy Alkenes

It is thought that ozonolysis of *E*-2-hexene and Alkene **19** have rate constants high enough (~10^{-16} cm^3 s^{-1}) that they will not only deplete tropospheric alkenes but also generate important bimolecular reaction products.[12,14] Determining the Γ_{THEO} values of the different CIs is important because, to the author's knowledge, there is no experimental data on product yields for O_3 + Alkene **19** (or O_3 + *E*-2-hexene either).[12] The Γ_{THEO} values of CIs obtained herein are vital to atmospheric models, potentially being stabilised to sCIs (explored in Chapters 4 & 5) or fragmenting to produce secondary yields of OH radical (see Introduction Section 1.5 for more details).[12,15,19,42,91,113,136,165–174] Experimental ozonolysis yields for similar alkenes have been measured, with high sCI yields from the reaction of O_3 + 1-pentene (0.29 — 0.45) and the substantial OH radical yields from the ozonolysis of 1-pentene and *E*- & *Z*-2-pentene (>0.25).[30,38,95,175,176] This provides further evidence that determining the full set of Γ_{THEO} values for O_3 reactions with Alkene **19** and other similar lengthy alkenes, such as 1-pentene, *E*-2-hexene and 2-methyl-2-hexene, is incredibly useful.

It has been noted in the literature that increasing an alkene substituent chain length beyond 3 carbons long, does not substantially change the alkene's ozonolysis chemistry, having a minimal effect on k_{EXP} and Γ_{EXP} values.[48,95] This makes the lengthening of the —R_1 chain from —Et to —nPr much more important because all "—CH_2-CH_2-CR_3" alkyl chains may be included in a single taxonomic group. Examples of this would be that the k_{THEO} & Γ_{THEO} results for O_3 + 1-pentene, *E*-2-hexene, Alkene **19** & 2-methyl-2-hexene would also apply to O_3 + 1-hexene, *E*- & *Z*-2-heptene & 2-methyl-2-heptene, respectively. This amplifies the value of any model derived herein to describe these alkene sets.

4.2 Use of FESP model 1 on Smaller Alkenes

To determine the accuracy of FESP model 1, and the MESMER projection technique that it is based on, were both separately validated by comparing the results obtained from applying the MESMER projection technique and then later FESP model 1 as a whole. These are applied to 1-butene, *E*-2-pentene, *Z*-2-pentene and 2-methyl-2-pentene (Alkenes **2**, **15**, **16** & **7**) using the MESMER input files and the energy adjustment from propene, *E*-2-butene, *Z*-2-butene and 2-methyl-2-butene (Alkenes **1**, **17**, **18** & **6**):

To test the reliability of both the MESMER Projection Technique were tested using calculated ΔG_{THEO} results medium alkenes (Alkenes **2**, **15**, **16** & **7**) and the Δ_{ADJ} values from the smaller alkenes (Alkenes **1**, **17**, **18** & **6**) to determine the ΔE_{ADJ} values to input into the MESMER input file, where the k_{TEST} & Γ_{TEST} are calculated.

4.2.1 Adjusted Data from MESMER projection Technique

*Table 147: Adjusted ΔE_{ADJ} values for each TS of O_3 + Alkenes **2** & **15** using ΔG_{THEO} results.*

O_3 + Alkene **2**			O_3 + Alkene **15**		
TS	**kJ mol^{-1}**		**TS**	**kJ mol^{-1}**	
	ΔG_{THEO}	**ΔE_{ADJ}**		**ΔG_{THEO}**	**ΔE_{ADJ}**
TS_{OZO} 1.1	56.93	11.55	TS_{OZO} 1.1	47.81	2.32
TS_{OZO} 1.2	57.88	12.51	TS_{OZO} 1.2	52.58	7.09
TS_{OZO} 1.3	56.40	11.02	TS_{OZO} 1.3	53.82	8.33
TS_{OZO} 2.1	61.15	15.97	TS_{OZO} 2.1	53.60	8.11
TS_{OZO} 2.2	63.98	18.80	TS_{OZO} 2.2	55.25	9.76
TS_{OZO} 2.3	58.39	13.22	TS_{OZO} 2.3	51.83	6.34
TS_{FO} 1.1	-108.70	-157.27	TS_{ANTI} 1.1	-113.92	-163.53
TS_{FO} 1.2	-108.04	-156.61	TS_{ANTI} 1.2	-120.06	-169.67
TS_{FO} 1.3	-109.21	-157.79	TS_{ANTI} 1.3	-122.47	-172.09
TS_{FO} 2.1	-106.39	-154.55	TS_{ANTI} 1.1	-114.76	-164.38
TS_{FO} 2.2	-106.68	-154.84	TS_{ANTI} 1.2	-121.89	-171.50
TS_{FO} 2.3	-107.63	-155.79	TS_{ANTI} 1.3	-122.54	-172.15
TS_{ANTI} 1	-113.30	-161.67	TS_{SYN} 1.1	-123.53	-173.99
TS_{ANTI} 2	-112.79	-161.16	TS_{SYN} 1.2	-120.22	-170.68
TS_{ANTI} 3	-115.45	-163.81	TS_{SYN} 1.3	-124.15	-174.61
TS_{SYN} 1	-112.36	-161.42	TS_{SYN} 2.1	-122.27	-172.73
TS_{SYN} 2	-100.89	-149.95	TS_{SYN} 2.2	-111.46	-161.91
TS_{SYN} 3	-113.34	-162.40	TS_{SYN} 2.3	-122.98	-173.44

*Table 148: Adjusted ΔE_{ADJ} values for each TS of O_3 + Alkenes **16** & **7** using ΔG_{THEO} results.*

O_3 + Alkene **16**			O_3 + Alkene **7**		
TS	**kJ mol^{-1}**		**TS**	**kJ mol^{-1}**	
	ΔG_{THEO}	**ΔE_{ADJ}**		**ΔG_{THEO}**	**ΔE_{ADJ}**
TS_{OZO} 1.1	49.57	4.96	TS_{OZO} 1.1	46.58	0.32
TS_{OZO} 1.2	62.29	17.67	TS_{OZO} 1.2	61.52	15.26
TS_{OZO} 1.3	46.58	1.97	TS_{OZO} 1.3	45.81	-0.45
TS_{OZO} 2.1	58.31	12.74	TS_{OZO} 2.1	53.58	5.86
TS_{OZO} 2.2	70.53	24.96	TS_{OZO} 2.2	65.35	17.62
TS_{OZO} 2.3	52.70	7.13	TS_{OZO} 2.3	48.56	0.83
TS_{ANTI} 1.1	-125.47	-176.74	TS_{DMFO} 1.1	-132.13	-185.44
TS_{ANTI} 1.2	-118.88	-170.15	TS_{DMFO} 1.2	-135.08	-188.38
TS_{ANTI} 1.3	-127.14	-178.41	TS_{DMFO} 1.3	-138.63	-191.93
TS_{ANTI} 1.1	-121.30	-172.57	TS_{DMFO} 2.1	-120.45	-173.49
TS_{ANTI} 1.2	-125.68	-176.95	TS_{DMFO} 2.2	-121.51	-174.55
TS_{ANTI} 1.3	-127.56	-178.83	TS_{DMFO} 2.3	-129.55	-182.59
TS_{SYN} 1.1	-111.34	-163.22	TS_{ANTI} 1	-117.98	-170.48
TS_{SYN} 1.2	-98.21	-150.09	TS_{ANTI} 2	-121.25	-173.75
TS_{SYN} 1.3	-115.02	-166.90	TS_{ANTI} 3	-127.80	-180.30
TS_{SYN} 2.1	-115.56	-167.44	TS_{SYN} 1	-117.61	-171.04
TS_{SYN} 2.2	-109.03	-160.91	TS_{SYN} 2	-103.99	-157.43
TS_{SYN} 2.3	-116.44	-168.32	TS_{SYN} 3	-119.90	-173.33

4.2.2 Comparing MESMER projection technique to Computational results

Table 149: Testing the rates MESMER projection technique *(k_{TEST}) with full computational analysis (k_{COMP}) (10^{-18} cm^3 s^{-1}) and product yields (Γ_{TEST} & Γ_{COMP}) of O_3 + alkene **2** by both subchannel (TS .1, TS .2 & TS .3) and overall channel (**Σ(TS)**)*

Channel	**k_{PROJ} [10^{-18} cm^3 s^{-1}]**				**k_{THEO} [10^{-18} cm^3 s^{-1}]**				**k_{PROJ} - k_{COMP}**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
TS_{OZO} 1	22.6	12.7	36.3	**71.6**	27.7	19.0	34.1	**80.8**	-9.2
TS_{OZO} 2	5.1	1.4	10.2	**16.6**	5.10	1.65	15.2	**21.9**	-5.3
Total *k*	**88.2**				**102.7**				-14.5
Channel	**Γ_{TEST}**				**Γ_{THEO}**				**$\Delta\Gamma$**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
Γ_{H_2COO} (1)	0.060	0.050	0.069	**0.179**	0.068	0.058	0.073	**0.199**	-0.020
Γ_{H_2COO} (2)	0.054	0.035	0.067	**0.156**	0.057	0.051	0.065	**0.173**	-0.017
$\Gamma_{anti\text{-}CH_3CHOO}$	0.142	0.119	0.164	**0.425**	0.130	0.108	0.188	**0.427**	-0.002
$\Gamma_{syn\text{-}CH_3CHOO}$	0.083	0.055	0.102	**0.240**	0.082	0.019	0.099	**0.201**	0.039

Table 150: Testing the rates MESMER projection technique *(k_{TEST}) with full computational analysis (k_{COMP}) (10^{-18} cm^3 s^{-1}) and product yields (Γ_{TEST} & Γ_{COMP}) of alkene **15** by both subchannel (TS .1, TS .2 & TS .3) and overall channel (**Σ(TS)**)*

Channel	k_{PROJ} [10^{-17} cm^3 s^{-1}]				k_{THEO} [10^{-17} cm^3 s^{-1}]				k_{TEST} - k_{COMP}
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
TS_{OZO} 1	14.74	6.65	23.09	**44.5**	66.2	22.2	9.78	**98.2**	-53.7
TS_{OZO} 2	11.80	5.86	32.22	**49.9**	6.22	4.98	3.36	**14.6**	35.3
Total *k*	**94.4**				**112.8**				-18.4
Channel	Γ_{PROJ}				Γ_{THEO}				**ΔΓ**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
$\Gamma_{anti\text{-}EtCHOO}$	0.091	0.074	0.102	**0.267**	0.029	0.072	0.128	**0.229**	0.038
$\Gamma_{syn\text{-}EtCHOO}$	0.079	0.065	0.088	**0.231**	0.087	0.016	0.101	**0.203**	0.028
$\Gamma_{anti\text{-}CH_3CHOO}$	0.086	0.072	0.111	**0.269**	0.035	0.105	0.126	**0.266**	0.003
$\Gamma_{syn\text{-}CH_3CHOO}$	0.074	0.063	0.096	**0.233**	0.120	0.058	0.124	**0.302**	-0.069

Table 151: Testing the rates MESMER projection technique *(k_{TEST}) with full computational analysis (k_{COMP}) (10^{-18} cm^3 s^{-1}) and product yields (Γ_{TEST} & Γ_{COMP}) of O_3 + alkene **16** by both subchannel (TS .1, TS .2 & TS .3) and overall channel (**Σ(TS)**)*

Channel	k_{PROJ} [10^{-17} cm^3 s^{-1}]				k_{COMP} [10^{-17} cm^3 s^{-1}]				k_{TEST} - k_{COMP}
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
TS_{OZO} 1	25.2	6.0	132.0	**163.2**	53.2	0.3	177.8	**231.3**	-68.1
TS_{OZO} 2	0.7	0.0	5.1	**5.9**	1.6	<0.1	15.2	**16.9**	-11
Total *k*	**169.1**				**248.2**				-79.1
Channel	Γ_{PROJ}				Γ_{COMP}				**ΔΓ**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
$\Gamma_{anti\text{-}EtCHOO}$	0.133	0.076	0.249	**0.458**	0.141	0.040	0.215	**0.395**	0.063
$\Gamma_{syn\text{-}EtCHOO}$	0.012	0.004	0.026	**0.042**	0.011	0.001	0.022	**0.034**	0.008
$\Gamma_{anti\text{-}CH_3CHOO}$	0.133	0.076	0.249	**0.458**	0.156	0.146	0.209	**0.510**	-0.052
$\Gamma_{syn\text{-}CH_3CHOO}$	0.012	0.004	0.026	**0.042**	0.022	0.008	0.030	**0.060**	-0.018

Table 152: Testing the rates MESMER projection technique *(k_{TEST}) with full computational analysis (k_{COMP}) (10^{-18} cm^3 s^{-1}) and product yields (Γ_{TEST} & Γ_{COMP}) of O_3 + alkene **7** by both subchannel (TS .1, TS .2 & TS .3) and overall channel (**Σ(TS)**)*

Channel	k_{PROJ} [10^{-18} cm^3 s^{-1}]				k_{COMP} [10^{-18} cm^3 s^{-1}]				k_{TEST} - k_{COMP}
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
TS_{OZO} 1	86.7	0.5	289.8	**377.0**	276.6	0.7	370.1	**647.4**	-270.4
TS_{OZO} 2	2.6	0.0	25.1	**27.8**	16.7	0.1	123.9	**140.7**	-112.9
Total *k*	**404.8**				**788.0**				-383.2
Channel	Γ_{PROJ}				Γ_{COMP}				**ΔΓ**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
$\Gamma_{(CH_3)_2COO}$ (1)	0.201	0.064	0.375	**0.640**	0.141	0.178	0.334	**0.653**	-0.013
$\Gamma_{(CH_3)_2COO}$ (2)	0.048	0.014	0.107	**0.169**	0.028	0.028	0.103	**0.158**	-0.008
$\Gamma_{anti\text{-}EtCHOO}$	0.046	0.014	0.089	**0.149**	0.023	0.027	0.102	**0.152**	0.018
$\Gamma_{syn\text{-}EtCHOO}$	0.012	0.003	0.026	**0.041**	0.014	0.002	0.021	**0.037**	0.003

4.2.3 Gibbs Free Energy Calculations using FESP model 1

Table 153: O_3 + 1-butene determining the ΔG_{PROJ} value.

		ΔG (kJ mol^{-1})				
$EtCHCH_2$		ΔG_{COMP}	$\Delta G_{TSX-POZ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G$
POZ	**TS_X**	[POZ]	(CH_3CHCH_2)			
POZ1.1	**TS_{OZO} 1.1**	-185.95	243.38	57.43	56.93	**-0.51**
	TS_{ANTI} 1		72.01	-113.94	-113.30	**0.64**
	TS_{FO} 1.1		78.28	-107.67	-108.70	**-1.02**
POZ1.2	**TS_{OZO} 1.2**	-184.52	243.38	58.86	57.88	**-0.98**
	TS_{ANTI} 2		72.01	-112.51	-112.79	**-0.28**
	TS_{FO} 1.2		78.28	-106.24	-108.04	**-1.79**
POZ1.3	**TS_{OZO} 1.3**	-187.13	243.38	56.26	56.40	**0.14**
	TS_{ANTI} 3		72.01	-115.11	-115.45	**-0.33**
	TS_{FO} 1.3		78.28	-108.85	-109.21	**-0.36**
POZ2.1	**TS_{OZO} 2.1**	-186.33	247.48	61.16	61.15	**-0.01**
	TS_{FO} 2.1		80.39	-105.94	-106.39	**-0.45**
	TS_{SYN} 1		74.26	-112.06	-112.36	**-0.30**
POZ2.2	**TS_{OZO} 2.2**	-183.07	247.48	64.41	63.98	**-0.44**
	TS_{FO} 2.2		80.39	-102.69	-106.68	***-3.99***
	TS_{SYN} 2		74.26	-108.81	-100.89	***7.92***
POZ2.3	**TS_{OZO} 2.3**	-188.04	247.48	59.45	58.39	**-1.05**
	TS_{FO} 2.3		80.39	-107.65	-107.63	**0.02**
	TS_{SYN} 3		74.26	-113.77	-113.34	**0.43**

*Table 154: The rate constants and product branching fractions for O_3 + Alkene **2** using the* FESP model 1 *(k_{PROJ} & Γ_{PROJ})* and *the full computational analysis from Chapter 3 (k_{THEO} & Γ_{THEO}) subdivided by subchannel (.1, .2 & .3) and aggregate across the channel (Σ); difference between the k_{PROJ} & k_{THEO} values [$\delta k_{TEST} = k_{PROJ} - k_{THEO}$]; difference between the Γ_{PROJ} & Γ_{THEO} values for each channel [$\delta\Gamma = \Gamma_{PROJ} - \Gamma_{THEO}$].*

Channel	***k_{PROJ}* [10^{-18} cm^3 s^{-1}]**				***k_{THEO}* [10^{-18} cm^3 s^{-1}]**				*δk*
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
TS_{OZO} 1	22.6	12.7	36.3	**71.6**	27.7	19.0	34.1	**80.8**	-9.2
TS_{OZO} 2	5.09	1.36	10.2	**16.6**	5.10	1.65	15.2	**21.9**	-5.3
Total *k*	88.2				102.7				-14.5
Channel	***Γ_{PROJ}***				***Γ_{THEO}***				**$\Delta\Gamma$**
	TS .1	TS .2	TS .3	**Σ(TS)**	TS .1	TS .2	TS .3	**Σ(TS)**	
Γ_{H_2COO} **(1)**	0.060	0.050	0.069	**0.179**	0.068	0.058	0.073	**0.199**	-0.020
Γ_{H_2COO} **(2)**	0.054	0.035	0.067	**0.156**	0.057	0.051	0.065	**0.173**	-0.017
$\Gamma_{anti\text{-}CH_3CHOO}$	0.142	0.119	0.164	**0.425**	0.130	0.108	0.188	**0.427**	-0.002
$\Gamma_{syn\text{-}CH_3CHOO}$	0.083	0.055	0.102	**0.240**	0.082	0.019	0.099	**0.201**	0.039

4.2.4 Comparing FESP model 1 results to Computational results

*Table 155: Ozonolysis of alkenes **15** (E-2-pentene), **16** (Z-2-pentene) and **7** (2-methyl-2-pentene), the ΔG of POZ + $\Delta G_{TSX-POZ}$ ($CH_3CHCR_3R_4$) projections [ΔG_{PROJ}]; comparison with computational ΔG_{TSX} of $EtCHCR_3R_4$ [ΔG_{PROJ}]; and difference between the two (δΔG)*

Alkene	**TS x.1** (kJ mol^{-1})			**TS x.2** (kJ mol^{-1})			**TS x.3** (kJ mol^{-1})		
15	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$
TS_{OZO} 1	52.80	47.81	**-4.99**	54.77	52.58	**-2.19**	51.68	53.82	**2.14**
TS_{OZO} 2	53.34	53.60	**0.25**	55.08	55.25	**0.17**	50.85	51.83	**0.98**
TS_{ANTI} 1	-120.84	-113.92	**6.91**	-118.87	-120.06	**-1.19**	-121.96	-122.47	**-0.51**
TS_{SYN} 2	-122.70	-123.53	**-0.83**	-120.73	-120.22	**0.51**	-123.82	-124.15	**-0.33**
TS_{ANTI} 2	-120.29	-114.76	**5.53**	-118.55	-121.89	**-3.33**	-122.78	-122.54	**0.24**
TS_{SYN} 1	-122.15	-122.27	**-0.12**	-120.42	-111.46	**8.96**	-124.64	-122.98	**1.67**
16	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$
TS_{OZO} 1	51.41	49.57	**-1.84**	54.98	62.29	**7.31**	47.31	46.58	**-0.72**
TS_{OZO} 2	60.17	58.31	**-1.86**	67.18	70.53	**3.36**	55.42	52.70	**-2.72**
TS_{ANTI} 1	-123.12	-125.47	**-2.35**	-119.55	-118.88	**0.67**	-127.23	-127.14	**0.09**
TS_{SYN} 2	-109.67	-115.56	**-5.89**	-102.67	-109.03	**-6.36**	-114.43	-116.44	**-2.01**
TS_{ANTI} 2	-123.12	-120.43	**2.69**	-119.55	-125.68	**-6.13**	-127.23	-127.56	**-0.33**
TS_{SYN} 1	-109.67	-111.34	**-1.67**	-102.67	-98.21	**4.46**	-114.43	-115.02	**-0.59**
7	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$	ΔG_{PROJ}	ΔG_{THEO}	$\delta\Delta G_{PROJ}$
TS_{OZO} 1	49.23	46.58	**-2.65**	56.20	61.52	**5.32**	45.37	45.81	**0.45**
TS_{OZO} 2	54.89	53.58	**-1.31**	62.23	65.35	**3.11**	50.13	48.56	**-1.57**
TS_{ANTI} 1	-123.04	-117.98	**5.06**	-116.07	-121.25	**-5.18**	-126.90	-127.80	**-0.90**
TS_{DMFO} 1	-133.53	-132.13	**1.39**	-126.56	-135.08	**-8.52**	-137.39	-138.63	**-1.24**
TS_{DMFO} 2	-124.43	-120.45	**3.98**	-117.08	-121.51	**-4.43**	-129.19	-129.55	**-0.36**
TS_{SYN} 1	-116.71	-117.61	**-0.89**	-109.37	-103.99	**5.38**	-121.48	-119.90	**1.58**

4.2.5 The accuracy of FESP model 1 results for the Ozonolysis *E*-2-pentene

Additional analysis of FESP model 1 is presented here for the ozonolysis of another alkene with an —Et substituent in the $—R_1$ position, Alkene **15**, using the adjusted MESMER files and ΔG_{TS-POZ} values extracted from equivalent alkenes with $—CH_3$ groups in the $—R_1$ position, Alkene **17**.

*Figure 25: Schematic of the chemical structures of Alkenes **15** & **17**.*

The TS structures in the O_3 + Alkene **15** reaction are likely to see some geometric distortions caused by interactions between the *E*-orientated —Et and $—CH_3$ substituents and therefore a greater number of deviations between the ΔG_{PROJ} & ΔG_{THEO} values, than O_3 + Alkene **2**. The FESP model 1 results of O_3 + Alkene **15** can be observed in the Table below:

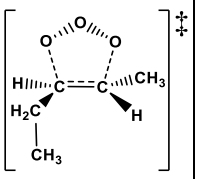
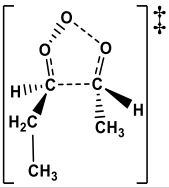
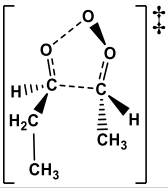
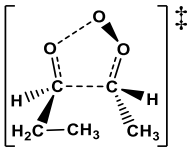
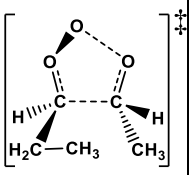
*Table 156: The rate constants and product branching fractions for O_3 + Alkene **15** using FESP model 1 (k_{PROJ} & Γ_{PROJ}) and the full computational analysis from Chapter 3 (k_{THEO} & Γ_{THEO}) subdivided by subchannel (.1, .2 & .3) and aggregate across the channel (Σ); difference between the k_{PROJ} & k_{THEO} values [$\delta k_{TEST} = k_{PROJ} - k_{THEO}$]; difference between the Γ_{PROJ} & Γ_{THEO} values for each channel [$\delta\Gamma = \Gamma_{PROJ} - \Gamma_{THEO}$].*

Alkene 15	k_{PROJ} [10^{-17} cm^3 s^{-1}]				k_{THEO} [10^{-17} cm^3 s^{-1}]				δk_{PROJ}
Channel	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
TS_{OZO} 1	14.7	6.65	23.1	44.5	66.2	22.2	9.8	98.2	-53.7
TS_{OZO} 2	11.8	5.86	32.2	49.9	6.2	5.0	3.4	14.6	+35.3
Total	94.4				112.7				-18.3
Channel	Γ_{PROJ}				Γ_{THEO}				$\Delta\Gamma_{PROJ}$
	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
$\Gamma_{anti\text{-}EtCHOO}$	0.091	0.074	0.102	**0.267**	0.029	0.072	0.128	**0.229**	0.038
$\Gamma_{syn\text{-}EtCHOO}$	0.079	0.065	0.088	**0.231**	0.087	0.016	0.101	**0.203**	0.028
$\Gamma_{anti\text{-}CH_3CHOO}$	0.086	0.072	0.111	**0.269**	0.035	0.105	0.126	**0.266**	0.003
$\Gamma_{syn\text{-}CH_3CHOO}$	0.074	0.063	0.096	**0.233**	0.120	0.058	0.124	**0.302**	-0.069

The difference between the overall k_{PROJ} value (9.44×10^{-16} cm^3 s^{-1}) is the overall k_{THEO} value (1.13×10^{-15} cm^3 s^{-1}) for O_3 + Alkene **15** is well within the 1 order of magnitude margin, but some of the distribution between channels is more distorted. As seen in the Table Above, the distortion is greatest between the k_{PROJ} & k_{THEO} values for reaction via the TS_{OZO} 1.1 structure, because the ΔG_{PROJ} [TS_{OZO} 1.1] value is ~5 kJ mol^{-1} higher than that of ΔG_{THEO} [TS_{OZO} 1.1], possibly due to an inductive effect. Of the cycloaddition structures, only the TS_{OZO} 1.1 structure sees a $\delta\Delta G_{PROJ}$ > 2.5 kJ mol^{-1} meaning that the proportion of the rate constant provided by the TS_{OZO} 1.1 mechanism, shifts from ~58% of the k_{THEO} value to only ~16% of the k_{PROJ} value. While reaction via TS_{OZO} 1.2 & TS_{OZO} 1.3 also sees

distortions, these $\delta\Delta G_{PROJ}$ values are small (-2.2 & 2.1 kJ mol^{-1}) and they balance out in k_{PROJ} calculations.

*Table 157: Transition States for the O_3 + Alkene **15** reaction with distinctive differences between the relative theoretical Gibbs free energy [ΔG_{THEO}] and projected relative Gibbs Free energy using FESP model 1 [ΔG_{PROJ}]; and the difference between the ΔG_{THEO} & ΔG_{PROJ} values for the TS structure [$\delta\Delta G_{PROJ} = \Delta G_{THEO} - \Delta G_{PROJ}$]. Gibbs Free energy values in kJ mol^{-1}.*

Label	TS_{OZO} 1.1	TS_{ANTI} 1.1	TS_{ANTI} 2.1	TS_{ANTI} 2.2	TS_{SYN} 1.2
Structure					
ΔG_{THEO}	47.8	-113.9	-114.8	-121.9	-111.4
ΔG_{PROJ}	52.8	-120.8	-120.3	-118.6	-120.4
$\delta\Delta G_{PROJ}$	**-5.0**	**6.9**	**5.5**	**-3.3**	**9.0**
CI Product	N/A	*anti*-EtCHOO	*anti*-CH_3CHOO	*anti*-CH_3CHOO	*syn*-CH_3CHOO

The Γ_{PROJ} values for O_3 + Alkene **15** have a similarly even distribution of CI products to that of Γ_{THEO} values from Chapter 3, but the distortions between these values are larger than those seen for O_3 + Alkene **2**. The differences in ΔG_{PROJ} & ΔG_{THEO} values for most POZ fragmentation barriers for O_3 + Alkene **15** are small (< 2 kJ mol^{-1}). However, notable differences between ΔG_{PROJ} & ΔG_{THEO} values are seen in four key POZ fragmentation barriers: TS_{ANTI} 1.1, TS_{ANTI} 2.1, TS_{ANTI} 2.2 & TS_{SYN} 1.2 (featured in Table 1.52 above). These emerge from the observation, noted for O_3 + Alkene **2**, that the ΔG_{PROJ} values in FESP model 1 do not always accommodate changes in steric interaction caused by the adjustments of the —Et substituent with the TS structures.

For example, the interaction of the —Et group and the central oxygen in the 1,2,3 trioxolane segment of the structure appears to cause the ΔG_{PROJ} values of TS_{ANTI} 2.2 & TS_{SYN} 1.2 to deviate from their ΔG_{THEO} values. A comparable steric interaction materialised for TS_{FO} 2.2 & TS_{SYN} 2 structures in O_3 + Alkene **2** and this generates parallel ΔG_{PROJ} deviations. The increased steric interaction in TS_{SYN} 1.2 contributes to why FESP model 1 overestimates the Γ_{PROJ} branching fraction for *syn*-EtCHOO + CH_3CHO.

FESP model 1 overestimates the ΔG_{PROJ} value for TS_{ANTI} 2.2 but this is too balanced out by ΔG_{PROJ} value for TS_{ANTI} 2.1 being underestimated and therefore the overall Γ_{PROJ} & Γ_{THEO} values for *anti*-CH_3CHOO + EtCHO are fairly similar. The steric changes that cause this underestimated ΔG_{PROJ} values for TS_{ANTI} 1.1 & 2.1 appear to be the inverse to the phenomenon seen for TS_{OZO} 1.1. These TS geometries feature a POZ-to-TS structural change where the lengthy —Et substituent diverges or converges with the *E*-orientated —CH_3 substituent. While, the Γ_{PROJ} & Γ_{THEO} values are similar for *anti*-EtCHOO + CH_3CHO, the

variances between them (and the consequential alterations to the Γ_{PROJ} & Γ_{THEO} values for *syn*-CH_3CHOO + EtCHO) are ascribed to the convergences and divergences of —Et substituent with other parts of the TS structure.

As mentioned in the discussion of O_3 + Alkene **2**, these distortions in steric interactions and the consequential effect the overestimating/underestimating of ΔG_{PROJ} values in FESP models is discussed in Thesis Section 6.6. The fact that the k_{PROJ} & k_{THEO} values are well within an order of magnitude to each other and that they have a relatively even distribution, despite these deviations, provides evidence that FESP model 1 is reasonably accurate.

4.2.6 The accuracy of FESP model 1 results for the Ozonolysis *Z*-2-pentene

Of the analysis of FESP model 1 here of the four with alkenes with —Et substituents in the $-R_1$ position, O_3 + Alkene **16** is of overriding importance because of its structural similarities between Alkene **19**, the alkene of interest of this chapter. Any inconsistencies in FESP modelling for O_3 + Alkene **16** are of particular interest as they may also apply to O_3 + Alkene **19**. The implementation of FESP model 1 for O_3 + Alkene **16** uses the adjusted MESMER files and ΔG_{TS-POZ} values extracted from equivalent alkenes with a $-CH_3$ group in the $-R_1$ position, Alkene **18**. Structures for Alkenes **16**, **18** & **19** are in Figure 19, below.

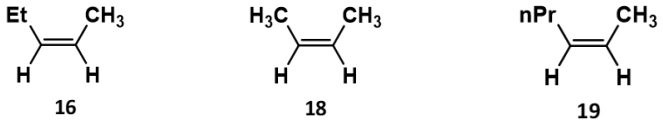


*Figure 26: Schematic of the chemical structures of Alkenes **16**, **18** & **19**.*

Increased barrier heights in certain cycloaddition structures (TS_{OZO} 1.2 & 2.2) have already been reported in Thesis Section 3.5.2, due to the steric interaction between the *Z*-orientated large and bulky —Et and $-CH_3$ substituents in O_3 + Alkene **16**. Another more moderate deviation between ΔG_{THEO} & ΔG_{PROJ} values is provided by TS_{OZO} 2.3, which is marginal in size ($\delta\Delta G_{PROJ}$ ~2.72 kJ mol^{-1}), but it does have a small effect on reactivity. While the steric changes in TS_{OZO} 1.2 & 2.2 & TS_{OZO} 2.3 barriers cause deviations between their ΔG_{THEO} & ΔG_{PROJ} values, these have a minor impact on the k_{PROJ} or k_{THEO} values, as shown in Table 153. Therefore, the k_{PROJ} value for O_3 + Alkene **16** (1.69×10^{-15} cm^3 s^{-1}) is still fairly close to the k_{THEO} value (2.48×10^{-15} cm^3 s^{-1}) and the proportions of each TS_{OZO} pathway are similar.

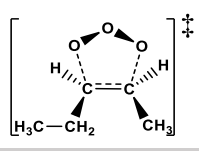
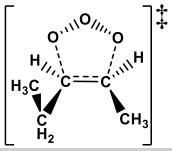
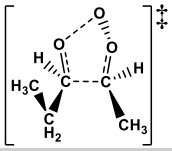
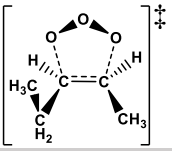
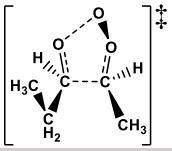
*Table 158: The rate constants and product branching fractions for O_3 + Alkene **15** using FESP model 1 (k_{PROJ} & Γ_{PROJ}) and the full computational analysis from Chapter 3 (k_{THEO} & Γ_{THEO}) subdivided by subchannel (.1, .2 & .3)*

and aggregate across the channel (Σ); difference between the k_{PROJ} & k_{THEO} values [$\delta k_{TEST} = k_{PROJ} - k_{THEO}$]; difference between the Γ_{PROJ} & Γ_{THEO} values for each channel [$\delta\Gamma = \Gamma_{PROJ} - \Gamma_{THEO}$].

Alkene 16	k_{PROJ} [10^{-16} cm^3 s^{-1}]				k_{THEO} [10^{-16} cm^3 s^{-1}]				δk_{PROJ}
Channel	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
TS_{OZO} 1	2.5	0.6	13.2	**16.3**	5.3	<0.1	17.8	**23.1**	-6.8
TS_{OZO} 2	<0.1	<0.1	0.5	**0.6**	0.2	<0.1	1.5	**1.7**	-1.1
Total	16.9				24.8				-7.9
Channel	Γ_{PROJ}				Γ_{THEO}				$\Delta\Gamma_{PROJ}$
	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
Γ_{anti}-EtCHOO	0.133	0.076	0.249	**0.458**	0.141	0.040	0.215	**0.395**	0.063
Γ_{syn}-EtCHOO	0.012	0.004	0.026	**0.042**	0.011	0.001	0.022	**0.034**	0.008
Γ_{anti}-CH_3CHOO	0.133	0.076	0.249	**0.458**	0.156	0.146	0.209	**0.510**	-0.052
Γ_{syn}-CH_3CHOO	0.012	0.004	0.026	**0.042**	0.022	0.008	0.030	**0.060**	-0.018

The Γ_{PROJ} values for *anti*-EtCHOO & *syn*-EtCHOO are the same as that for *anti*-CH_3CHOO & *syn*-CH_3CHOO, respectively because each pair of POZ fragmentation TS structures has the same ΔG_{PROJ} value. The symmetrical ΔG_{PROJ} values for these TS structures (e.g. ~ -123.1 kJ mol^{-1} for TS_{ANTI} 1.1 & 2.1) are due to being produced from the same ΔG_{THEO} value of the same POZ (e.g. ~ -190.5 kJ mol^{-1} for POZ 1.1) and the same ΔG_{TS-POZ} value of the same TS structure in O_3 + Alkene **18** (~67.35 kJ mol^{-1} for TS_{ANTI}). However, this set of symmetrical values actually produces a Γ_{PROJ} distribution for O_3 + Alkene **16** which is very similar to the Γ_{THEO} values calculated in Thesis Chapter 3, with the most significant deviation being that *anti*-CH_3CHOO has a larger Γ_{THEO} value (~0.510) than that of *anti*-EtCHOO (~0.395).

*Table 159: Example Transition States for the O_3 + Alkene **15** reaction with the differences between the relative theoretical Gibbs free energy [ΔG_{THEO}] and projected relative Gibbs Free energy using FESP model 1 [ΔG_{PROJ}]; and the difference between the ΔG_{THEO} & ΔG_{PROJ} values for the TS structure [$\delta\Delta G_{PROJ} = \Delta G_{THEO} - \Delta G_{PROJ}$]. Gibbs Free energy values in kJ mol^{-1}.*

Label	**TS_{OZO} 2.3**	**TS_{OZO} 1.2**	**TS_{ANTI} 2.2**	**TS_{OZO} 2.2**	**TS_{SYN} 2.2**
Structure					
ΔG_{THEO}	52.7	62.3	-125.7	70.5	-109.0
ΔG_{PROJ}	55.4	55.0	-119.6	67.2	-102.7
$\delta\Delta G_{PROJ}$	**2.7**	**7.3**	**-6.1**	**3.3**	**-6.3**
CI Product	N/A	N/A	*anti*-CH_3CHOO	N/A	*syn*-CH_3CHOO

However, one very important factor that can be noted, particularly when observing the deviations between their ΔG_{THEO} & ΔG_{PROJ} values for O_3 + Alkene **16**, is that the steric impacts appear to form convergence/divergence pairs, such as TS_{OZO} 1.2 & TS_{ANTI} 1.2, paired in Table 154 above. These pairs of TS structures exhibit the same —Et substituent rotational movement during transition that causes the —Et substituent to converge (TS_{OZO} 1.2) or diverge (TS_{ANTI} 1.2), with a near structural feature (the —CH_3 substituent) an respectively increase or decrease the ΔG_{THEO} value by a similar energy (here ~6 kJ mol^{-1}). It

is this drop ~6 kJ mol^{-1} between the ΔG_{PROJ} & ΔG_{THEO} values that is principally responsible for the larger Γ_{THEO} value for *anti*-CH_3CHOO, given in Table 154 above. Similar parings of steric interactions are seen for other TS structures in the O_3 + Alkene **16** reaction, such as TS_{OZO} 2.2 & TS_{SYN} 2.2, but they have little impact on k_{PROJ} or Γ_{THEO} values and are therefore explored only in Thesis Section 6.6 in conjunction with those seen for O_3 + Alkenes **2** & **15**. The fact that these k_{PROJ} & Γ_{PROJ} values for O_3 + Alkene **16** are similar to the k_{THEO} & Γ_{THEO} values determined in Chapter 3, provides more evidence that FESP model 1 is quite accurate.

4.2.7 The Accuracy of FESP model 1 for the Ozonolysis of 2-methyl-2-pentene

The key structural detail of a —CH_3 group in the *Z*-position to the principle —R_1 group for both Alkenes **16** & **19** is also seen for Alkene **7**, meaning discrepancies seen for O_3 + Alkene **7**, may also be of interest. The FESP model 1 for O_3 + Alkene **7** uses the adjusted MESMER files and ΔG_{TS-POZ} values extracted from the O_3 + Alkene **6** reaction.

*Figure 27: Schematic of the chemical structures of Alkenes **6** & **7**.*

While the TS_{OZO} 1.2 & 2.2 structures have deviations between the ΔG_{THEO} & ΔG_{PROJ} barriers for O_3 + Alkene **7**, the only important cycloaddition structure with such a difference in ΔG values was TS_{OZO} 1.1 ($\delta\Delta G_{PROJ}$ ~2.7 kJ mol^{-1}). The underestimation of the ΔG_{PROJ} barriers for TS_{OZO} 1.1, similar to one seen for O_3 + Alkene **15**, is the main contributing factor to the small difference in the k_{PROJ} & k_{THEO} values for O_3 + Alkene **7** (see Table 155 below).

*Table 6.160: The rate constants and product branching fractions for O_3 + Alkene **15** using FESP model 1 (k_{PROJ} & Γ_{PROJ}) the full computational analysis from Chapter 3 (k_{THEO} & Γ_{THEO}) subdivided by subchannel (.1, .2 & .3) and aggregate across the channel (Σ); difference between the k_{PROJ} & k_{THEO} values [$\delta k_{TEST} = k_{PROJ} - k_{THEO}$]; difference between the Γ_{PROJ} & Γ_{THEO} values for each channel [$\delta_{PROJ} = \Gamma_{PROJ} - \Gamma_{THEO}$].*

Alkene 7	k_{PROJ} [10^{-16} cm^3 s^{-1}]				k_{THEO} [10^{-16} cm^3 s^{-1}]				δk_{PROJ}
Channel	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
TS_{OZO} 1	8.7	<0.1	29.0	**37.7**	18.0	<0.1	24.0	**42.1**	-4.4
TS_{OZO} 2	0.3	<0.1	2.5	**2.8**	1.1	<0.1	8.0	**9.1**	-6.3
Total	**40.5**				**51.2**				-10.7
Channel	Γ_{PROJ}				Γ_{THEO}				$\Delta\Gamma_{PROJ}$
	(.1)	(.2)	(.3)	**Σ**	(.1)	(.2)	(.3)	**Σ**	
$\Gamma_{(CH_3)_2COO\,(1)}$	0.201	0.064	0.375	**0.640**	0.141	0.178	0.334	**0.653**	-0.013
$\Gamma_{(CH_3)_2COO\,(2)}$	0.048	0.014	0.107	**0.149**	0.028	0.028	0.103	**0.158**	-0.009
$\Gamma_{anti\text{-}EtCHOO}$	0.046	0.014	0.089	**0.169**	0.023	0.027	0.102	**0.152**	0.017
$\Gamma_{syn\text{-}EtCHOO}$	0.012	0.003	0.026	**0.041**	0.014	0.002	0.021	**0.037**	0.004

Table 155 (above) also shows that the Γ_{PROJ} & Γ_{THEO} distributions are also fairly similar and where there are overestimations in the product distribution, such as for the TS_{DMFO} 1.2 & 2.2 subchannels, the yield of $(CH_3)_2COO$ from the underestimated TS_{DMFO} 1.1 & 2.1 subchannels balances this out. Other discontinuities do exist between the ΔG_{THEO} & ΔG_{PROJ} barriers of other POZ fragmentation structures however they have little effect on the Γ_{PROJ} & Γ_{THEO} distributions. Many of these steric repulsion-related disparities between ΔG_{THEO} & ΔG_{PROJ} values for TS barriers found for O_3 + Alkene **7** are of interest and are explored in conjunction with those of O_3 + Alkenes **2**, **15** & **16**. Once again, the k_{PROJ} & Γ_{PROJ} for O_3 + Alkene **16** are similar to the k_{THEO} & Γ_{THEO} values, calculated in Chapter 3, implying that FESP Model 1 is relatively accurate.

4.2.9 Steric Factor extracted from Different TS structures

*Table 161: Compiled convergences and divergences take place all O_3 + Alkenes **2**, **7**, **15** & **16** reaction by Steric (Δ_{STERIC}) and hindered internal rotation (Δ_{ROT}) factors by: Label; number of the Alkene reactant; TS structure they emerged from; angle change of the critical bond rotation (Δ_{ANGLE}); change in energy that results ($\delta\Delta G$); Average change in energy from each factor (Average Δ_{DIV} / Δ_{CON}).*

$\Delta_{ROT}/\Delta_{STERIC}$ Label	Alkene No	TS	Δ_{ANGLE} (^{O})	kJ mol^{-1}	
				δΔG	Average Δ_{DIV} / Δ_{CON}
Δ_{DIV} (—Et,^{c}O,—H)	2	TS_{FO} 2.2	+23.42	-3.99	-3.66 (± 0.33)
	15	TS_{ANTI} 2.2	+21.17	-3.33	
Δ_{CON} (—Et,^{c}O,—H)	2	TS_{SYN} 2	-19.10	7.89	8.43 (± 0.54)
	15	TS_{SYN} 2.2	-19.19	8.96	
Δ_{DIV} (—Et,^{t}O,—CH_3)	16	TS_{ANTI} 2.2	+9.20	-6.13	-6.61 (± 1.91)
	7	TS_{ANTI} 2	+19.19	-5.18	
	7	TS_{DMFO} 1.2	+0.81	-8.52	
Δ_{CON} (—Et,^{t}O,—CH_3)	16	TS_{OZO} 1.2	23.05	7.31	6.32 (± 0.99)
	7	TS_{OZO} 1.2	39.82	5.32	
Δ_{DIV} (—Et,^{c}O,—CH_3)	16	TS_{SYN} 2.2	+24.62	-6.36	-5.40 (± 0.97)
	7	TS_{DMFO} 2.2	+25.83	-4.43	
Δ_{CON} (—Et,^{c}O,—CH_3)	16	TS_{OZO} 2.2	32.95	3.36	3.24 (± 0.13)
	7	TS_{OZO} 2.2	51.48	3.11	
Δ_{DIV} (—Et,—CH_3)	15	TS_{OZO} 1.1	-24.04	-4.99	-3.97 (± 1.92)
	7	TS_{OZO} 1.1	-55.19	-2.65	
	16	TS_{ANTI} 1.1	-21.11	-2.35	
	16	TS_{SYN} 2.1	-27.41	-5.89	
Δ_{CON} (—Et,—CH_3)	15	TS_{ANTI} 1.1	13.47	6.91	5.37 (± 1.54)
	15	TS_{ANTI} 2.1	5.31	5.53	
	7	TS_{ANTI} 1	12.85	5.06	
	7	TS_{DMFO} 2.1	10.41	3.98	
Δ_{DIV} (*syn*—Et,^{c}O,—CH_3)	16	TS_{SYN} 1.2	-8.122	4.46	4.92 (± 0.46)
	7	TS_{SYN} 2	-6.856	5.38	
$\Delta_{DIV}/\Delta_{CON}$ (—Et,^{t}O)	16	TS_{OZO} 2.3	-2.01	-2.72	±2.37 (± 0.36)
	16	TS_{SYN} 2.3	-13.25	-2.01	

*Table 162: Summary of converging (Δ_{CON}) and diverging (Δ_{DIV}) steric and rotational factors labels including: their nomenclature; an example of an O_3 + Alkene TS structures the $\Delta_{DIV}/\Delta_{CON}$ steric factor is derived from; the quantised numerical factor; whether FESP model 2 uses it for the ozonolysis chemistry of Alkene **19**.*

$\Delta_{ROT}/\Delta_{STERIC}$ Label	O_3 + Alkene Example Alkene No	TS	Δ_{DIV} / Δ_{CON} values (kJ mol^{-1})	Applied to O_3 + Alkene 19?
Δ_{DIV} (−Et,^{c}O,−H)	15	TS_{ANTI} 2.2	-3.7 (± 0.3)	N
Δ_{CON} (−Et,^{c}O,−H)	15	TS_{SYN} 2.2	8.4 (± 0.5)	N
Δ_{DIV} (−Et,^{t}O,−CH_3)	16	TS_{ANTI} 2.2	-6.6 (± 1.9)	N
Δ_{CON} (−Et,^{t}O,−CH_3)	16	TS_{OZO} 1.2	6.3 (± 1.0)	Y
Δ_{DIV} (−Et,^{c}O,−CH_3)	16	TS_{SYN} 2.2	-5.4 (± 1.0)	N
Δ_{CON} (−Et,^{c}O,−CH_3)	16	TS_{OZO} 2.2	3.2 (± 0.1)	Y
Δ_{DIV} (−Et,−CH_3)	15	TS_{OZO} 1.1	-4.0 (± 1.9)	Y
Δ_{CON} (−Et,−CH_3)	15	TS_{ANTI} 1.1	5.4 (± 1.5)	Y
Δ_{DIV} (*syn*−Et,^{c}O,−CH_3)	16	TS_{SYN} 1.2	4.9 (± 0.5)	Y
$\Delta_{DIV}/\Delta_{CON}$ (−Et,^{t}O)	16	TS_{SYN} 2.3	±2.4 (±0.4)	Y (Δ_{DIV} & Δ_{CON})

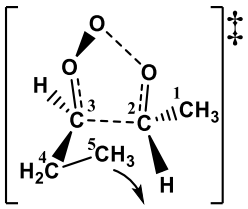
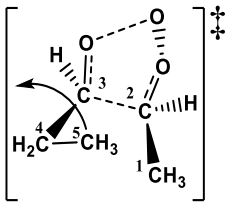
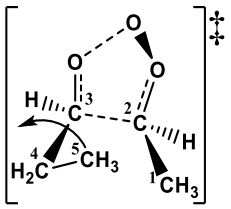
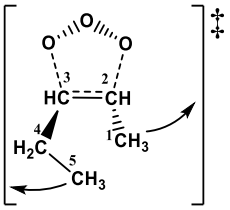
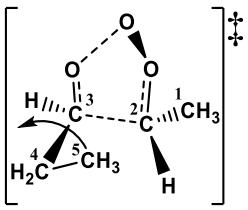
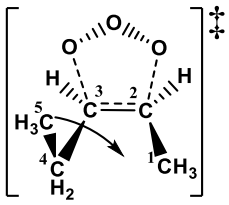
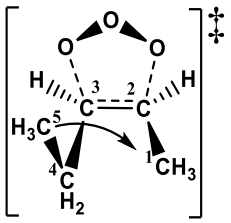
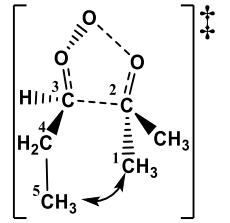
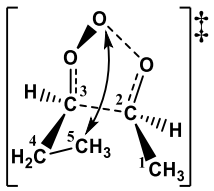
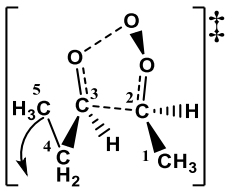
Δ_{DIV} (−Et,^{c}O,−H)	Δ_{DIV} (−Et,^{t}O,−CH_3)	Δ_{DIV} (−Et,^{c}O,−CH_3)	Δ_{DIV} (−Et,−CH_3)
			
-8.4 ± 0.5	-6.6 ± 1.9	-5.4 ± 1.0	-3.8 ± 1.2
Δ_{CON} (−Et,^{c}O,−H)	Δ_{CON} (−Et,^{t}O,−CH_3)	Δ_{CON} (−Et,^{c}O,− CH_3)	Δ_{CON} (−Et,− CH_3)
			
3.7 ± 0.3	6.3 ± 1.0	3.2 ± 0.1	5.4 ± 1.5
	Δ_{DIV} (*syn*−Et,^{c}O,−CH_3)	$\Delta_{DIV}/\Delta_{CON}$ (−Et,^{t}O)	
			
	4.9 ± 0.5	±2.4 ± 0.4	

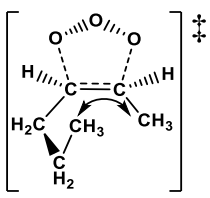
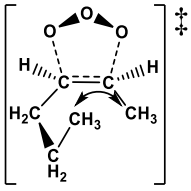
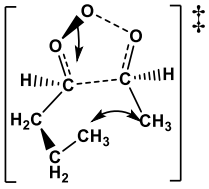
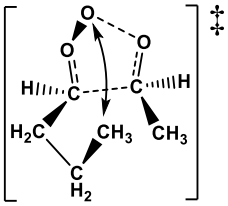
*Figure 28: Steric Factors extracted from the Ozonolyses of Alkenes **2**, **7**, **15**, & **16***

4.2.10 Apply Steric Factors to Inconsequential TS structures

In chapter 6 many different transition states applied different steric factors, but most only applied one of the following: **Δ_{DIV} (—Et,—CH_3)**, **Δ_{CON} (—Et,—CH_3)**, **Δ_{CON} (—Et,^{t}O)** or **Δ_{DIV} (—Et,^{t}O)**. However, a few transition states had other factors applied to them (TS_{OZO} 1.5, TS_{OZO} 2.5, TS_{SYN} 1.5 & TS_{SYN} 1.6) but their energies so high they make very little difference to the overall chemistry and so were not fully described in the main body of the thesis. This is a fuller description of those steric interactions seen in those minor transition states:

The **Δ_{CON} (—Et,^{t}O,—CH_3)** factor is only applies to one TS structure in the O_3 + Alkene **19** reaction, TS_{OZO} 1.5, because the TS_{OZO} 1.5 structure (displayed in Table 6.18) incorporates an unusual mixture of factors. The —nPr group converging with the —CH_3 group with increased proximity to the terminal oxygen of the 1,2,3 trioxolane segment and this raises the energy of the TS_{OZO} 1.5 barrier significantly. The steric trap factor, **Δ_{CON} (—Et,^{c}O,—CH_3)**, is similar to this but it involves interaction with a the —nPr group converging with the —CH_3 group with increased proximity to the central oxygen of the 1,2,3 trioxolane segment instead. This is only applied sparingly for O_3 + Alkene **19**, with those two structures, TS_{OZO} 2.5 & TS_{SYN} 1.5, where the increased steric repulsion further raises already high energy barriers. While these **Δ_{CON} (—Et,^{t}O,—CH_3)** & **Δ_{CON} (—Et,^{c}O,—CH_3)** factors have divergent equivalent in O_3 + Alkene **16**, such a divergence does not appear for any of the TS structures in O_3 + Alkene **19** reaction.

*Table 163: Steric changes for a variety TS structures of the O_3 + Alkene **19** reaction, the changes in energy that steric interaction causes (Δ_{STERIC}) and the ΔG_{PROJ} & ΔG_{STERIC} values of those TSs. Gibbs Free energy values in kJ mol^{-1}.*

Alkene	**O_3 + Alkene 19**			
TS Label	**TS_{OZO} 1.5**	**TS_{OZO} 2.5**	**TS_{SYN} 1.5**	**TS_{SYN} 1.6**
Δ_{STERIC} Label	**Δ_{DIV} (—Et,^{t}O,—CH_3)**	**Δ_{CON} (—Et,^{c}O,—CH_3)**		**Δ_{DIV} (*syn*—Et,^{c}O,—CH_3)**
Structure				
ΔG_{PROJ}	-109.0	83.8	-84.9	-116.4
Δ_{STERIC} value	6.3	3.2	3.2	4.9
ΔG_{STERIC}	83.7	87.1	-81.7	-85.8

The last of the Δ_{STERIC} factors is referred to as **Δ_{DIV} (*syn*—Et,^{c}O,—CH_3)** and only applies to TS_{SYN} 1.6 in the O_3 + Alkene **19** reaction because it requires the *cis*—CH_3 group restricting the—nPr movement, while a *syn*-nPrCHOO species is forming. As shown in Table 6.18 TS_{SYN} 1.6 involves a convergence of the —nPr group and the central oxygen in the 1,2,3

trioxolane segment and no divergent equivalent has either been identified or used in this study, if one is even needed due to the unique nature of this factor.

4.3 Relative Energies of Calculated Minima for O_3 + *Z*-2-hexene

Minima	(kJ mol^{-1})			
	ΔE	**ΔZPE**	**$\Delta H_{298.15}$**	**$\Delta G_{298.15}$**
O_3 + Alkene **19** Con 1	0.00	0.00	0.00	0.00
O_3 + Alkene **19** Con 2	0.65	0.42	0.64	0.08
O_3 + Alkene **19** Con 3	3.18	3.47	3.51	3.01
O_3 + Alkene **19** Con 4	15.82	16.27	16.32	16.89
POZ 1.1	-259.29	-241.46	-246.64	-189.41
POZ 1.2	-255.47	-237.42	-242.64	-185.79
POZ 1.3	-253.57	-235.24	-240.82	-181.99
POZ 1.4	-255.25	-237.65	-242.79	-185.37
POZ 1.5	-245.23	-226.31	-232.07	-171.86
POZ 1.6	-252.01	-233.92	-239.27	-180.55
POZ 1.7	-262.83	-245.38	-250.43	-193.73
POZ 1.8	-258.61	-240.98	-246.22	-189.08
POZ 1.9	-260.24	-242.39	-247.55	-191.15
POZ 2.1	-257.36	-239.92	-245.11	-187.73
POZ 2.2	-253.40	-235.72	-240.93	-183.91
POZ 2.3	-249.70	-232.44	-237.50	-179.90
POZ 2.4	-249.82	-232.10	-237.47	-179.18
POZ 2.5	-240.26	-221.84	-227.49	-167.87
POZ 2.6	-243.90	-225.98	-231.34	-173.65
POZ 2.7	-260.49	-243.21	-248.44	-191.26
POZ 2.8	-255.20	-237.87	-243.17	-186.51
POZ 2.9	-258.33	-240.72	-246.04	-189.13
CH_3CHO + *Anti*-nPrCHOO Con 1	-258.70	-260.03	-259.47	-262.83
CH_3CHO + *Anti*-nPrCHOO Con 2	-261.03	-262.67	-261.96	-265.20
CH_3CHO + *Anti*-nPrCHOO Con 3	-261.47	-263.03	-262.51	-265.50
CH_3CHO + *Anti*-nPrCHOO Con 4	-261.72	-263.80	-263.20	-265.64
CH_3CHO + *Anti*-nPrCHOO Con 5	-260.92	-262.67	-262.25	-264.18
CH_3CHO + *Syn*-nPrCHOO Con 1	-258.70	-260.03	-259.47	-262.83
CH_3CHO + *Syn*-nPrCHOO Con 2	-261.03	-262.67	-261.96	-265.20
CH_3CHO + *Syn*-nPrCHOO Con 3	-261.47	-263.03	-262.51	-265.50
CH_3CHO + *Syn*-nPrCHOO Con 4	-261.72	-263.80	-263.20	-265.64
CH_3CHO + *Syn*-nPrCHOO Con 5	-260.92	-262.67	-262.25	-264.18
Anti-CH_3CHO + nPrCHOO Con 1	-262.81	-264.57	-264.29	-266.73
Anti-CH_3CHO + nPrCHOO Con 2	-262.63	-264.01	-263.95	-265.60
Anti-CH_3CHO + nPrCHOO Con 3	-260.06	-261.45	-260.96	-264.50
Anti-CH_3CHO + nPrCHOO Con 4	-260.34	-261.77	-261.48	-264.57
Anti-CH_3CHO + nPrCHOO Con 5	-255.56	-256.74	-256.19	-261.32
syn-CH_3CHO + nPrCHOO Con 1	-277.66	-278.59	-278.98	-280.43
syn-CH_3CHO + nPrCHOO Con 2	-277.48	-278.03	-278.65	-279.29
syn-CH_3CHO + nPrCHOO Con 3	-274.91	-275.47	-275.65	-278.19
syn-CH_3CHO + nPrCHOO Con 4	-275.19	-275.79	-276.17	-278.26
syn-CH_3CHO + nPrCHOO Con 5	-270.41	-270.76	-270.89	-275.02
TSanti 1.8	-187.12	-178.27	-182.80	-126.39
TSsyn 1.8	-171.70	-161.77	-166.70	-109.02

4.4 Use of FESP models 2 & 3 for O_3 + *Z*-2-hexene

MESMER calculations of FESP model 2 & 3 are mostly found in the main body of the Thesis the steric and empirical factors (Δ_{STERIC} & Δ_{EMP}) is covered in the Table below:

Table 164: Applying the steric and empirical factors (Δ_{STERIC} & Δ_{EMP}) to the Projected relative Gibbs Free energy (ΔG_{PROJ}) to produce steric and empirically adjusted relative Gibbs Free energy (ΔG_{STERIC} & ΔG_{EMP})

POZ	TS	ΔG_{PROJ}	Steric factor applied	Δ_{STERIC}	ΔG_{STERIC}	ΔG_{EMP}
		kJ mol^{-1}			kJ mol^{-1}	
POZ 1.2	TS_{OZO} 1.2	54.25	Δ_{DIV} (—Et,—CH_3)	-3.97	**50.28**	**47.69**
	TS_{ANTI} 1.2	-120.79	Δ_{DIV} (—Et,—CH_3)	-3.97	**-124.76**	**-127.35**
	TS_{ANTI} 2.2	-116.62	Δ_{DIV} (—Et,—CH_3)	-3.97	**-120.59**	**-123.18**
POZ 1.3	TS_{OZO} 1.3	58.05	Δ_{CON} (—Et,—CH_3)	5.37	63.42	60.84
	TS_{ANTI} 1.3	-116.99	Δ_{CON} (—Et,—CH_3)	5.37	-111.62	-114.21
	TS_{ANTI} 2.3	-112.82	Δ_{CON} (—Et,—CH_3)	5.37	-107.45	-110.04
POZ 1.5	TS_{OZO} 1.5	77.33	Δ_{CON} (—Et,^{t}O,—CH_3)	6.32	83.65	81.07
	TS_{ANTI} 1.5	-103.84	Δ_{CON} (—Et,—CH_3)	5.37	-98.47	-101.05
	TS_{ANTI} 2.5	-110.64	Δ_{DIV} (—Et,—CH_3)	-3.97	**-114.61**	**-117.20**
POZ 1.6	TS_{OZO} 1.6	68.63	Δ_{CON} (—Et,^{t}O)	2.37	71.00	68.42
	TS_{ANTI} 1.6	-112.53	Δ_{DIV} (—Et,^{t}O)	-2.37	**-114.90**	**-117.49**
	TS_{ANTI} 2.6	-119.33	Δ_{CON} (—Et,^{t}O)	2.37	**-116.96**	**-119.55**
POZ 1.8	TS_{OZO} 1.8	52.08	Δ_{CON} (—Et,^{t}O)	2.37	54.45	51.86
	TS_{ANTI} 1.8	-121.64	Δ_{DIV} (—Et,^{t}O)	-2.37	-124.01	-126.60
	TS_{ANTI} 2.8	-122.06	Δ_{DIV} (—Et,^{t}O)	-2.37	-124.43	-127.02
POZ 1.9	TS_{OZO} 1.9	50.01	-	-	50.01	50.01
	TS_{ANTI} 1.9	-123.72	Δ_{DIV} (—Et,—CH_3)	-3.97	**-127.69**	**-130.28**
	TS_{ANTI} 2.9	-124.13	Δ_{DIV} (—Et,—CH_3)	-3.97	**-128.10**	**-130.69**
POZ 2.2	TS_{OZO} 2.2	62.58	Δ_{DIV} (—Et,—CH_3)	-3.97	**58.61**	**56.02**
	TS_{SYN} 1.2	-107.07	Δ_{DIV} (—Et,—CH_3)	-3.97	**-111.04**	**-113.63**
	TS_{SYN} 2.2	-111.29	-	-	-111.29	-111.29
POZ 2.3	TS_{OZO} 2.3	66.59	Δ_{CON} (—Et,—CH_3)	5.37	71.96	69.37
	TS_{SYN} 1.3	-103.06	Δ_{CON} (—Et,—CH_3)	5.37	-97.69	-100.28
	TS_{SYN} 2.3	-107.28	-	-	-107.28	-107.28
POZ 2.5	TS_{OZO} 2.5	83.84	Δ_{CON} (—Et,^{c}O,—CH_3)	3.24	87.08	84.49
	TS_{SYN} 1.5	-84.90	Δ_{CON} (—Et,^{c}O,—CH_3)	3.24	-81.66	-84.25
	TS_{SYN} 2.5	-95.72	Δ_{CON} (—Et,—CH_3)	5.37	-90.35	-92.94
POZ 2.6	TS_{OZO} 2.6	78.06	Δ_{CON} (—Et,^{t}O)	2.37	80.43	77.84
	TS_{SYN} 1.6	-90.68	Δ_{DIV} (*syn*—Et,^{c}O,—CH_3)	4.92	-85.76	-88.35
	TS_{SYN} 2.6	-101.50	Δ_{CON} (—Et,^{t}O)	2.37	**-99.13**	**-101.72**
POZ 2.8	TS_{OZO} 2.8	59.12	Δ_{CON} (—Et,^{t}O)	2.37	61.49	58.91
	TS_{SYN} 1.8	-108.60	Δ_{CON} (—Et,^{t}O)	2.37	-106.23	-108.81
	TS_{SYN} 2.8	-110.02	Δ_{DIV} (—Et,^{t}O)	-2.37	-112.39	-114.97
POZ 2.9	TS_{OZO} 2.9	56.50	-	-	56.50	56.50
	TS_{SYN} 1.9	-111.22	Δ_{DIV} (—Et,—CH_3)	-3.97	**-115.19**	**-117.78**
	TS_{SYN} 2.9	-112.64	-	-	-112.64	-112.64

4.4.1 Impacts of inputting calculated ΔG_{THEO} (TS) values and imaginary frequencies

During Chapter 6 of the Thesis, the rate constants and product branching fractions for O_3 + Alkene **19** was calculated using FESP Models 1-3 only projected values for the TS structures and the Eckart function was derived using the imaginary frequencies from the respective TSs in the O_3 + Alkene **16** reaction. Two further derivatives of model 3 have also been adopted. Model 3a uses the computational ΔG_{THEO} (TS), -126.39 & -109.02 kJ mol^{-1}, to derive an adjusted ΔZPE (-178.27 & -161.77 kJ mol^{-1}) of TS_{ANTI} 1.8 and TS_{SYN} 1.8. The yields had only negligible changes, as shown in Table 6.15, and did not have a significant overall effect on the different yields. This helps to verify the reliability of Model 3.

Table 165: A comparison of models 1-3b in the effective way of calculating product yields and Eckart functions with grain size 50-60 cm^{-1}.

Models	Grain size	TS_{ANTI} 1.8		TS_{SYN} 1.8		Overall	
		ΔG_{TS}	Γ_{PROJ}	ΔG_{TS}	Γ_{PROJ}	Γanti- *nPrCHOO*	Γsyn-*nPrCHOO*
1	60	-121.64	0.058	-108.60	0.004	0.455	0.031
2	60	-124.01	0.069	-106.23	0.001	0.480	0.025
3	60	-126.60	0.081	-108.81	0.003	0.478	0.032
3a	50	-126.39	0.080	-109.02	0.001	0.482	0.028
3b	50		0.078		0.003	0.472	0.035

For models 1-3a, the imaginary frequencies used for TS_{ANTI} 1.8 and TS_{SYN} 1.8 were the respective imaginary frequencies of *Z*-2-pentene, TS_{ANTI} 1.3 (-442.19 cm^{-1}) and TS_{SYN} 1.3 (-462.01 cm^{-1}). Model 3b, uses the imaginary frequencies of TS_{ANTI} 1.8 (-443.08 cm^{-1}) and TS_{SYN} 1.8 (-467.61 cm^{-1}), which have been calculated using the optimised structures for O_3 + *Z*-2-hexene instead. As shown in table 6.15, this change in imaginary frequencies causes only negligible changes in Γ_{EMP}. This helps to verify that the use of the imaginary frequencies of *Z*-2-pentene compared to the actual imaginary frequency, in these Eckart functions, has negligible impact. Therefore, use of the imaginary frequencies is for models 1-3 is much more likely to produce reliable Eckart functions and therefore reliable product yields.

4.5 Rate Constants for All Three FESP Models

4.5.1 FESP Model 1 for O_3 + *Z*-2-hexene

Table 166: Canonical Rate constants (k_{CAN}) for FESP Model 3, breakdown by Transition State across a variety of Temperatures

T (K)	k_{ME}	Total k_{CAN}	TS_{ozo} 1.1	TS_{ozo} 1.2	TS_{ozo} 1.3	TS_{ozo} 1.4	TS_{ozo} 1.5	TS_{ozo} 1.6	TS_{ozo} 1.7	TS_{ozo} 1.8	TS_{ozo} 1.9
200	9.59E-16	9.46E-16	9.78E-17	1.11E-17	1.13E-18	2.58E-20	0.00E+00	1.43E-21	6.53E-16	2.49E-17	1.38E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			8.97E-19	8.98E-20	8.06E-21	4.16E-22	4.61E-25	1.49E-23	1.41E-17	8.12E-19	3.92E-18
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
275	2.02E-15	1.95E-15	2.72E-16	5.60E-17	1.06E-17	6.79E-19	0.00E+00	8.14E-20	1.09E-15	7.26E-17	3.53E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			8.18E-18	1.53E-18	2.66E-19	2.25E-20	1.59E-22	1.99E-21	5.63E-17	7.05E-18	2.22E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
298	2.48E-15	2.39E-15	3.48E-16	8.10E-17	1.75E-17	1.38E-18	0.00E+00	1.93E-19	1.26E-15	9.26E-17	4.44E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			1.34E-17	2.85E-18	5.65E-19	5.29E-20	5.49E-22	5.66E-21	7.76E-17	1.14E-17	3.28E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
325	3.11E-15	2.98E-15	4.52E-16	1.19E-16	2.91E-17	2.84E-18	0.00E+00	4.62E-19	1.48E-15	1.19E-16	5.69E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			2.21E-17	5.36E-18	1.22E-18	1.26E-19	1.91E-21	1.62E-20	1.09E-16	1.87E-17	4.94E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
400	5.53E-15	5.22E-15	8.41E-16	2.84E-16	9.06E-17	1.36E-17	0.00E+00	3.00E-18	2.24E-15	2.12E-16	1.03E-15
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			6.78E-17	2.14E-17	6.43E-18	8.18E-19	2.72E-20	1.55E-19	2.35E-16	5.65E-17	1.24E-16

4.5.2 FESP Model 2 for O_3 + *Z*-2-hexene

Table 167: Canonical Rate constants (k_{CAN}) for FESP Model 3, breakdown by Transition State across a variety of Temperatures

T (K)	k_{ME}	Total k_{CAN}	TS_{ozo} 1.1	TS_{ozo} 1.2	TS_{ozo} 1.3	TS_{ozo} 1.4	TS_{ozo} 1.5	TS_{ozo} 1.6	TS_{ozo} 1.7	TS_{ozo} 1.8	TS_{ozo} 1.9
200	1.03E-15	1.03E-15	9.78E-17	1.21E-16	4.49E-20	2.58E-20	-	1.06E-22	6.53E-16	-	1.38E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			8.94E-19	9.78E-19	3.19E-22	4.16E-22	6.56E-26	3.58E-24	1.41E-17	1.94E-19	3.92E-18
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
275	2.13E-15	2.13E-15	2.72E-16	3.18E-16	1.02E-18	6.79E-19	-	6.70E-21	1.09E-15	-	3.51E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			8.16E-18	8.71E-18	2.54E-20	2.25E-20	3.86E-23	7.08E-22	5.63E-17	2.49E-18	2.22E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
298	2.60E-15	2.60E-15	3.48E-16	4.02E-16	2.00E-18	1.38E-18	-	1.61E-20	1.26E-15	-	4.41E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			1.33E-17	1.41E-17	6.47E-20	5.29E-20	1.48E-22	2.17E-21	7.76E-17	4.37E-18	3.28E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
325	3.24E-15	3.23E-15	4.52E-16	5.17E-16	3.99E-18	2.84E-18	-	3.88E-20	1.48E-15	-	5.63E-16
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			2.21E-17	2.33E-17	1.67E-19	1.26E-19	5.76E-22	6.75E-21	1.09E-16	7.76E-18	4.94E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
400	5.60E-15	5.58E-15	8.41E-16	9.37E-16	1.80E-17	1.36E-17	-	2.51E-19	2.24E-15	-	1.00E-15
			TS_{ozo} 2.1	**TS_{ozo} 2.2**	**TS_{ozo} 2.3**	**TS_{ozo} 2.4**	**TS_{ozo} 2.5**	**TS_{ozo} 2.6**	**TS_{ozo} 2.7**	**TS_{ozo} 2.8**	**TS_{ozo} 2.9**
			6.77E-17	7.08E-17	1.28E-18	8.18E-19	1.03E-20	7.59E-20	2.35E-16	2.76E-17	1.24E-16

4.5.3 FESP Model 3 for O_3 + *Z*-2-hexene

Table 168: Canonical Rate constants (k_{CAN}) for FESP Model 3, breakdown by Transition State across a variety of Temperatures

T (K)	k_{ME}	Total k_{CAN}	TS_{ozo} 1.1	TS_{ozo} 1.2	TS_{ozo} 1.3	TS_{ozo} 1.4	TS_{ozo} 1.5	TS_{ozo} 1.6	TS_{ozo} 1.7	TS_{ozo} 1.8	TS_{ozo} 1.9
200	1.53E-15	1.55E-15	9.93E-17	5.81E-16	2.17E-19	2.64E-20	0.00E+00	1.55E-21	6.63E-16	3.66E-17	1.40E-16
			TS_{ozo} 2.1	TS_{ozo} 2.2	TS_{ozo} 2.3	TS_{ozo} 2.4	TS_{ozo} 2.5	TS_{ozo} 2.6	TS_{ozo} 2.7	TS_{ozo} 2.8	TS_{ozo} 2.9
			9.15E-19	4.75E-18	1.56E-21	4.25E-22	3.20E-25	1.75E-23	1.44E-17	9.43E-19	4.00E-18
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
275	2.98E-15	2.95E-15	2.74E-16	9.89E-16	3.17E-18	6.85E-19	0.00E+00	7.82E-20	1.10E-15	1.08E-16	3.54E-16
			TS_{ozo} 2.1	TS_{ozo} 2.2	TS_{ozo} 2.3	TS_{ozo} 2.4	TS_{ozo} 2.5	TS_{ozo} 2.6	TS_{ozo} 2.7	TS_{ozo} 2.8	TS_{ozo} 2.9
			8.25E-18	2.73E-17	7.97E-20	2.27E-20	1.21E-22	2.23E-21	5.67E-17	7.81E-18	2.24E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
298	3.58E-15	3.53E-15	3.49E-16	1.14E-15	5.71E-18	1.39E-18	0.00E+00	1.80E-19	1.27E-15	1.38E-16	4.44E-16
			TS_{ozo} 2.1	TS_{ozo} 2.2	TS_{ozo} 2.3	TS_{ozo} 2.4	TS_{ozo} 2.5	TS_{ozo} 2.6	TS_{ozo} 2.7	TS_{ozo} 2.8	TS_{ozo} 2.9
			1.34E-17	4.06E-17	1.86E-19	5.33E-20	4.27E-22	6.25E-21	7.80E-17	1.25E-17	3.30E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
325	4.40E-15	4.31E-15	4.54E-16	1.35E-15	1.04E-17	2.85E-18	0.00E+00	4.17E-19	1.49E-15	1.79E-16	5.65E-16
			TS_{ozo} 2.1	TS_{ozo} 2.2	TS_{ozo} 2.3	TS_{ozo} 2.4	TS_{ozo} 2.5	TS_{ozo} 2.6	TS_{ozo} 2.7	TS_{ozo} 2.8	TS_{ozo} 2.9
			2.22E-17	6.12E-17	4.39E-19	1.27E-19	1.52E-21	1.78E-20	1.09E-16	2.04E-17	4.96E-17
T (K)	**k_{ME}**	**Total k_{CAN}**	**TS_{ozo} 1.1**	**TS_{ozo} 1.2**	**TS_{ozo} 1.3**	**TS_{ozo} 1.4**	**TS_{ozo} 1.5**	**TS_{ozo} 1.6**	**TS_{ozo} 1.7**	**TS_{ozo} 1.8**	**TS_{ozo} 1.9**
400	7.41E-15	7.15E-15	8.43E-16	2.04E-15	3.93E-17	1.37E-17	0.00E+00	2.51E-18	2.24E-15	3.22E-16	1.00E-15
			TS_{ozo} 2.1	TS_{ozo} 2.2	TS_{ozo} 2.3	TS_{ozo} 2.4	TS_{ozo} 2.5	TS_{ozo} 2.6	TS_{ozo} 2.7	TS_{ozo} 2.8	TS_{ozo} 2.9
			6.80E-17	1.55E-16	2.80E-18	8.21E-19	2.25E-20	1.66E-19	2.36E-16	6.04E-17	1.24E-16

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Phase Reactions of CH2OO with H2S and H2S–H2O, Respectively. See DOI: 10.1039/C7sc01797a Click Here for Additional Data File. Click Here for Additional Data File. Click Here for Additional Data File. Click Here for Additional Data File. Click Here for Additional Data File. *Chem Sci* **2017**, *8* (8), 5385–5391. https://doi.org/10.1039/c7sc01797a.
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6.0 Cartesian Coordinates And IRCs for Chapter 3: Ozonolysis of Alkenes

6.1 Reactants

6.1.1 Ozone

Compound: O_3	**Energy (kJ mol^{-1}):** -225.232118853147
Reaction Coordinates: 8 -0.000000 0.000000 0.429077 8 0.000000 1.077304 -0.214539 8 -0.000000 -1.077304 -0.214539	**Frequencies (cm^{-1}):** 745.8860, 1189.8635, 1249.1307

6.1.2 Alkenes

Compound: 1-Propene (Alkene 1)	**Energy (kJ mol^{-1}):** -117.734202583006
Reaction Coordinates: 6 -1.230938 0.162150 0.000000 6 0.133754 -0.452181 0.000000 6 1.278183 0.219838 0.000000 1 2.233452 -0.287527 0.000000 1 1.300084 1.303347 0.000000 1 0.166634 -1.537973 0.000000 1 -1.180079 1.250999 -0.000004 1 -1.803043 -0.153849 -0.876177 1 -1.803039 -0.153842 0.876181	**Frequencies (cm^{-1}):** 204.9479, 425.8636, 592.517, 924.196, 947.717, 950.3007, 1027.4886, 1075.0243, 1192.5587, 1330.7287, 1409.8921, 1452.5855, 1479.5898, 1494.4211, 1708.0283, 3014.1612, 3054.976, 3090.0181, 3122.2949, 3128.6327, 3208.6582

Compound: 1-Butene con 1 (Alkene 2)	**Energy (kJ mol^{-1}):** -156.990868091369
Reaction Coordinates: 6 -0.536459 -0.517092 0.305759 6 0.720848 0.298931 0.330086 6 1.858817 -0.019671 -0.274312 1 1.960541 -0.935339 -0.845149 1 2.729712 0.619667 -0.219444 1 0.667703 1.230181 0.888931 6 -1.728322 0.242406 -0.290499 1 -2.633603 -0.365138 -0.259588 1 -1.925489 1.162189 0.263200 1 -1.537492 0.514803 -1.329163 1 -0.363084 -1.438686 -0.254199 1 -0.787596 -0.815119 1.329209	**Frequencies (cm^{-1}):** 109.5259, 228.1782, 317.2718, 433.7871, 654.5041, 797.6579, 857.8692, 950.0516, 991.6019, 1019.2921, 1035.3656, 1095.9436, 1201.3788, 1291.9326, 1324.9038, 1347.1325, 1409.6417, 1459.0333, 1483.6329, 1498.3084, 1506.7266, 1703.7339, 3001.7445, 3024.8565, 3045.1892, 3085.1411, 3091.1432, 3111.3755, 3126.3992, 3207.0069

Compound: 1-Butene con 2 (Alkene 2)	**Energy (kJ mol^{-1}):** -156.990759930222
Reaction Coordinates: 6 0.638811 0.717833 0.000002 6 -0.854431 0.555674 -0.000001 6 -1.533105 -0.585545 0.000001 1 -1.044066 -1.550718 0.000003 1 -2.614680 -0.591931 -0.000001 1 -1.413272 1.487408 -0.000005 6 1.454633 -0.570783 -0.000001 1 2.521758 -0.347745 0.000001 1 1.242067 -1.177482 0.881388 1 1.242069 -1.177476 -0.881395 1 0.915341 1.327440 -0.867565 1 0.915339 1.327437 0.867571	**Frequencies (cm^{-1}):** 160.259, 257.6184, 275.4325, 547.3184, 564.6587, 805.1812, 837.0941, 947.1934, 998.2798, 1032.782, 1038.5949, 1110.213, 1146.5461, 1293.5114, 1334.6517, 1381.0385, 1411.6583, 1456.0652, 1475.7496, 1499.0556, 1508.9344, 1703.3793, 2995.8815, 3008.4799, 3029.2014, 3087.4202, 3091.1398, 3117.9322, 3140.3888, 3214.7309

Compound: 3-methyl-1-Butene con 1 (Alkene 3)	**Energy (kJ mol^{-1}):** -196.250016454020
Reaction Coordinates: 6 -0.369797 -0.000000 -0.307860 6 0.949413 -0.000003 0.412744 6 2.145751 -0.000001 -0.161515 1 3.056614 -0.000003 0.422167 1 2.257390 0.000004 -1.239614 1 0.886880 -0.000008 1.499171 1 -0.165906 0.000000 -1.382726 6 -1.174768 -1.264206 0.028387 1 -0.628045 -2.165889 -0.248287 1 -1.387431 -1.316605 1.098771 1 -2.129533 -1.267701 -0.500422 6 -1.174763 1.264209 0.028389 1 -0.628035 2.165890 -0.248285 1 -2.129527 1.267709 -0.500419 1 -1.387425 1.316608 1.098773	**Frequencies (cm^{-1}):** 98.8235, 222.6742, 239.6225, 313.4523, 321.4543, 347.0894, 504.5264, 697.5098, 801.1446, 930.7808, 932.2227, 951.0227, 963.7819, 1007.3587, 1036.2437, 1115.241, 1185.2275, 1218.5117, 1322.1315, 1337.3236, 1342.1606, 1396.8721, 1416.4007, 1461.1698, 1488.9058, 1489.881, 1501.9278, 1510.7555, 1701.7048, 3009.9448, 3016.5794, 3020.9294, 3073.2624, 3079.7035, 3090.4561, 3091.8414, 3102.8104, 3125.4857, 3205.8722

Compound: 3-methyl-1-Butene con 2 (Alkene 3)	**Energy (kJ mol^{-1}):** -196.249609684300
Reaction Coordinates: 6 0.471638 -0.018352 -0.417232 6 -0.896450 -0.628921 -0.257404 6 -1.985773 -0.052916 0.237060 1 -2.918762 -0.595435 0.310334 1 -1.994966 0.971569 0.584568 1 -0.966572 -1.663115 -0.585257 1 0.708452 -0.064473 -1.487926 6 0.562071 1.443577 0.017004 1 -0.142226 2.070983 -0.530164 1 0.352517 1.552418 1.083076 1 1.565193 1.831589 -0.163949 6 1.521043 -0.879191 0.306284 1 1.478788 -1.918362 -0.023504 1 2.528122 -0.506270 0.113506 1 1.354279 -0.864087 1.385038	**Frequencies (cm^{-1}):** 114.6497, 235.0579, 260.5161, 286.8624, 350.9344, 382.2605, 539.2118, 674.5589, 781.4482, 923.1806, 932.5024, 950.0535, 969.3309, 1033.2886, 1043.7479, 1117.0369, 1154.9103, 1207.1747, 1319.3983, 1339.8844, 1369.4212, 1399.9641, 1416.4501, 1457.613, 1490.4591, 1493.7712, 1503.9212, 1513.9373, 1699.5984, 2972.0167, 3019.9562, 3025.481, 3080.4557, 3084.0765, 3086.0992, 3090.2351, 3110.3928, 3140.0824, 3214.3701

Compound: 3,3-dimethyl-1-Butene (Alkene 4)	**Energy (kJ mol^{-1}):** -235.509880163998
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.351150 -0.001909 -0.000000 6 1.009060 0.660323 0.000000 6 2.201853 0.078085 0.000000 1 2.326643 -0.996421 -0.000000 1 3.108508 0.668311 -0.000000 1 0.969826 1.747386 0.000000 6 -1.115401 0.467384 -1.254902 1 -2.127636 0.058245 -1.262419 1 -1.193783 1.555680 -1.284174 1 -0.609550 0.142645 -2.165026 6 -0.262357 -1.531765 0.000002 1 -1.263343 -1.965983 0.000003 1 0.260348 -1.901743 -0.883122 1 0.260348 -1.901740 0.883127 6 -1.115403 0.467388 1.254900 1 -2.127638 0.058248 1.262417 1 -0.609553 0.142651 2.165025 1 -1.193785 1.555684 1.284168	104.7515, 226.713, 264.1669, 285.0811, 291.744, 314.8559, 350.0099, 385.3784, 402.5624, 526.5443, 699.9181, 714.1615, 883.0131, 927.0951, 938.5748, 951.0736, 963.7101, 1016.7692, 1039.6134, 1050.5989, 1091.827, 1222.6682, 1231.8623, 1291.626, 1341.9136, 1395.8354, 1399.3707, 1423.351, 1457.8098, 1481.6925, 1488.1651, 1491.7312, 1504.8251, 1504.9522, 1522.0759, 1697.4588, 3016.3606, 3019.0744, 3027.0225, 3076.5819, 3080.1217, 3085.1923, 3085.4136, 3089.3936, 3089.6833, 3104.2194, 3139.7976, 3213.9846

Compound: Methyl Vinyl Ketone (Alkene 5) Con 1	**Energy (kJ mol^{-1}):** -230.947246392397
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.745082 -0.601228 0.000001 6 -0.443184 0.165775 -0.000002 6 0.804450 -0.656380 -0.000002 6 2.012398 -0.101726 0.000001 1 2.913228 -0.699634 0.000002 1 2.117137 0.975614 0.000003 1 0.689509 -1.734043 -0.000003 8 -0.413644 1.379339 -0.000000 1 -2.586099 0.086258 -0.000007 1 -1.798052 -1.250785 -0.877062 1 -1.798056 -1.250767 0.877077	91.2067, 125.0188, 267.7951, 416.1738, 459.9243, 601.345, 686.5542, 778.0401, 959.5856, 1019.3789, 1027.227, 1047.4258, 1085.647, 1196.2019, 1329.7897, 1385.1429, 1439.4219, 1464.5645, 1474.0063, 1667.5026, 1764.2385, 3025.0855, 3075.4149, 3139.8447, 3141.3414, 3155.0215, 3231.2254

Compound: Methyl Vinyl Ketone (Alkene 5) Con 2	**Energy (kJ mol^{-1}):** -230.948123255856
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.862592 1.290436 0.000000 6 0.541735 -0.188772 -0.000000 6 -0.876762 -0.629762 0.000000 6 -1.935118 0.176610 -0.000000 1 -2.941959 -0.218702 0.000000 1 -1.840063 1.254225 -0.000001 1 -0.997314 -1.706492 0.000002 8 1.425408 -1.024458 -0.000000 1 1.941376 1.417331 -0.000003 1 0.440003 1.779118 -0.879457 1 0.440009 1.779115 0.879462	115.3929, 125.8373, 279.3674, 434.0748, 492.6237, 538.0067, 701.2258, 760.6503, 946.7066, 997.4841, 1043.5912, 1051.9594, 1075.0319, 1271.0386, 1311.8244, 1390.2797, 1448.5287, 1473.5799, 1479.6845, 1681.4643, 1740.3039, 3036.7015, 3090.9528, 3141.4545, 3142.9025, 3164.6944, 3223.3275

Compound: 2-methyl-2-Butene (Alkene 6)	**Energy (kJ mol^{-1}):** -196.253938354277
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.624503 1.452410 0.000000 6 -0.447140 -0.041432 -0.000000 6 0.730526 -0.670603 0.000000 1 0.707689 -1.757034 0.000000 6 2.106934 -0.077806 0.000000 1 2.671834 -0.409494 0.875668 1 2.671834 -0.409494 -0.875668 1 2.106436 1.010167 -0.000000 6 -1.736975 -0.818574 0.000000 1 -1.562432 -1.893791 0.000000 1 -2.343659 -0.571524 0.876361 1 -2.343659 -0.571524 -0.876361 1 0.315041 1.998972 -0.000000 1 -1.198069 1.769879 -0.875725 1 -1.198068 1.769879 0.875725	119.287, 142.8596, 184.9092, 265.3825, 296.142, 384.9177, 457.0872, 527.2405, 770.054, 832.394, 957.7479, 968.7794, 1018.083, 1066.3741, 1068.8734, 1105.8277, 1129.4731, 1234.5111, 1376.8706, 1411.2291, 1415.4366, 1423.97, 1472.9828, 1481.779, 1483.9397, 1492.3166, 1496.9433, 1498.3233, 1733.8621, 3003.315, 3010.4859, 3012.6748, 3040.3203, 3044.1971, 3044.5477, 3095.0622, 3099.7183, 3115.5834, 3123.0159

Compound: 2-methyl-2-pentene (Alkene 7) con 1	**Energy (kJ mol^{-1}):** -235.510710308254
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.520310 0.221336 -0.523304 6 -0.234286 -0.525718 -0.322966 6 0.979796 -0.045824 -0.041200 6 2.155079 -0.971745 0.130221 1 2.945285 -0.739424 -0.590032 1 2.599420 -0.861198 1.123880 1 1.871746 -2.015220 -0.001392 6 1.312561 1.411770 0.128122 1 1.755509 1.590707 1.112078 1 2.060720 1.721688 -0.607412 1 0.451197 2.066543 0.024353 1 -0.327786 -1.605616 -0.414792 1 -1.363805 1.298498 -0.469677 1 -1.892183 0.018473 -1.533586 6 -2.603355 -0.188153 0.484308 1 -3.543315 0.327818 0.282390 1 -2.795928 -1.261654 0.438934 1 -2.297778 0.049388 1.504166	51.8385, 134.0678, 155.563, 211.3092, 213.2614, 306.3294, 360.6327, 413.2072, 486.1891, 512.7563, 751.3242, 825.2312, 864.3378, 915.4111, 962.8715, 1013.2655, 1020.6581, 1082.2278, 1094.991, 1105.6605, 1141.043, 1231.6042, 1293.7294, 1338.8625, 1390.3168, 1407.4913, 1412.798, 1421.2303, 1473.0816, 1479.5445, 1490.5559, 1492.0726, 1497.0068, 1498.9707, 1507.1527, 1728.9667, 2997.3477, 3003.3894, 3011.1735, 3022.168, 3040.5651, 3044.3677, 3062.2916, 3084.0155, 3087.4197, 3094.8892, 3103.9654, 3119.1194

Compound: 2-methyl-2-pentene (Alkene 7) con 2	**Energy (kJ mol^{-1}):** -235.503965311762
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.587139 -0.824293 -0.000001 6 -0.081647 -0.918267 -0.000000 6 0.912688 -0.025175 0.000000 6 2.343751 -0.505934 0.000002 1 2.410754 -1.592876 0.000003 1 2.881410 -0.131116 -0.876192 1 2.881410 -0.131114 0.876194 6 0.803464 1.476984 0.000000 1 1.315239 1.889798 0.874584 1 1.315248 1.889799 -0.874579 1 -0.212815 1.848888 -0.000005 1 0.238029 -1.958104 0.000000 1 -1.939778 -1.398553 -0.864851 1 -1.939779 -1.398552 0.864850 6 -2.299938 0.526588 -0.000002 1 -3.379324 0.366789 -0.000002	49.3885, 126.9372, 178.6736, 240.3712, 261.9161, 312.6675, 336.2853, 394.4681, 465.0377, 618.9179, 748.0852, 774.9348, 878.4081, 891.3665, 960.6299, 1023.4086, 1032.3807, 1075.0986, 1104.4448, 1111.0341, 1145.5448, 1214.3884, 1313.6081, 1377.6798, 1398.9989, 1410.8834, 1420.1532, 1427.8634, 1474.1226, 1477.3024, 1485.5748, 1492.4022, 1499.7359, 1510.3612, 1515.345, 1731.9196, 2985.1506, 2994.8608, 3002.3228, 3010.713, 3030.2095, 3038.2199, 3040.7653, 3082.8631, 3091.5868, 3096.9833, 3101.0623, 3177.4209

1 -2.058735 1.117812 0.883316 1 -2.058734 1.117811 -0.883319	

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 1	**Energy (kJ mol^{-1}):** -274.769873729866
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.247137 0.237315 -0.000023 6 0.055240 -0.516336 0.000036 6 1.304219 -0.044270 0.000000 6 2.483373 -0.981511 0.000076 1 3.116709 -0.814425 -0.876310 1 3.116702 -0.814291 0.876442 1 2.171798 -2.025197 0.000155 6 1.676813 1.413854 -0.000112 1 2.287634 1.652389 0.875439 1 2.287647 1.652251 -0.875692 1 0.817731 2.079795 -0.000171 1 -0.064196 -1.598538 0.000122 1 -1.048296 1.310326 -0.000120 6 -2.059584 -0.087816 -1.263421 1 -1.512045 0.185139 -2.165993 1 -2.280533 -1.156454 -1.318240 1 -3.010384 0.448795 -1.265264 6 -2.059568 -0.087590 1.263445 1 -1.512019 0.185529 2.165960 1 -3.010369 0.449020 1.265201 1 -2.280514 -1.156218 1.318458	40.2249, 121.1126, 149.4513, 199.6047, 207.6406, 226.1775, 255.9976, 301.8987, 397.8943, 400.2782, 449.0185, 504.6168, 514.9766, 806.8098, 857.8554, 875.9431, 929.9461, 952.8705, 960.5746, 964.6545, 1019.0613, 1088.314, 1105.6218, 1114.5094, 1138.028, 1192.67, 1236.2331, 1330.4358, 1338.1236, 1392.9908, 1395.7476, 1409.608, 1418.7341, 1421.6929, 1473.2079, 1485.7607, 1488.1608, 1489.7061, 1492.0437, 1495.6178, 1502.5374, 1509.3166, 1727.2033, 3003.3271, 3010.867, 3014.1397, 3018.2239, 3035.8106, 3040.5823, 3044.3118, 3070.1314, 3078.284, 3086.8013, 3087.8307, 3091.1843, 3098.6926, 3117.9913

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 2	**Energy (kJ mol^{-1}):** -274.764773946885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.338433 -0.567560 0.000010 6 0.151295 -0.871346 0.000013 6 1.201254 -0.045119 0.000000 6 2.605061 -0.593296 0.000008 1 3.160641 -0.246154 -0.876346 1 3.160641 -0.246130 0.876353 1 2.616229 -1.682291 0.000023 6 1.139328 1.459171 -0.000022 1 1.658226 1.860516 0.875499 1 1.658232 1.860490 -0.875551 1 0.128892 1.853883 -0.000031 1 0.385053 -1.932121 0.000028 1 -1.833136 -1.542711 0.000028 6 -1.817961 0.150147 1.272820 1 -1.517384 -0.398512 2.166038 1 -1.410784 1.157939 1.352519 1 -2.906959 0.231618 1.277280 6 -1.817964 0.150102 -1.272825 1 -1.517391 -0.398590 -2.166024 1 -2.906961 0.231577 -1.277284 1 -1.410783 1.157890 -1.352561	66.9975, 125.3714, 167.3352, 197.0113, 208.3577, 234.3454, 237.9794, 308.8628, 376.8418, 393.88, 406.0858, 495.3459, 620.8043, 769.1911, 838.2769, 853.7765, 930.0836, 959.0098, 961.2789, 977.2296, 1015.9067, 1076.2022, 1105.3816, 1123.0582, 1129.0872, 1205.0421, 1226.7452, 1357.6722, 1380.4474, 1384.5308, 1398.2498, 1410.817, 1419.5341, 1423.837, 1473.4915, 1483.5955, 1487.1637, 1490.7858, 1493.4414, 1500.0646, 1505.225, 1511.4668, 1719.997, 3003.0185, 3005.6275, 3011.4461, 3022.5044, 3026.9414, 3040.039, 3044.0641, 3079.6144, 3082.613, 3094.0631, 3096.8454, 3097.0983, 3113.8644, 3143.5006

Compound: 2,4-dimethyl-2-pentene (Alkene 8) con 3	**Energy (kJ mol^{-1}):** -274.763016073451

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.354661 -0.223774 -0.415572 6 -0.094184 -0.657937 -0.362243 6 -1.244757 -0.062819 -0.031566 6 -1.455245 1.355444 0.429559 1 -2.147931 1.871342 -0.242215 1 -0.548740 1.942733 0.494055 1 -1.929641 1.358110 1.415440 6 -2.532425 -0.848604 -0.098538 1 -2.370389 -1.873330 -0.429355 1 -3.241417 -0.376719 -0.785509 1 -3.022654 -0.878803 0.879146 1 -0.189436 -1.703443 -0.648756 1 1.711274 -0.559693 -1.397350 6 1.684710 1.267854 -0.327831 1 1.503045 1.669764 0.669539 1 1.114195 1.856119 -1.046219 1 2.744118 1.416640 -0.544683 6 2.165233 -1.012286 0.630230 1 1.876956 -0.717367 1.641064 1 3.234763 -0.826539 0.513981 1 1.997901 -2.086085 0.536625	35.6181, 112.23, 149.6262, 212.6158, 225.555, 262.282, 307.951, 329.8406, 358.5092, 409.1844, 425.0623, 505.6342, 613.6757, 770.3826, 844.3845, 874.9328, 931.9043, 954.6786, 960.6706, 976.4238, 1023.5399, 1084.2207, 1100.8448, 1105.1482, 1144.7, 1207.7566, 1227.8653, 1326.0417, 1376.3833, 1395.1516, 1402.1973, 1410.7867, 1422.7879, 1428.191, 1474.0691, 1484.0705, 1488.9555, 1495.1297, 1496.138, 1500.0458, 1511.7552, 1517.2955, 1725.4607, 2968.4206, 3002.7538, 3011.2398, 3017.7296, 3026.6285, 3038.9404, 3041.6594, 3076.0373, 3081.171, 3083.6741, 3088.9647, 3096.5764, 3100.5859, 3178.7312

Compound: 2,4,4-trimethyl-2-pentene (Alkene 9) con 1	**Energy (kJ mol^{-1}):** -314.024563428501
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.137021 -0.070215 0.000000 6 -0.259379 -0.689851 0.000001 6 -1.471838 -0.127696 0.000001 6 -2.706834 -0.992971 -0.000001 1 -3.328600 -0.786757 0.876368 1 -3.328602 -0.786750 -0.876367 1 -2.460715 -2.053740 -0.000005 6 -1.777139 1.346640 0.000001 1 -2.379148 1.607658 -0.875378 1 -2.379196 1.607648 0.875349 1 -0.896633 1.979490 0.000028 1 -0.251207 -1.776368 0.000001 6 2.159436 -1.222334 -0.000016 1 2.038628 -1.853302 -0.882604 1 2.038636 -1.853320 0.882560 1 3.179848 -0.835652 -0.000017 6 1.381325 0.778784 -1.263983 1 1.232401 0.181059 -2.164341 1 0.712537 1.635696 -1.321966 1 2.406761 1.155494 -1.275302 6 1.381335 0.778758 1.263999 1 1.232421 0.181014 2.164346 1 2.406769 1.155471 1.275316 1 0.712543 1.635666 1.322006	64.6822, 125.8305, 167.2823, 186.8965, 206.5533, 231.1321, 251.6629, 291.7571, 307.6043, 324.4647, 353.3254, 377.9719, 425.5823, 444.5562, 507.1322, 563.6174, 763.512, 822.3046, 852.0831, 926.4871, 929.8539, 947.305, 960.7913, 962.3601, 1016.111, 1050.8404, 1050.9084, 1102.2743, 1105.3059, 1178.0627, 1223.8857, 1250.4395, 1272.6268, 1390.6545, 1398.7861, 1400.4123, 1411.3526, 1423.0565, 1433.9231, 1473.2339, 1481.7288, 1482.5287, 1489.4142, 1489.436, 1493.4063, 1497.3553, 1507.9296, 1508.2509, 1520.1388, 1714.1334, 3003.1763, 3011.9746, 3016.3659, 3019.786, 3026.3564, 3040.1157, 3044.466, 3075.8264, 3077.4012, 3080.487, 3085.2659, 3097.2579, 3103.8216, 3105.2391, 3109.5045, 3148.4459

Compound: 2,4,4-trimethyl-2-pentene (Alkene 9) con 2	**Energy (kJ mol^{-1}):** -314.022840256808
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.153931 -0.048669 -0.000000 6 -0.259750 -0.606740 0.000000	37.8322, 101.7978, 141.0677, 207.7913, 226.2622, 241.0601,

6 -1.493679 -0.091407 0.000000 6 -1.908958 1.356708 -0.000000 1 -2.533187 1.564475 -0.874234 1 -1.088057 2.060881 -0.000004 1 -2.533181 1.564477 0.874237 6 -2.680455 -1.026650 0.000000 1 -2.378564 -2.072788 0.000001 1 -3.312543 -0.853912 -0.876221 1 -3.312544 -0.853911 0.876221 1 -0.228806 -1.694896 0.000000 6 1.866263 -0.602670 -1.253503 1 2.918543 -0.310396 -1.258443 1 1.820595 -1.692529 -1.283641 1 1.402786 -0.222853 -2.165068 6 1.297257 1.478281 0.000006 1 0.850274 1.929994 0.885386 1 0.850277 1.930000 -0.885373 1 2.357218 1.740226 0.000008 6 1.866266 -0.602679 1.253498 1 1.402792 -0.222868 2.165066 1 2.918546 -0.310405 1.258436 1 1.820598 -1.692538 1.283628	279.2297, 282.177, 331.5456, 352.9526, 362.9578, 394.6266, 425.29, 447.2463, 523.6109, 571.5711, 759.7664, 816.9911, 886.0609, 919.5083, 921.9658, 952.2851, 959.7541, 963.041, 1024.7654, 1047.0804, 1049.2022, 1102.2659, 1105.0826, 1175.1177, 1218.0621, 1242.0655, 1293.024, 1395.1699, 1395.2076, 1402.1578, 1411.0855, 1425.6459, 1434.4024, 1474.1451, 1482.1272, 1483.267, 1487.6212, 1493.7567, 1495.2499, 1501.5745, 1505.6236, 1513.9309, 1524.0001, 1720.2484, 3002.9985, 3011.4962, 3014.5969, 3017.7374, 3027.3661, 3038.9553, 3041.8064, 3074.9884, 3075.9104, 3081.1704, 3084.0698, 3084.7163, 3088.8554, 3099.5563, 3100.8475, 3183.575

Compound: Mesityl oxide (Alkene 10) Con 1	**Energy (kJ mol^{-1}):** -309.465790128374
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.817766 1.181570 0.000004 6 1.405239 -0.276388 0.000000 6 -0.006648 -0.723675 0.000002 6 -1.179688 -0.066779 0.000000 6 -2.458820 -0.860839 0.000002 1 -3.064594 -0.611789 0.875663 1 -3.064593 -0.611795 -0.875662 1 -2.276783 -1.933168 0.000006 6 -1.408062 1.417055 -0.000004 1 -2.002887 1.696951 -0.873831 1 -2.002883 1.696956 0.873824 1 -0.505647 2.013372 -0.000008 1 -0.048320 -1.807120 0.000003 8 2.271136 -1.136768 -0.000004 1 2.903580 1.226157 0.000009 1 1.437161 1.699458 -0.881230 1 1.437152 1.699457 0.881235	31.6247, 80.284, 143.1236, 213.5149, 230.804, 244.7836, 321.059, 373.1935, 471.6983, 524.2838, 583.3977, 584.7874, 781.0513, 876.1255, 885.7522, 956.6211, 1006.7854, 1015.2786, 1050.1668, 1092.0784, 1104.8031, 1202.7335, 1285.404, 1375.525, 1390.6008, 1409.8701, 1419.9382, 1467.8219, 1470.9895, 1483.6426, 1484.0559, 1495.1889, 1501.6001, 1683.5878, 1710.2959, 3012.6049, 3021.673, 3036.5958, 3051.1468, 3056.0309, 3095.4893, 3115.1414, 3134.563, 3146.8775, 3184.7417

Compound: Mesityl oxide (Alkene 10) Con 2	**Energy (kJ mol^{-1}):** -309.469316688066
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.560147 -0.799843 -0.000136 6 1.332280 0.091641 0.000049 6 0.040736 -0.632293 0.000085 6 -1.203331 -0.120263 -0.000002 6 -2.391119 -1.040052 0.000042 1 -3.018807 -0.851288 0.875172 1 -3.018660 -0.851563 -0.875252 1 -2.103278 -2.089720 0.000231 6 -1.539236 1.340342 -0.000146 1 -2.153759 1.574849 -0.874336	5.8179, 86.0289, 114.2669, 145.7257, 205.0671, 210.6334, 339.0034, 375.819, 442.647, 469.8649, 601.5013, 628.5367, 825.3514, 856.2612, 913.0507, 957.5863, 970.9409, 1005.165, 1042.746, 1096.5757, 1108.4228, 1188.3377, 1241.1667, 1381.198, 1390.1797, 1413.3283, 1415.1672, 1463.24, 1467.3951, 1473.9688, 1476.0118,

1 -2.153184 1.575136 0.874378 1 -0.657914 1.969542 -0.000496 1 0.133320 -1.712859 0.000161 8 1.450441 1.304942 0.000166 1 3.459067 -0.189878 -0.000173 1 2.556494 -1.450538 0.877320 1 2.556331 -1.450413 -0.877685	1487.7439, 1503.8996, 1660.1472, 1744.6457, 3010.4657, 3017.3443, 3025.9074, 3047.5875, 3056.8968, 3077.1295, 3107.6752, 3136.3004, 3139.6793, 3169.7428

Compound: HFO-1234yf (Alkene 11)	**Energy (kJ mol^{-1}):** -514.464460739210
Reaction Coordinates: 6 -0.585281 -0.043725 -0.000000 6 0.922986 -0.027137 -0.000000 6 1.716238 -1.077688 -0.000001 1 2.788511 -0.953648 -0.000000 1 1.298487 -2.070706 -0.000001 9 1.389017 1.232144 -0.000000 9 -1.057966 -1.299622 0.000000 9 -1.077228 0.584609 1.083539 9 -1.077230 0.584609 -1.083538	**Frequencies (cm^{-1}):** 66.5226, 234.0701, 236.7274, 365.1414, 415.2527, 493.7216, 570.3112, 611.2868, 679.7835, 755.144, 787.2174, 932.9654, 956.2932, 1141.1345, 1151.7237, 1178.4052, 1353.311, 1423.1767, 1747.7183, 3179.6402, 3276.2088

Compound: HFO-1345fz (Alkene 12) con 1	**Energy (kJ mol^{-1}):** -652.907119469829
Reaction Coordinates: 6 -0.406520 0.464064 0.041056 6 -1.522801 -0.339034 0.631669 6 -2.575775 -0.740538 -0.061205 1 -2.684659 -0.515610 -1.112637 1 -3.364589 -1.307849 0.411851 1 -1.404735 -0.563074 1.683356 6 0.950218 -0.293991 -0.013799 9 1.922772 0.493908 -0.477940 9 1.293377 -0.712595 1.214935 9 0.854506 -1.364889 -0.812109 9 -0.680637 0.869707 -1.226395 9 -0.191880 1.585372 0.793853	**Frequencies (cm^{-1}):** 65.4496, 74.8184, 198.6928, 219.6502, 276.1685, 313.3121, 354.3534, 378.6851, 459.1658, 522.8383, 564.6134, 580.3317, 645.5624, 729.0861, 768.6396, 1006.1183, 1021.6304, 1023.5818, 1037.8805, 1126.2012, 1182.7922, 1193.0461, 1246.4826, 1313.0904, 1326.6004, 1455.9826, 1714.5074, 3154.9201, 3185.8, 3241.5178

Compound: HFO-1345fz (Alkene 12) con 2	**Energy (kJ mol^{-1}):** -652.904303093187
Reaction Coordinates: 6 -0.373774 0.636304 -0.000001 6 -1.766832 0.091752 0.000022 6 -2.127041 -1.181547 -0.000001 1 -1.418307 -1.996261 -0.000041 1 -3.174403 -1.448473 0.000018 1 -2.505479 0.884601 0.000061 6 0.805569 -0.372781 0.000002 9 1.971435 0.276945 -0.000013 9 0.761617 -1.156981 1.087333 9 0.761605 -1.157009 -1.087307 9 -0.198970 1.436160 -1.095537 9 -0.198947 1.436192 1.095505	**Frequencies (cm^{-1}):** 75.3476, 82.8866, 175.3097, 217.682, 288.051, 308.1011, 346.8878, 415.779, 426.4018, 498.141, 573.3491, 587.1223, 651.4742, 710.5058, 760.9488, 980.9817, 1000.8456, 1023.0824, 1090.7632, 1132.2297, 1182.4404, 1183.2641, 1198.8206, 1316.4318, 1376.3369, 1472.9663, 1719.0547, 3157.1139, 3167.5889, 3242.3767

Compound: HFO-1233zd (Alkene 13)	**Energy (kJ mol^{-1}):** -874.459906302694

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.304166 0.037365 0.000000 6 -0.124015 0.475233 0.000000 6 -1.124569 -0.388198 0.000000 17 -2.785458 0.098196 -0.000000 1 -0.988720 -1.458223 0.000001 1 -0.277597 1.544740 -0.000001 9 1.958514 0.511736 -1.083528 9 1.958515 0.511740 1.083526 9 1.448039 -1.301504 0.000002	81.6682, 155.5861, 167.9512, 299.2645, 393.6749, 400.4923, 547.4506, 563.4267, 660.1194, 833.3308, 851.3053, 872.8286, 968.2956, 1117.8281, 1125.0475, 1261.1857, 1285.3608, 1322.7518, 1697.9469, 3203.4882, 3220.3034

Compound: HFO-1234ze(E) (Alkene 14)	**Energy (kJ mol^{-1}):** -514.467255920440
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.843476 0.031705 0.000000 6 -0.560694 0.526254 -0.000001 6 -1.592866 -0.296119 -0.000000 9 -2.847722 0.166306 -0.000000 1 -1.543881 -1.375091 0.000000 1 -0.689768 1.598797 -0.000001 9 1.521177 0.474285 -1.082808 9 1.521177 0.474288 1.082807 9 0.926942 -1.314295 0.000002	85.0572, 191.9601, 193.4258, 386.5226, 409.7951, 418.4184, 554.7289, 577.4385, 690.8616, 869.6416, 879.7608, 963.0113, 1084.8443, 1116.9275, 1187.7224, 1257.587, 1321.8206, 1346.0002, 1742.5088, 3208.2322, 3218.0848

Compound: *E*-2-pentene (Alkene 15) con 1	**Energy (kJ mol^{-1}):** -196.251071480094
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.295855 0.556837 -0.220006 6 0.066116 -0.044855 -0.400279 6 1.169904 0.338239 0.233138 1 1.102628 1.160771 0.941527 6 2.527626 -0.268169 0.055375 1 3.250426 0.475332 -0.291259 1 2.912725 -0.659893 1.000639 1 2.509533 -1.084536 -0.667014 1 0.130587 -0.869626 -1.107825 6 -2.338349 -0.455703 0.270882 1 -3.323589 0.005142 0.355288 1 -2.423089 -1.298008 -0.418354 1 -2.064921 -0.854290 1.248704 1 -1.235300 1.394648 0.478403 1 -1.635656 0.972367 -1.174770	95.1208, 174.4694, 207.0285, 212.393, 302.7287, 410.1315, 488.8208, 766.8394, 817.5183, 884.3052, 949.8826, 1000.5831, 1029.2249, 1072.7703, 1080.2898, 1102.139, 1179.992, 1278.1465, 1322.7711, 1338.3681, 1369.4151, 1409.1436, 1414.9778, 1479.9028, 1483.1445, 1493.0503, 1497.8229, 1505.8295, 1731.9048, 2998.0422, 3010.7105, 3022.8968, 3041.7622, 3049.2851, 3082.4761, 3085.5294, 3088.4103, 3097.267, 3111.8101

Compound: *E*-2-pentene (Alkene 15) con 2	**Energy (kJ mol^{-1}):** -196.250612583247
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.396132 0.663057 0.000001 6 -0.105953 0.719991 -0.000000 6 -0.948189 -0.308269 0.000000 1 -0.553348 -1.319353 0.000002 6 -2.442134 -0.192208 -0.000000 1 -2.877019 -0.680561 -0.876242 1 -2.877019 -0.680548 0.876250 1 -2.762895 0.849873 -0.000007 1 -0.524143 1.724290 -0.000002	130.3313, 201.3828, 203.2816, 221.8668, 292.7763, 366.5152, 583.9821, 717.6484, 835.4658, 855.006, 951.5287, 1007.0597, 1039.5076, 1072.8252, 1082.5013, 1109.8349, 1145.4322, 1294.0792, 1323.984, 1342.7188, 1382.2184, 1413.543, 1417.3128, 1478.2158, 1480.4696, 1494.103, 1499.2672,

6 2.019655 -0.729366 -0.000000 1 3.107809 -0.660621 0.000001 1 1.723368 -1.300060 0.881425 1 1.723371 -1.300058 -0.881429 1 1.761409 1.223907 -0.867778 1 1.761408 1.223905 0.867781	1507.7024, 1732.3268, 2992.3715, 3003.9092, 3010.0394, 3027.5453, 3048.3419, 3085.3026, 3085.8294, 3088.8917, 3102.4869, 3133.8875

Compound: *Z*-2-pentene (Alkene 16) con 1	**Energy (kJ mol^{-1}):** -196.249290990363
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.010746 -0.198222 0.561353 6 0.013678 0.811731 0.134129 6 1.302108 0.614454 -0.141415 1 1.882671 1.481361 -0.442343 6 2.071878 -0.670389 -0.086180 1 2.529282 -0.887960 -1.054905 1 2.891397 -0.599267 0.634145 1 1.457110 -1.523846 0.192647 1 -0.365072 1.825551 0.033681 1 -0.563596 -1.186428 0.670085 1 -1.385389 0.078640 1.552669 6 -2.199758 -0.275580 -0.405698 1 -2.952628 -0.978457 -0.046177 1 -2.679137 0.698708 -0.517042 1 -1.877596 -0.600271 -1.395899	56.5887, 136.8691, 214.5953, 260.9216, 300.6178, 474.1665, 572.161, 720.4797, 795.9926, 863.0838, 935.7132, 1013.6785, 1025.7052, 1051.4266, 1067.852, 1093.8952, 1172.2047, 1282.5784, 1302.9043, 1340.4758, 1406.7983, 1411.0139, 1442.7749, 1482.5483, 1484.6711, 1494.972, 1498.104, 1507.0336, 1721.314, 3000.5883, 3015.1258, 3023.4597, 3050.2094, 3061.1266, 3085.2081, 3088.8849, 3102.8509, 3109.9953, 3132.9181

Compound: *Z*-2-pentene (Alkene 16) con 2	**Energy (kJ mol^{-1}):** -196.243578385811
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.346035 0.530063 -0.000000 6 -0.042625 1.114177 -0.000001 6 -1.264818 0.580769 0.000000 1 -2.082808 1.296181 0.000001 6 -1.727065 -0.846757 -0.000000 1 -2.354640 -1.039431 0.874611 1 -2.354674 -1.039418 -0.874590 1 -0.921974 -1.572409 -0.000021 1 -0.017015 2.201089 -0.000001 1 1.870389 0.952186 -0.865216 1 1.870386 0.952185 0.865219 6 1.547001 -0.983835 0.000000 1 2.613861 -1.212224 0.000005 1 1.112653 -1.452330 0.883057 1 1.112661 -1.452329 -0.883061	70.7599, 118.6826, 241.8645, 305.955, 324.6422, 411.6616, 677.3082, 681.0786, 792.0716, 810.5278, 924.8355, 1023.3636, 1048.4103, 1056.5721, 1069.0422, 1110.8488, 1144.3627, 1310.0689, 1316.5031, 1394.6609, 1406.1158, 1417.3797, 1448.2938, 1475.2148, 1486.6778, 1493.1653, 1507.6348, 1514.9225, 1727.0842, 2988.5174, 2999.203, 3015.111, 3030.9911, 3045.5051, 3084.559, 3094.3334, 3097.6924, 3119.4895, 3159.5188

Compound: *E*-2-butene (Alkene 17)	**Energy (kJ mol^{-1}):** -156.994340303979
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.956867 -0.079076 0.000000 6 0.535689 0.393027 -0.000000 6 -0.535689 -0.393028 -0.000000 1 -0.389176 -1.470660 -0.000000 6 -1.956867 0.079076 0.000000 1 -2.496480 -0.289912 -0.876354 1 -2.496480 -0.289912 0.876354	176.4585, 229.7314, 245.7757, 281.793, 501.7962, 763.4185, 874.6193, 990.2857, 998.622, 1071.1443, 1072.9916, 1074.3046, 1167.8269, 1334.2191, 1336.5376, 1414.0301, 1415.6287, 1479.5634, 1480.1443, 1488.9859, 1497.3116,

1 -2.016423 1.167743 0.000000 1 0.389176 1.470659 -0.000000 1 2.016423 -1.167742 -0.000001 1 2.496480 0.289913 -0.876353 1 2.496480 0.289912 0.876354	1736.0464, 3010.5495, 3010.8238, 3048.8673, 3049.5438, 3084.2729, 3085.8189, 3106.0668, 3115.5896

Compound: *Z*-2-butene (Alkene 18)	**Energy (kJ mol^{-1}):** -156.992617941268
Reaction Coordinates: 6 1.587222 -0.520466 -0.000000 6 0.665981 0.661426 -0.000000 6 -0.665981 0.661426 -0.000000 1 -1.160946 1.627759 0.000000 6 -1.587222 -0.520466 -0.000000 1 -2.241381 -0.500797 0.875770 1 -2.241383 -0.500795 -0.875768 1 -1.059134 -1.471929 -0.000002 1 1.160946 1.627759 0.000000 1 1.059134 -1.471929 -0.000004 1 2.241384 -0.500794 -0.875768 1 2.241379 -0.500798 0.875771	**Frequencies (cm^{-1}):** 126.2, 142.7478, 287.1418, 400.5225, 572.897, 698.0489, 867.8641, 978.3282, 1010.4684, 1025.3172, 1067.0026, 1067.6084, 1160.0865, 1295.2903, 1395.5841, 1418.5863, 1440.7993, 1482.7723, 1485.7588, 1489.9577, 1495.1634, 1726.0624, 3014.0643, 3016.1249, 3049.918, 3050.1832, 3096.2508, 3110.3152, 3117.6898, 3139.0122

Compound: *Z*-2-pentene (Alkene 19) con 1	**Energy (kJ mol^{-1}):** -235.506682457045
Reaction Coordinates: 6 -0.484550 -0.779889 -0.638230 6 0.525983 -0.847958 0.469686 6 1.696144 -0.218366 0.564952 1 2.289756 -0.408075 1.454327 6 2.316438 0.730764 -0.415159 1 2.526540 1.692914 0.059377 1 3.275525 0.345477 -0.771905 1 1.688328 0.916275 -1.284034 1 0.248846 -1.503141 1.291820 6 -1.881700 -0.342377 -0.162983 6 -1.943829 1.106751 0.315921 1 -1.261216 1.279437 1.148810 1 -1.667935 1.796144 -0.485117 1 -2.949401 1.369846 0.647015 1 -2.589075 -0.485136 -0.983701 1 -2.208956 -1.008607 0.640698 1 -0.149721 -0.113664 -1.435121 1 -0.573613 -1.775028 -1.087295	**Frequencies (cm^{-1}):** 41.2889, 109.1277, 138.6313, 200.7807, 254.3338, 306.0596, 362.8515, 478.4332, 574.6806, 710.7203, 774.1094, 859.1837, 893.2596, 913.9097, 971.1405, 1016.7575, 1058.8693, 1066.8111, 1068.3942, 1096.9851, 1172.2002, 1248.8115, 1285.6173, 1303.9926, 1352.9883, 1376.1035, 1409.2313, 1414.0569, 1441.3499, 1481.0826, 1484.2795, 1491.0118, 1493.7543, 1500.092, 1507.7222, 1721.092, 2997.5177, 3011.7554, 3015.048, 3021.8142, 3037.2674, 3049.8747, 3058.0268, 3078.8452, 3089.2331, 3100.7837, 3109.1404, 3131.3534

Compound: *Z*-2-pentene (Alkene 19) con 2	**Energy (kJ mol^{-1}):** -235.506435572184
Reaction Coordinates: 6 0.434966 -0.117017 0.541223 6 -0.768923 -0.917198 0.140474 6 -1.998500 -0.479536 -0.127223 1 -2.738429 -1.222625 -0.409177 6 -2.506265 0.930013 -0.085721 1 -2.920030 1.219735 -1.055210 1 -3.319095 1.026870 0.639157 1 -1.736662 1.652390 0.178752	**Frequencies (cm^{-1}):** 49.398, 89.8889, 131.3736, 200.6305, 237.2598, 284.6984, 367.1046, 472.5868, 573.9975, 716.265, 749.0739, 874.3506, 897.4234, 914.7403, 996.5133, 1016.423, 1046.2213, 1064.9359, 1067.7578, 1112.9827, 1173.4844, 1258.5156, 1296.0617, 1307.5407,

1 -0.594362 -1.986289 0.053094 6 1.602087 -0.256493 -0.448454 6 2.853014 0.499733 -0.006021 1 2.652727 1.568128 0.098353 1 3.213119 0.136792 0.958923 1 3.663324 0.384110 -0.727068 1 1.839604 -1.316616 -0.574572 1 1.280249 0.101120 -1.429809 1 0.185006 0.938803 0.656687 1 0.776276 -0.459438 1.525215	1327.4771, 1377.8452, 1409.382, 1413.0443, 1441.3848, 1481.8697, 1484.5099, 1492.062, 1495.9796, 1499.292, 1509.8532, 1721.1738, 2989.8003, 3013.0685, 3014.9788, 3019.3197, 3036.2808, 3050.028, 3059.6606, 3078.2852, 3082.9867, 3101.9921, 3110.5017, 3132.9048

Compound: *Z*-2-pentene (Alkene 19) con 3	**Energy (kJ mol^{-1}):** -235.505472702575
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.387333 -0.463961 0.701236 6 0.465392 0.714968 0.330713 6 1.730961 0.707319 -0.087526 1 2.184208 1.668259 -0.312315 6 2.630709 -0.473982 -0.290862 1 2.983197 -0.515716 -1.324889 1 3.522305 -0.393583 0.336840 1 2.147545 -1.422526 -0.065533 1 -0.016601 1.683692 0.414440 6 -1.568144 -0.714092 -0.257091 6 -2.602649 0.410309 -0.293766 1 -3.008865 0.603567 0.701753 1 -2.175461 1.342466 -0.664852 1 -3.437593 0.151168 -0.946170 1 -1.177074 -0.884773 -1.263410 1 -2.060679 -1.642297 0.044550 1 0.216477 -1.369984 0.755883 1 -0.791076 -0.303631 1.707472	34.3897, 103.3731, 134.5315, 214.2817, 240.4438, 292.9596, 379.8072, 506.8255, 563.1399, 726.9086, 753.4922, 864.2882, 874.0456, 921.5376, 976.0881, 1019.525, 1054.0488, 1067.4956, 1069.3503, 1115.1616, 1159.276, 1254.0333, 1286.6668, 1309.7021, 1351.7153, 1373.443, 1408.4598, 1415.8675, 1443.9916, 1483.8179, 1484.6204, 1490.4358, 1496.0546, 1502.4863, 1508.8898, 1718.1454, 2993.7939, 3013.0809, 3015.0794, 3021.7087, 3042.6046, 3049.9742, 3066.3489, 3079.0806, 3088.2713, 3103.7062, 3117.7216, 3139.4572

Compound: *Z*-2-pentene (Alkene 19) con 4	**Energy (kJ mol^{-1}):** -235.500658574891
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.577039 0.946865 0.000000 6 -0.916425 1.144905 -0.000000 6 -1.956113 0.309862 -0.000000 1 -2.932908 0.786052 0.000000 6 -2.028114 -1.188752 0.000000 1 -2.583132 -1.539328 0.874654 1 -2.583145 -1.539328 -0.874646 1 -1.060683 -1.677803 -0.000007 1 -1.177357 2.200314 0.000000 1 0.973702 1.492334 -0.865662 1 0.973702 1.492333 0.865663 6 1.181178 -0.457355 -0.000001 6 2.709439 -0.418085 0.000000 1 3.132589 -1.423346 -0.000000 1 3.091038 0.102388 -0.880903 1 3.091036 0.102385 0.880906 1 0.836567 -1.010323 0.876289 1 0.836569 -1.010321 -0.876293	66.6089, 98.5924, 158.6739, 174.6908, 243.1529, 288.2919, 375.6707, 405.2788, 677.6753, 691.5656, 774.183, 816.3684, 889.4815, 912.7182, 991.5727, 1024.0328, 1052.5046, 1068.8351, 1075.9989, 1128.5062, 1151.1806, 1278.6814, 1306.2328, 1333.9822, 1339.9285, 1407.242, 1410.6888, 1415.8065, 1447.3686, 1471.9223, 1489.4133, 1490.9556, 1498.713, 1500.125, 1513.8684, 1726.4224, 2977.137, 2988.1787, 3014.9054, 3019.1809, 3024.2171, 3045.3647, 3052.6144, 3080.9261, 3084.2604, 3094.2598, 3119.4523, 3158.768

Compound: Isobutene (Alkene 20)	**Energy (kJ mol^{-1}):**
Reaction Coordinates: 6 -1.272479 -0.676792 0.000000 6 0.000000 0.123854 0.000000 6 0.000001 1.454624 0.000000 1 0.922183 2.021321 0.000000 1 -0.922183 2.021320 0.000000 6 1.272479 -0.676794 0.000000 1 2.153824 -0.037282 0.000000 1 1.321461 -1.329357 0.876282 1 1.321461 -1.329357 -0.876282 1 -2.153825 -0.037281 0.000000 1 -1.321462 -1.329356 -0.876282 1 -1.321462 -1.329356 0.876282	**Frequencies (cm^{-1}):** 172.7829, 211.2397, 381.0088, 439.3224, 442.8878, 706.3756, 814.459, 924.6733, 961.7242, 988.287, 1022.3943, 1086.1878, 1108.4808, 1296.388, 1409.6995, 1415.2186, 1444.6997, 1471.8573, 1483.628, 1489.6004, 1502.8985, 1712.7565, 3007.5773, 3013.0906, 3047.6689, 3050.2723, 3100.6528, 3102.2216, 3129.5895, 3206.5032

6.2 Products

6.2.1 Criegee Intermediates

Compound: sCI1 (HCHOO)	**Energy (kJ mol^{-1}):** -189.400847568329
Reaction Coordinates: 6 -1.068412 0.202194 -0.000000 8 -0.003231 -0.459294 -0.000000 8 1.179333 0.194958 0.000000 1 -1.021445 1.284352 -0.000000 1 -1.976903 -0.382830 0.000002	**Frequencies (cm^{-1}):** 527.7609,673.7578, 912.8476, 951.0664, 1242.0554, 1402.0013, 1543.5428, 3118.1651, 3267.9600

Compound: *Anti*-CH_3CHOO	**Energy (kJ mol^{-1}):** -228.668481416675
Reaction Coordinates: 6 1.768337 -0.098013 0.000000 6 0.380636 0.408005 -0.000001 8 -0.571402 -0.409277 -0.000001 8 -1.854416 0.073325 0.000001 1 0.119269 1.462625 -0.000001 1 2.303633 0.275054 0.877345 1 1.786152 -1.185114 -0.000027 1 2.303652 0.275101 -0.877313	**Frequencies (cm^{-1}):** 159.9851, 257.6665, 324.381, 553.5978, 867.7539, 893.0654, 968.3519, 1067.3161, 1157.1901, 1344.2119, 1414.9461, 1458.644, 1462.7974, 1577.2586, 3019.4822, 3060.7084, 3131.6411, 3145.1519

Compound: *Syn*-CH_3CHOO	**Energy (kJ mol^{-1}):** -228.674137895205
Reaction Coordinates: 6 1.364404 -0.472563 -0.000000 6 0.481825 0.697474 0.000000 8 -0.774763 0.588713 -0.000000 8 -1.295881 -0.676150 0.000000 1 0.816554 1.727871 0.000000 1 2.410795 -0.181137 -0.000003 1 1.130215 -1.098354 0.866933 1 1.130211 -1.098357 -0.866930	**Frequencies (cm^{-1}):** 185.3271, 295.7077, 460.8721, 674.8786, 756.9638, 900.7617, 982.6906, 1046.5977, 1110.553, 1349.2256, 1398.9588, 1437.3442, 1460.4744, 1559.818, 3015.3924, 3049.5183, 3140.3388, 3177.8251

Compound: *Anti*-EtCHOO con 1	**Energy (kJ mol^{-1}):** -267.925413397257
Reaction Coordinates: 6 -1.238387 0.671859 0.000001 6 0.243293 0.716298 -0.000001 8 0.906784 -0.346617 0.000001 8 2.280006 -0.267327 -0.000000 1 0.808677 1.644807 -0.000003 1 -1.577933 1.251548 0.867130 1 -1.577935 1.251550 -0.867126 6 -1.855251 -0.723194 -0.000000 1 -1.551814 -1.289222 -0.879384 1 -1.551811 -1.289225 0.879380 1 -2.941441 -0.647683 0.000001	**Frequencies (cm^{-1}):** 130.9388, 193.1388, 202.5138, 272.6768, 419.6176, 620.8898, 744.3949, 897.1681, 918.3676, 925.3618, 1025.6913, 1105.3439, 1123.1071, 1275.1458, 1339.7654, 1387.5666, 1425.6198, 1450.0468, 1498.9388, 1504.5907, 1574.7551, 2994.2524, 3005.7603, 3048.8185, 3114.4836, 3114.5196, 3135.7266

Compound: *Anti*-EtCHOO con 2	**Energy (kJ mol^{-1}):** -267.924722060814
Reaction Coordinates: 6 1.131391 0.597027 0.114323 6 -0.186195 -0.013288 0.406647 8 -1.174188 0.269041 -0.313495 8 -2.384882 -0.310259 -0.030725 1 -0.357920 -0.717017 1.217757 1 1.021985 1.290943 -0.718380 1 1.434653 1.179175 0.991339 6 2.208737 -0.460271 -0.182091 1 2.315531 -1.161616 0.645772 1 1.963229 -1.027476 -1.078988 1 3.171487 0.024934 -0.337014	**Frequencies (cm^{-1}):** 79.1142, 195.2713, 205.3122, 327.0348, 409.9348, 538.219, 777.8747, 908.9061, 921.1754, 935.6995, 1017.6514, 1089.1869, 1177.5842, 1277.7692, 1321.9142, 1366.6797, 1416.2125, 1471.0462, 1499.8413, 1504.8533, 1566.5471, 3007.5733, 3039.1061, 3086.2792, 3107.0306, 3111.9258, 3132.8426

Compound: *Syn*-EtCHOO con 1	**Energy (kJ mol^{-1}):** -267.929199725584
Reaction Coordinates: 6 0.923269 0.426502 0.547182 6 -0.273025 0.951814 -0.133366 8 -1.335917 0.288133 -0.280028 8 -1.378535 -0.987515 0.215939 1 -0.343576 1.943872 -0.565754 1 0.578050 -0.104376 1.437841 1 1.555704 1.264174 0.840694 6 1.714340 -0.561104 -0.339827 1 2.094886 -0.069777 -1.234859 1 2.563010 -0.947994 0.222458 1 1.080044 -1.394116 -0.631598	**Frequencies (cm^{-1}):** 112.796, 197.0713, 243.4832, 323.9713, 537.4759, 652.1667, 811.3089, 833.6176, 890.6056, 905.7836, 1009.4333, 1081.9342, 1145.8927, 1289.6824, 1331.79, 1370.0543, 1401.7209, 1460.3766, 1495.3906, 1511.5641, 1558.8684, 3032.0107, 3044.775, 3087.3063, 3106.9797, 3135.4246, 3164.4414

Compound: *Syn*-EtCHOO con 2	**Energy (kJ mol^{-1}):** -267.930089984566
Reaction Coordinates: 6 -0.773628 -0.439742 0.000000 6 0.143905 0.707537 0.000000 8 1.397747 0.574971 -0.000000 8 1.895135 -0.701219 -0.000000 1 -0.172097 1.745490 0.000000 1 -0.499810 -1.066484 0.857959 1 -0.499809 -1.066484 -0.857958 6 -2.249706 -0.054174 -0.000000 1 -2.510613 0.531063 -0.882579 1 -2.873539 -0.946390 -0.000000 1 -2.510613 0.531063 0.882579	**Frequencies (cm^{-1}):** 94.1884, 200.9246, 218.1471, 362.392, 465.8496, 689.645, 707.4179, 830.1912, 890.317, 935.7901, 1047.473, 1098.5582, 1140.771, 1248.8554, 1320.9428, 1370.6582, 1424.9606, 1430.752, 1503.458, 1505.6674, 1561.5455, 3000.6382, 3006.4657, 3036.0444, 3092.694, 3108.5153, 3159.5381

Compound: *Anti*-iPrCHOO con 1	**Energy (kJ mol^{-1}):** -307.183903025558
Reaction Coordinates: 6 -0.965724 -0.022320 -0.415928 6 0.451044 -0.471047 -0.343096 8 1.340114 0.284155 0.114105 8 2.635957 -0.175402 0.163739 1 0.771661 -1.457371 -0.671117 1 -1.230765 -0.073551 -1.480983 6 -1.862506 -1.041551 0.316090	**Frequencies (cm^{-1}):** 86.4377, 189.3429, 195.2162, 220.6261, 257.4231, 334.5273, 436.9484, 442.9461, 601.9411, 826.139, 920.3659, 928.242, 940.115, 971.1987, 975.1866, 1108.5286, 1140.3406, 1205.1665, 1300.8512, 1342.4565, 1373.2338,

1 -1.662940 -1.031784 1.387934 1 -2.910430 -0.786411 0.161324 1 -1.704546 -2.055839 -0.051424 6 -1.180802 1.407058 0.078694 1 -0.932701 1.496751 1.136303 1 -0.565070 2.118627 -0.469045 1 -2.225846 1.686708 -0.050311	1407.8302, 1429.2624, 1488.4416, 1492.5379, 1504.3735, 1510.6035, 1563.7815, 2968.5051, 3033.1315, 3042.4617, 3098.7008, 3102.9851, 3106.8174, 3112.9375, 3128.3525

Compound: *Anti*-iPrCHOO con 2	**Energy (kJ mol^{-1}):** -307.183504223503
Reaction Coordinates: 6 0.887613 0.000000 -0.323680 6 -0.461359 0.000004 0.300578 8 -1.485439 -0.000003 -0.422869 8 -2.720692 0.000002 0.178783 1 -0.621403 0.000012 1.377128 1 0.743561 -0.000001 -1.405313 6 1.653916 1.271480 0.084187 1 1.786741 1.320883 1.166272 1 2.642925 1.267849 -0.374361 1 1.131562 2.171757 -0.237300 6 1.653908 -1.271483 0.084190 1 1.786732 -1.320886 1.166275 1 1.131549 -2.171758 -0.237296 1 2.642918 -1.267859 -0.374358	**Frequencies (cm^{-1}):** 67.3615, 184.8015, 204.221, 214.3213, 266.4091, 317.491, 416.6544, 477.3281, 523.4987, 851.3703, 925.6943, 939.2119, 947.0572, 947.6788, 968.204, 1099.3011, 1182.723, 1198.2556, 1322.2851, 1333.6178, 1365.1658, 1401.9082, 1423.0427, 1488.3999, 1490.9307, 1502.5096, 1510.1752, 1566.1929, 3029.6121, 3031.5752, 3054.3653, 3091.6977, 3098.037, 3105.4845, 3106.3581, 3123.2305

Compound: *Syn*-iPrCHOO con 1	**Energy (kJ mol^{-1}):** -307.187971815102
Reaction Coordinates: 6 0.685393 0.034039 -0.266093 6 -0.344387 -0.746961 0.451159 8 -1.585539 -0.578006 0.306437 8 -2.016369 0.391930 -0.560956 1 -0.114839 -1.533111 1.164189 6 0.802253 1.443751 0.358578 1 1.186654 1.387829 1.377879 1 1.496498 2.039857 -0.233659 1 -0.164773 1.940955 0.364631 1 0.294160 0.167642 -1.279557 6 2.024152 -0.706031 -0.288280 1 1.937024 -1.684752 -0.761394 1 2.759440 -0.129507 -0.848813 1 2.416638 -0.849099 0.720696	**Frequencies (cm^{-1}):** 97.301, 196.6638, 208.2676, 232.3478, 275.8028, 335.1623, 411.9805, 546.8364, 672.2183, 838.1781, 850.88, 889.9471, 939.4327, 950.3204, 975.7047, 1109.0713, 1173.5297, 1192.4754, 1308.2468, 1321.5635, 1371.7229, 1393.551, 1423.2907, 1486.691, 1494.8823, 1502.364, 1514.2539, 1559.3308, 3019.6062, 3027.3683, 3035.1978, 3086.2642, 3096.0502, 3100.9662, 3127.9019, 3149.0892

Compound: *Syn*-iPrCHOO con 2	**Energy (kJ mol^{-1}):** -307.184639319810
Reaction Coordinates: 6 -0.878257 -0.000001 0.485811 6 0.510830 -0.000004 1.017271 8 1.575267 -0.000002 0.342536 8 1.514281 0.000004 -1.025788 1 0.720729 -0.000010 2.082327 6 -1.177955 1.278802 -0.323492 1 -0.549243 1.326970 -1.208037 1 -2.225039 1.263930 -0.627045	**Frequencies (cm^{-1}):** 106.1975, 196.259, 198.7294, 229.4144, 235.9845, 341.1971, 417.1591, 539.501, 742.4056, 798.3226, 843.7334, 886.6389, 941.3455, 964.4005, 971.288, 1097.8197, 1123.9389, 1195.8952, 1336.5111, 1368.1737, 1388.3097, 1393.6817, 1417.9274, 1482.0393,

1 -1.013352 2.175651 0.274198 1 -1.521789 -0.000004 1.368946 6 -1.177958 -1.278799 -0.323500 1 -1.013357 -2.175652 0.274185 1 -2.225042 -1.263922 -0.627054 1 -0.549245 -1.326963 -1.208045	1493.91, 1502.4489, 1522.3991, 1558.6615, 3028.4394, 3037.2438, 3039.1962, 3094.1619, 3095.4681, 3138.4912, 3140.7073, 3150.7961

Compound: *Anti*-tBuCHOO	**Energy (kJ mol^{-1}):** -346.443987742296
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.789980 -0.001899 0.000000 6 -0.622216 -0.490941 0.000001 8 -1.586526 0.307444 0.000001 8 -2.866746 -0.202482 0.000000 1 -0.868477 -1.551112 0.000002 6 1.474988 -0.578024 1.260488 1 1.413826 -1.666766 1.287820 1 2.529747 -0.300726 1.258757 1 1.020181 -0.186446 2.170246 6 1.474983 -0.578019 -1.260493 1 1.020172 -0.186437 -2.170247 1 2.529741 -0.300720 -1.258765 1 1.413821 -1.666760 -1.287829 6 0.864650 1.528339 0.000003 1 0.381929 1.950817 -0.880399 1 0.381933 1.950814 0.880409 1 1.908986 1.840905 0.000002	72.1401, 188.151, 188.2131, 214.2437, 266.0175, 267.9342, 327.4276, 336.7752, 351.7125, 453.0763, 462.9141, 555.678, 774.9509, 910.7703, 922.1565, 926.7502, 954.2772, 959.5186, 972.3446, 1042.6824, 1064.7891, 1212.059, 1227.8809, 1295.2272, 1357.7122, 1399.7857, 1408.0789, 1435.3288, 1480.5727, 1487.9721, 1488.4896, 1503.0707, 1504.3892, 1518.7856, 1561.5817, 3027.2938, 3029.8872, 3040.5647, 3091.6685, 3095.4354, 3100.5416, 3100.793, 3105.6391, 3110.5258, 3121.737

Compound: *Syn*-tBuCHOO	**Energy (kJ mol^{-1}):** -346.444793572179
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.674006 0.018836 0.000000 6 -0.425399 -0.994158 0.000003 8 -1.667963 -0.782312 0.000003 8 -2.155760 0.497368 -0.000001 1 -0.213619 -2.059710 0.000006 6 0.570336 0.896137 1.269013 1 0.678505 0.293952 2.172053 1 1.379325 1.627869 1.253432 1 -0.382295 1.416647 1.304163 6 0.570338 0.896124 -1.269022 1 1.379325 1.627858 -1.253445 1 0.678513 0.293930 -2.172055 1 -0.382294 1.416630 -1.304181 6 2.009587 -0.742745 0.000005 1 2.110730 -1.374102 -0.884612 1 2.837661 -0.034600 0.000001 1 2.110729 -1.374091 0.884630	114.1607, 194.1886, 205.8697, 232.2877, 242.8082, 264.5474, 311.7319, 373.5137, 391.4703, 393.826, 547.4009, 663.0079, 788.1158, 844.621, 883.7145, 925.5938, 937.5768, 946.5911, 973.0925, 1045.3904, 1059.5755, 1212.9554, 1234.9867, 1273.5478, 1387.4046, 1388.6852, 1398.869, 1427.9961, 1474.7784, 1491.2046, 1492.4225, 1498.8999, 1508.6258, 1525.3289, 1552.4378, 3023.8797, 3030.5664, 3033.6024, 3083.1399, 3088.7935, 3089.4156, 3101.4749, 3138.0935, 3139.3703, 3141.242

Compound: *Anti*-OCH-CHOO con 1	**Energy (kJ mol^{-1}):** -341.874794351903
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.380256 1.277703 -0.000000 1 -0.955960 1.770134 0.876375 1 -0.955957 1.770135 -0.876373	89.6551, 146.6518, 186.4248, 224.6185, 399.2977, 500.0396, 564.1078, 570.7829, 831.647, 915.5553, 1012.7049, 1032.2613,

1 -2.460742 1.386745 -0.000002 6 -1.036272 -0.186163 0.000000 6 0.387585 -0.587014 0.000002 8 1.273575 0.315950 0.000000 8 2.568387 -0.027599 -0.000001 1 0.693149 -1.627188 0.000001 8 -1.860316 -1.079225 -0.000001	1049.9935, 1243.359, 1341.157, 1401.107, 1462.5227, 1471.3513, 1484.672, 1737.9924, 3041.5794, 3095.8339, 3149.8163, 3178.9853

Compound: *Anti*-OCH-CHOO con 2	**Energy (kJ mol^{-1}):** -341.869209743485
Reaction Coordinates: 6 2.127294 -0.803805 -0.000000 1 2.079125 -1.451555 0.878536 1 2.079127 -1.451553 -0.878537 1 3.064887 -0.256073 0.000001 6 0.975759 0.169274 -0.000000 6 -0.372747 -0.463275 -0.000000 8 -1.386227 0.292533 -0.000000 8 -2.603355 -0.254499 0.000000 1 -0.548493 -1.533793 0.000002 8 1.107522 1.371942 0.000000	**Frequencies (cm^{-1}):** 102.3254, 112.5058, 191.0887, 212.4039, 376.1871, 466.8569, 565.8761, 617.4788, 888.5896, 915.1229, 943.8324, 1043.1568, 1059.09, 1199.1456, 1355.7011, 1393.137, 1461.9568, 1471.3795, 1484.65, 1758.0848, 3027.5069, 3078.7494, 3148.8069, 3160.3167

Compound: *Syn*-OCH-CHOO con 1	**Energy (kJ mol^{-1}):** -341.871502609295
Reaction Coordinates: 6 0.824684 1.415296 0.000001 1 0.252348 1.748952 0.866525 1 1.823703 1.843568 0.000003 1 0.252351 1.748953 -0.866524 6 0.938768 -0.075163 -0.000000 6 -0.264153 -0.958412 0.000001 8 -1.493315 -0.652057 0.000001 8 -1.908490 0.625605 -0.000002 1 -0.094945 -2.028110 0.000003 8 1.998149 -0.674010 -0.000002	**Frequencies (cm^{-1}):** 53.3101, 199.8905, 242.9936, 325.1407, 348.3545, 498.05, 591.87, 671.4057, 819.5133, 854.8213, 929.5827, 1042.2661, 1048.7575, 1258.0221, 1357.3156, 1402.6209, 1440.6406, 1453.1665, 1487.5244, 1727.3454, 3041.8082, 3094.7872, 3143.9874, 3190.0379

Compound: *Syn*-OCH-CHOO con 2	**Energy (kJ mol^{-1}):** -341.862276812340
Reaction Coordinates: 6 2.212569 -0.366213 -0.000000 1 2.378486 -0.992625 -0.879375 1 2.922410 0.455584 -0.000001 1 2.378487 -0.992624 0.879375 6 0.805815 0.192945 0.000000 6 -0.249500 -0.850623 0.000000 8 -1.514104 -0.688513 0.000000 8 -2.085057 0.507733 -0.000000 1 0.007673 -1.902228 -0.000001 8 0.561616 1.377686 0.000000	**Frequencies (cm^{-1}):** 56.8625, 95.6231, 211.2354, 295.931, 342.9427, 470.109, 603.6244, 693.3941, 806.2389, 873.8416, 987.0687, 1009.6464, 1039.5672, 1182.516, 1373.8337, 1390.1633, 1461.4244, 1473.5334, 1484.3973, 1748.4762, 3027.9802, 3080.2331, 3147.2836, 3182.6552

Compound: $(CH_3)_2COO$	**Energy (kJ mol^{-1}):** -267.942546539936
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.072626 1.465423 -0.000000 6 -0.377947 0.024683 -0.000000 8 0.567304 -0.816015 -0.000001 8 1.858053 -0.326037 0.000001 6 -1.751450 -0.541461 0.000000 1 -2.301504 -0.192862 -0.877682 1 -1.721850 -1.628087 -0.000001 1 -2.301501 -0.192865 0.877685 1 -0.976897 2.068002 -0.000002 1 0.555520 1.695182 0.865234 1 0.555523 1.695181 -0.865232	154.7878, 180.6109, 277.8128, 307.6135, 363.4465, 483.1866, 597.9012, 812.4888, 924.0134, 934.3173, 985.9827, 1070.4539, 1093.8612, 1305.1876, 1393.4045, 1409.3403, 1438.2555, 1458.0039, 1469.8151, 1476.4709, 1560.106, 3020.3234, 3025.0231, 3060.3596, 3065.9584, 3134.9818, 3137.2227

Compound: *Anti*-CF_3CF_2CHOO con 1	**Energy (kJ mol^{-1}):** -763.819838560287
Reaction Coordinates: 6 0.069149 0.627138 0.022159 6 -1.236224 0.079680 0.533411 8 -2.153739 -0.114622 -0.301088 8 -3.332105 -0.597276 0.118248 1 -1.394430 -0.148462 1.580273 9 -0.061230 1.131744 -1.217459 9 0.470150 1.617642 0.864146 6 1.205189 -0.440766 -0.006928 9 1.356875 -0.964924 1.217947 9 0.885110 -1.420835 -0.855647 9 2.354927 0.108299 -0.387810	**Frequencies (cm^{-1}):** 44.3986, 57.0473, 153.6216, 185.5355, 220.3238, 244.4913, 329.0152, 354.6629, 373.6292, 403.3591, 478.9045, 533.1629, 588.2807, 625.4113, 728.0104, 825.9083, 883.5367, 987.1218, 1053.852, 1139.4701, 1192.9705, 1206.8077, 1241.3348, 1298.0137, 1341.3819, 1534.4801, 3187.8179

Compound: *Anti*-CF_3CF_2CHOO con 2	**Energy (kJ mol^{-1}):** -763.818682766641
Reaction Coordinates: 6 -0.209949 0.769713 -0.000001 6 1.290692 0.714352 0.000016 8 1.865913 -0.400862 -0.000009 8 3.206432 -0.449944 0.000003 1 1.873935 1.628647 0.000047 9 -0.609897 1.470190 1.094503 9 -0.609877 1.470174 -1.094524 6 -0.963428 -0.591937 0.000002 9 -0.648973 -1.297686 -1.088456 9 -0.648980 -1.297676 1.088469 9 -2.277449 -0.364442 -0.000003	**Frequencies (cm^{-1}):** 54.871, 70.3267, 116.3479, 177.129, 217.1967, 256.1066, 336.8535, 365.3074, 376.2775, 393.3915, 477.5585, 530.2372, 590.7708, 641.6927, 692.4777, 787.0862, 887.8686, 984.3691, 1107.5422, 1114.7433, 1175.4569, 1209.0797, 1211.1947, 1337.2608, 1347.8549, 1544.616, 3173.6706

Compound: *Syn*-CF_3CF_2CHOO con 1	**Energy (kJ mol^{-1}):** -763.816355614179
Reaction Coordinates: 6 -0.003801 0.701424 -0.128518 6 1.241007 0.658922 0.730098 8 2.241648 -0.082513 0.545868 8 2.274088 -0.974731 -0.450052 1 1.322895 1.331879 1.571843 9 0.288532 0.805216 -1.437493 9 -0.663474 1.832436 0.250099 6 -1.007627 -0.478856 0.080434 9 -1.264414 -0.596419 1.394913 9 -2.148787 -0.207742 -0.554718	**Frequencies (cm^{-1}):** 27.0324, 94.7261, 149.4391, 189.9634, 212.3468, 276.2901, 314.8169, 354.514, 426.5154, 464.8876, 494.3785, 559.4939, 582.4453, 648.1925, 750.1928, 774.9641, 830.5958, 945.864, 1066.2727, 1126.2644, 1181.1031, 1213.9794, 1227.7939, 1289.1019, 1369.3086, 1532.2685, 3212.718

9 -0.525885 -1.629365 -0.367297	

Compound: *Syn*-CF_3CF_2CHOO con 2	**Energy (kJ mol^{-1}):** -763.816743925882
Reaction Coordinates: 6 0.151655 -0.282103 0.000000 6 1.047244 0.934668 0.000000 8 2.306717 0.869749 0.000000 8 2.931888 -0.310367 -0.000000 1 0.652384 1.939972 0.000000 9 0.361554 -1.039417 1.099463 9 0.361554 -1.039418 -1.099462 6 -1.345243 0.140891 0.000000 9 -1.609795 0.881573 -1.086690 9 -2.134980 -0.926063 -0.000000 9 -1.609795 0.881573 1.086690	**Frequencies (cm^{-1}):** 63.5645, 71.6863, 136.7132, 216.3012, 216.6225, 246.917, 298.1751, 360.9537, 404.6534, 470.2807, 542.1749, 556.7641, 594.1608, 602.749, 751.3958, 767.793, 875.8626, 958.276, 1030.5662, 1141.6776, 1183.7528, 1188.334, 1237.0489, 1326.2237, 1377.1304, 1533.5921, 3218.195

Compound: *Anti*-CF_3CHOO	**Energy (kJ mol^{-1}):** -526.205978402574
Reaction Coordinates: 6 -0.814124 -0.010987 0.000000 6 0.599627 -0.529934 0.000001 8 1.532385 0.307937 -0.000000 8 2.803565 -0.122750 -0.000000 1 0.814702 -1.591587 0.000002 9 -0.871266 1.317793 -0.000001 9 -1.465219 -0.472475 -1.084562 9 -1.465219 -0.472472 1.084563	**Frequencies (cm^{-1}):** 53.4225, 186.5103, 191.8874, 388.9843, 394.1412, 416.4183, 552.7580, 560.7356, 699.8777, 883.4653, 889.1822, 988.9465, 1131.2630, 1171.7198, 1270.0033, 1355.9541, 1546.1599, 3188.0668

Compound: *Syn*-CF_3CHOO	**Energy (kJ mol^{-1}):** -526.205009675300
Reaction Coordinates: 6 0.544326 0.408563 0.000000 6 -0.965669 0.489858 0.000000 8 -1.720767 -0.517005 -0.000000 8 -1.205470 -1.752491 -0.000000 1 -1.466000 1.447260 0.000000 9 1.014961 -0.207422 1.087387 9 1.014961 -0.207422 -1.087387 9 1.014961 1.672420 0.000000	**Frequencies (cm^{-1}):** 83.4264, 179.3385, 247.1426, .2827, 478.5065, 507.3023, ,536.2006, 591.5612, 758.0400, 772.8798, 885.1813, 947.2031, 1151.7894, 1176.1918, 1243.1084, 1364.7774, 1539.7613, ,3220.6741

Compound: *Anti*-ClCHOO	**Energy (kJ mol^{-1}):** -648.567491157440
Reaction Coordinates: 6 0.000000 0.446097 0.000000 17 -1.534775 -0.276709 0.000000 1 0.093739 1.524821 0.000000 8 1.012621 -0.284105 -0.000000 8 2.237057 0.346936 -0.000000	**Frequencies (cm^{-1}):** 229.5392, 303.4732, 458.6682, 865.92, 891.9082, 915.5859, 1291.2838, 1476.5172, 3188.0722

Compound: *Syn*-ClCHOO	**Energy (kJ mol^{-1}):** -648.572181521575

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.000000 0.842892 -0.000000 17 -1.279322 -0.251963 -0.000000 1 -0.196377 1.904658 -0.000000 8 1.205128 0.491035 0.000000 8 1.537978 -0.825865 0.000000	241.5659, 471.9135, 657.3934, 752.0452, 869.6006, 902.2343, 1330.4159, 1460.2303, 3220.2157

Compound: *Anti*-FCHOO	**Energy (kJ mol^{-1}):** -288.578114161732
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.000000 0.583824 -0.000000 9 -1.138700 1.222551 0.000000 1 0.914897 1.162472 -0.000000 8 -0.034852 -0.649166 0.000000 8 1.201527 -1.309381 -0.000000	268.0562, 334.6853, 573.9602, 880.5495, 899.7337, 1214.4299, 1317.8767, 1591.5708, 3211.2991

Compound: *Syn*-FCHOO	**Energy (kJ mol^{-1}):** -288.580107921778
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.000000 0.819490 0.000000 9 1.262219 0.529738 -0.000000 1 -0.281417 1.862464 0.000000 8 -0.878953 -0.056851 0.000000 8 -0.505866 -1.386529 -0.000000	290.6308, 484.5048, 767.7453, 782.9853, 845.1627, 1204.4974, 1343.3329, 1593.0432, 3233.2806

Compound: *Anti*-CF_3CFOO	**Energy (kJ mol^{-1}):** -625.3783361
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.277404 -0.919423 0.000000 6 0.018963 0.571292 0.000000 8 1.190937 0.987253 0.000000 8 1.417147 2.337638 0.000000 9 -0.997920 1.369496 0.000000 9 0.847756 -1.621862 0.000000 9 -0.997920 -1.235503 1.084149 9 -0.997920 -1.235503 -1.084149	41.8080, 154.2443, 183.9192, 293.0541, 346.5294, 372.3393, 406.8758, 515.4784, 576.4030, 659.0393, 728.8220, .5490, 906.9387, 1155.2541, 1155.7283, 1229.1869, 1400.7892, 1601.0242

Compound: *Syn*-CF_3CFOO	**Energy (kJ mol^{-1}):** -625.3731138
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.267347 0.734443 0.000000 6 -0.668190 -0.480912 0.000000 8 -0.317071 -1.670141 0.000000 8 1.031885 -1.966693 0.000000 9 -1.951916 -0.250006 0.000000 9 1.031885 0.735046 1.087938 9 1.031885 0.735046 -1.087938 9 -0.480015 1.843635 0.000000	58.8820, 180.2110, 218.4479, 269.2791, 292.9260, ,363.8515, 484.2548, 493.0742, 582.0033, 631.0249, 653.9584, 780.2000, 927.2456, 1158.8972, 1195.1079, 1198.3764, 1398.0465, 1580.9318

Compound: *Anti*-nPrCHOO con 1	**Energy (kJ mol^{-1}):** -307.181067012075
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.512711 0.900051 0.352587 6 -0.628351 -0.044175 0.360780 8 -1.716841 0.306294 -0.158476 8 -2.763993 -0.578758 -0.157008 1 -0.595133 -1.044241 0.783547 1 0.162162 1.860325 -0.024729 1 0.838722 1.047214 1.388447 6 1.718464 0.404885 -0.478611 6 2.382827 -0.859440 0.063106 1 3.259263 -1.116297 -0.531656 1 1.712335 -1.719384 0.037988 1 2.712380 -0.722061 1.094869 1 1.396438 0.248513 -1.509889 1 2.446591 1.217711 -0.501882	57.3891, 98.1852, 175.8113, 241.148, 301.1324, 334.5312, 458.2627, 544.0796, 763.1513, 849.6596, 856.3487, 940.4958, 944.6979, 1007.685, 1050.9046, 1112.5895, 1152.3069, 1253.9629, 1290.3338, 1328.9757, 1361.0412, 1386.524, 1422.7998, 1470.609, 1493.4645, 1503.5391, 1508.228, 1561.8709, 3002.7804, 3027.4275, 3034.0535, 3062.0201, 3088.5795, 3090.9573, 3095.4269, 3144.4718

Compound: *Anti*-nPrCHOO con 2	**Energy (kJ mol^{-1}):** -307.181954702062
Reaction Coordinates: 6 -0.510416 -0.533809 0.254420 6 0.840671 0.037982 0.448086 8 1.770608 -0.289874 -0.328431 8 3.012643 0.262072 -0.141466 1 1.086723 0.754922 1.227730 1 -0.472029 -1.276942 -0.542405 1 -0.796891 -1.051416 1.177147 6 -1.567881 0.545744 -0.055130 6 -2.969708 -0.045433 -0.182435 1 -3.699685 0.732311 -0.406218 1 -3.277932 -0.536078 0.742463 1 -3.015348 -0.785044 -0.983366 1 -1.554761 1.301450 0.733842 1 -1.292079 1.056298 -0.979674	**Frequencies (cm^{-1}):** 65.6742, 89.2984, 168.4161, 243.394, 300.3373, 336.3777, 384.6076, 578.5347, 746.1612, 846.8403, 880.0363, 938.8091, 948.3238, 1020.8924, 1041.6515, 1105.6554, 1178.063, 1258.6457, 1293.9097, 1328.312, 1357.0746, 1379.8877, 1418.2676, 1469.9779, 1494.2577, 1500.3118, 1508.8923, 1564.8337, 3000.1766, 3026.0869, 3029.1671, 3055.7101, 3083.0873, 3092.4341, 3096.6082, 3133.3991

Compound: *Anti*-nPrCHOO con 3	**Energy (kJ mol^{-1}):** -307.182121254065
Reaction Coordinates: 6 -0.583661 -1.015023 -0.296147 6 0.655972 -0.483752 0.314407 8 1.529564 0.052851 -0.409267 8 2.668870 0.538519 0.182102 1 0.863698 -0.521736 1.381395 1 -0.529327 -0.889808 -1.377961 1 -0.623362 -2.089912 -0.087585 6 -1.857765 -0.353276 0.271306 6 -1.987456 1.124798 -0.088758 1 -2.911020 1.540876 0.313614 1 -2.001321 1.266544 -1.170706 1 -1.158714 1.712369 0.309177 1 -2.715896 -0.907662 -0.112369 1 -1.874067 -0.478120 1.356905	**Frequencies (cm^{-1}):** 62.869, 105.9322, 178.42, 247.2197, 279.0519, 351.7739, 450.114, 537.3536, 779.941, 818.5202, 880.1877, 936.78, 946.9433, 992.711, 1057.1994, 1095.1244, 1175.9777, 1240.3839, 1283.5495, 1334.2517, 1363.6115, 1384.7879, 1424.3973, 1467.8791, 1491.9958, 1501.1848, 1504.7684, 1565.4296, 3004.7632, 3026.2427, 3029.5516, 3057.3638, 3083.074, 3091.2354, 3096.2382, 3129.9569

Compound: *Anti*-nPrCHOO con 4	**Energy (kJ mol^{-1}):** -307.182218473013
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.559948 0.837680 -0.000000 6 -0.918625 0.737439 0.000000 8 -1.477565 -0.384116 -0.000000 8 -2.852427 -0.435356 0.000000 1 -1.571559 1.606789 0.000000 1 0.843478 1.448114 -0.867398 1 0.843478 1.448115 0.867397 6 1.322417 -0.486724 0.000000 1 1.026689 -1.072181 0.871978 1 1.026688 -1.072181 -0.871977 6 2.834935 -0.276625 -0.000000 1 3.159938 0.279201 -0.881610 1 3.159939 0.279202 0.881610 1 3.359235 -1.231903 0.000000	80.3561, 138.497, 143.0562, 240.1337, 251.5122, 326.4856, 403.5991, 665.0471, 720.2753, 833.6513, 861.1925, 937.5239, 940.597, 998.8708, 1045.9112, 1121.6527, 1140.4928, 1253.3391, 1318.7091, 1328.0623, 1356.1445, 1408.6418, 1420.5347, 1447.5595, 1493.6704, 1502.631, 1509.4189, 1572.6658, 2984.0156, 2995.7929, 3024.5283, 3042.6179, 3064.2164, 3088.9886, 3096.4366, 3133.4776

Compound: *Anti*-nPrCHOO con 5	**Energy (kJ mol^{-1}):** -307.181910880642
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.646564 1.168582 -0.106263 6 0.768963 0.764035 -0.290550 8 1.199600 -0.297590 0.216017 8 2.527302 -0.619712 0.046251 1 1.487956 1.366564 -0.840453 1 -0.630307 2.096041 0.481611 1 -1.028713 1.471754 -1.088351 6 -1.574819 0.138873 0.543976 1 -1.135445 -0.201561 1.482741 1 -2.501802 0.652459 0.804851 6 -1.892095 -1.060996 -0.349071 1 -2.356891 -0.742406 -1.284364 1 -0.996497 -1.630938 -0.593310 1 -2.586423 -1.736456 0.150573	91.5103, 128.6726, 165.1414, 234.3122, 257.2545, 335.2353, 437.5822, 621.3027, 783.9881, 804.6133, 853.8654, 931.7261, 944.3601, 979.8758, 1064.9686, 1098.3415, 1142.0294, 1243.1641, 1299.4352, 1342.5786, 1382.6938, 1397.2192, 1421.2839, 1446.0822, 1492.1839, 1502.4825, 1509.8679, 1575.5467, 2983.9653, 3006.4971, 3029.6857, 3040.2365, 3068.1115, 3091.056, 3106.8837, 3131.9858

Compound: *Syn*-nPrCHOO con 1	**Energy (kJ mol^{-1}):** -307.186319485581
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.285432 0.668228 0.497870 6 -1.049098 0.941684 -0.057703 8 -1.935563 0.055268 -0.203460 8 -1.639564 -1.228243 0.172804 1 -1.383861 1.917230 -0.392884 1 0.151341 -0.015671 1.340227 1 0.723466 1.603842 0.847870 6 1.227476 -0.005676 -0.532167 6 2.575066 -0.359093 0.090501 1 2.452742 -1.064906 0.913237 1 3.231716 -0.819367 -0.648175 1 3.081132 0.526489 0.480114 1 0.737878 -0.902983 -0.907260 1 1.373348 0.668309 -1.378889	75.9689, 108.778, 192.5411, 242.726, 304.6045, 370.2883, 530.2874, 660.9098, 761.4841, 813.2105, 890.0174, 891.9084, 911.7306, 1005.6927, 1028.0212, 1100.0583, 1155.1074, 1267.776, 1303.4333, 1333.2206, 1362.6453, 1371.794, 1415.3463, 1458.7502, 1495.6888, 1499.5993, 1506.1713, 1555.9629, 3023.2799, 3024.8293, 3035.9697, 3072.9839, 3081.5503, 3093.742, 3104.0287, 3163.9706

Compound: *Syn*-nPrCHOO con 2	**Energy (kJ mol^{-1}):** -307.185660079521
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.255765 0.313774 0.974048 6 -0.680101 0.949916 0.031150 8 -1.668082 0.350781 -0.476881 8 -1.873039 -0.962135 -0.146435 1 -0.613517 1.980706 -0.298130 1 -0.350753 -0.266871 1.674525 1 0.794575 1.095047 1.511994 6 1.261262 -0.649544 0.291947 6 2.244554 0.048632 -0.644547 1 2.816105 0.820118 -0.123847 1 2.956281 -0.666984 -1.056694 1 1.735636 0.520847 -1.486956 1 1.806084 -1.156271 1.090092 1 0.695661 -1.412427 -0.240044	63.9642, 119.7899, 188.0012, 242.8649, 326.7743, 372.7058, 539.8268, 665.4507, 760.6731, 816.3104, 886.1695, 891.8698, 897.229, 987.3466, 1043.8406, 1103.3874, 1134.3635, 1258.1987, 1280.6656, 1344.6388, 1361.5194, 1380.9147, 1419.4438, 1457.1881, 1496.5986, 1502.6063, 1506.2974, 1555.4388, 3020.8301, 3023.7021, 3044.9949, 3069.0258, 3079.3221, 3090.5231, 3105.7184, 3166.487

Compound: *Syn*-nPrCHOO con 3	**Energy (kJ mol^{-1}):** -307.184497672213
Reaction Coordinates: 6 0.329268 0.946748 0.574690 6 -0.751053 0.871057 -0.426047 8 -1.657962 -0.005345 -0.447450 8 -1.670995 -0.987455 0.506390 1 -0.849684 1.579057 -1.242648 1 0.018056 0.383627 1.452914 1 0.457681 1.999678 0.838805 6 1.679790 0.406595 0.037861 6 1.673698 -1.090419 -0.260631 1 0.934583 -1.348461 -1.019795 1 2.651756 -1.409754 -0.622303 1 1.432513 -1.668026 0.630983 1 1.961357 0.967869 -0.856843 1 2.435180 0.634528 0.792128	**Frequencies (cm^{-1}):** 53.7657, 98.8056, 189.4119, 258.0978, 308.7251, 375.9105, 540.1885, 641.0404, 781.6319, 802.1913, 877.5309, 884.4448, 910.571, 974.2216, 1048.7562, 1097.0622, 1167.4631, 1247.3852, 1279.0684, 1345.898, 1366.9992, 1386.6266, 1428.171, 1462.0446, 1488.4836, 1499.0387, 1501.4274, 1559.5203, 3020.3561, 3029.6266, 3034.852, 3055.1886, 3093.766, 3104.5469, 3108.2332, 3155.7172

Compound: *Syn*-nPrCHOO con 4	**Energy (kJ mol^{-1}):** -307.187234925581
Reaction Coordinates: 6 0.262782 -0.150022 0.000003 6 -0.870210 0.784104 0.000002 8 -2.070834 0.399027 -0.000001 8 -2.298821 -0.951664 -0.000001 1 -0.773220 1.864746 0.000003 1 0.127021 -0.820901 -0.858749 1 0.127025 -0.820894 0.858761 6 1.632752 0.527182 -0.000003 1 1.718163 1.176460 0.875323 6 2.778302 -0.482165 -0.000000 1 2.736619 -1.125179 -0.880792 1 2.736623 -1.125170 0.880799 1 3.745086 0.020989 -0.000004 1 1.718160 1.176452 -0.875334	**Frequencies (cm^{-1}):** 84.7541, 97.7522, 149.1674, 245.1554, 319.834, 395.4879, 464.8931, 686.4635, 700.8163, 780.4966, 887.4962, 891.2703, 926.1719, 1034.4076, 1065.5998, 1114.2849, 1147.9493, 1237.0182, 1281.4425, 1323.1078, 1361.7626, 1396.2937, 1420.2587, 1428.2612, 1494.3379, 1500.9083, 1509.9075, 1560.8583, 2990.6098, 2996.2171, 3016.762, 3027.7137, 3044.8921, 3086.7411, 3095.499, 3159.215

Compound: *Syn*-nPrCHOO con 5	**Energy (kJ mol^{-1}):** -307.186732727465
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.205942 0.641897 -0.085374 6 0.590230 -0.557000 -0.380454 8 1.824682 -0.631311 -0.134533 8 2.418927 0.461411 0.440462 1 0.198132 -1.457442 -0.840990 1 0.274211 1.473455 -0.617889 1 -0.034583 0.893591 0.969095 6 -1.692408 0.511295 -0.420875 1 -1.806720 0.201905 -1.463399 6 -2.444352 -0.453842 0.495620 1 -2.381481 -0.132896 1.536793 1 -2.040316 -1.466844 0.440426 1 -3.499146 -0.508516 0.226356 1 -2.144142 1.501843 -0.351328	66.391, 116.9869, 184.1646, 246.6209, 298.8611, 434.6715, 463.449, 681.6291, 728.2433, 785.0073, 874.0906, 891.423, 913.6468, 1004.7568, 1070.0682, 1097.643, 1144.8899, 1220.7339, 1285.0691, 1339.4048, 1374.5446, 1379.9094, 1419.9597, 1428.1661, 1493.5375, 1501.8971, 1508.0264, 1560.9653, 2994.014, 3000.9149, 3023.5939, 3026.2834, 3057.6537, 3084.2212, 3094.2295, 3161.356

6.2.2 Aldehyde and Ketones

Compound: HCHO	**Energy (kJ mol^{-1}):** -114.386051813463
Reaction Coordinates: 6 -0.000000 -0.526970 -0.000000 8 0.000000 0.673271 0.000000 1 -0.000000 -1.112173 0.938294 1 -0.000000 -1.112173 -0.938294	**Frequencies (cm^{-1}):** 1198.1780, 1262.9587, 1530.2218, 1813.2454, 2885.3911, 2940.0951

Compound: CH_3CHO	**Energy (kJ mol^{-1}):** -153.656268371812
Reaction Coordinates: 6 -0.930255 -0.717875 -0.000000 6 -0.000000 0.459414 0.000000 8 1.202268 0.385569 0.000000 1 -0.496506 1.452140 0.000000 1 -0.376434 -1.653591 -0.000000 1 -1.581838 -0.666172 0.876235 1 -1.581838 -0.666172 -0.876235	**Frequencies (cm^{-1}):** 157.49, 509.7923, 774.8566, 886.2424, 1129.3368, 1135.746, 1379.3886, 1421.9604, 1459.9658, 1469.2145, 1805.3067, 2868.8104, 3021.8671, 3072.7019, 3134.3627

Compound: EtCHO con 1	**Energy (kJ mol^{-1}):** -192.913837029760
Reaction Coordinates: 6 -0.543174 0.724333 -0.000000 6 0.930840 0.419433 -0.000000 8 1.409880 -0.686094 0.000000 1 1.589155 1.313513 -0.000000 1 -0.730675 1.368894 0.867197 1 -0.730677 1.368896 -0.867194 6 -1.449528 -0.498268 -0.000000 1 -1.269156 -1.118012 -0.877396 1 -1.269148 -1.118018 0.877391 1 -2.497367 -0.199511 0.000006	**Frequencies (cm^{-1}):** 137.5718, 225.4743, 252.4946, 667.9491, 671.0327, 846.7328, 905.066, 1004.0188, 1110.2803, 1147.8003, 1282.794, 1365.2956, 1410.3368, 1424.1161, 1448.5397, 1494.3937, 1501.1112, 1800.8127, 2864.479, 3000.2219, 3017.4543, 3043.9519, 3106.2238, 3108.9258

Compound: EtCHO con 2	**Energy (kJ mol^{-1}):** -192.912338568899
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.471414 0.591563 0.144443 6 -0.783366 -0.223964 0.305786 8 -1.809862 -0.045796 -0.298860 1 -0.710126 -1.048102 1.048532 1 0.303006 1.346400 -0.622882 1 0.640985 1.108503 1.095741 6 1.686869 -0.286831 -0.176400 1 1.828702 -1.060701 0.579780 1 1.571813 -0.777932 -1.142881 1 2.595014 0.313595 -0.210385	77.0701, 211.6772, 328.3854, 508.5738, 759.2011, 873.8252, 921.0946, 1006.6118, 1133.4945, 1159.9478, 1273.7425, 1328.0464, 1410.4146, 1423.6601, 1467.8018, 1501.4797, 1505.8218, 1801.2012, 2850.7386, 3007.6748, 3032.5054, 3081.0494, 3099.782, 3103.2068

Compound: iPrCHO con 1	**Energy (kJ mol^{-1}):** -232.172228330803
Reaction Coordinates: 6 -0.424807 0.011130 0.411567 6 0.937214 -0.612380 0.203295 8 1.895814 -0.060080 -0.272802 1 1.009145 -1.672468 0.529672 6 -1.493645 -0.870458 -0.255268 1 -1.420692 -1.909310 0.070614 1 -2.491461 -0.511411 -0.004487 1 -1.391113 -0.848333 -1.341472 1 -0.591607 -0.042692 1.496286 6 -0.483246 1.465361 -0.041068 1 0.282622 2.063530 0.450349 1 -0.317857 1.543102 -1.116023 1 -1.458648 1.896299 0.186320	**Frequencies (cm^{-1}):** 94.38, 199.3595, 228.0336, 270.2049, 343.142, 400.1517, 638.9295, 791.9112, 913.8814, 925.7399, 945.4003, 974.5251, 1129.0298, 1154.3785, 1201.6496, 1304.4207, 1354.5164, 1404.0355, 1410.1452, 1431.8869, 1486.4235, 1490.7128, 1504.6756, 1509.354, 1798.0552, 2852.8215, 2972.8853, 3026.5846, 3037.3535, 3086.6913, 3095.4317, 3098.8093, 3108.0968

Compound: iPrCHO con 2	**Energy (kJ mol^{-1}):** -232.171466830656
Reaction Coordinates: 6 0.341720 0.000000 -0.340819 6 -0.997632 0.000023 0.357561 8 -2.071058 0.000007 -0.188449 1 -0.935722 0.000055 1.469066 6 1.115632 -1.269194 0.042815 1 0.585418 -2.169521 -0.268298 1 2.095803 -1.271210 -0.435015 1 1.273172 -1.323710 1.122300 1 0.142848 -0.000001 -1.413593 6 1.115677 1.269168 0.042806 1 0.585496 2.169513 -0.268310 1 1.273222 1.323684 1.122291 1 2.095848 1.271148 -0.435025	**Frequencies (cm^{-1}):** 69.7947, 205.9689, 225.4671, 330.2493, 331.4338, 352.8203, 544.3316, 843.4077, 911.982, 931.9916, 958.9973, 981.0885, 1132.403, 1180.9634, 1183.6461, 1320.7455, 1345.2516, 1398.9327, 1408.2364, 1426.0614, 1488.4443, 1491.9585, 1504.0805, 1511.3597, 1799.7755, 2838.1938, 3022.4608, 3025.208, 3052.1002, 3082.0856, 3089.2092, 3095.9544, 3096.6206

Compound: tBuCHO	**Energy (kJ mol^{-1}):** -271.432768566988
Reaction Coordinates: 6 0.327863 0.027002 0.000000 6 -1.038328 -0.639844 0.000003 8 -2.101561 -0.075616 0.000001 1 -0.996024 -1.751482 0.000005 6 1.069906 -0.463705 1.258254 1 1.127500 -1.553428 1.290144 1 2.089773 -0.076452 1.262388	**Frequencies (cm^{-1}):** 81.7708, 195.9456, 243.2167, 244.5766, 272.8523, 322.6699, 347.3042, 387.3488, 401.0632, 594.2683, 763.1273, 877.7581, 927.1989, 949.846, 961.6521, 968.464, 1056.6159, 1071.9643, 1226.8546, 1234.5254, 1290.9903,

1 0.574689 -0.122370 2.168152 6 1.069897 -0.463701 -1.258260 1 0.574675 -0.122362 -2.168153 1 2.089765 -0.076449 -1.262399 1 1.127490 -1.553424 -1.290154 6 0.194291 1.549358 0.000003 1 -0.349217 1.895976 -0.878376 1 -0.349210 1.895974 0.878387 1 1.181275 2.014285 -0.000001	1396.8823, 1403.7876, 1408.1713, 1436.9589, 1479.7446, 1486.5007, 1488.148, 1499.8075, 1506.854, 1519.3097, 1797.847, 2844.414, 3020.6027, 3023.7014, 3035.2588, 3082.3301, 3085.7412, 3090.5506, 3090.9174, 3097.7377, 3105.997

Compound: OCH-CHO con 1	**Energy (kJ mol^{-1}):** -266.852222733238
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.686244 -0.639816 0.000000 1 1.703444 -1.293431 -0.876216 1 2.564025 -0.000453 0.000000 1 1.703443 -1.293430 0.876217 6 0.432933 0.193453 -0.000001 6 -0.901455 -0.603806 -0.000000 8 -1.973369 -0.071325 0.000000 1 -0.799929 -1.708511 0.000001 8 0.413704 1.395930 0.000000	47.3713, 128.1887, 263.2023, 401.0914, 459.8692, 636.677, 798.6621, 875.4651, 969.6703, 1074.1133, 1175.5864, 1387.5164, 1401.8205, 1460.3017, 1467.9025, 1792.6692, 1827.3837, 2878.3114, 3022.7027, 3070.5679, 3146.1316

Compound: OCH-CHO con 2	**Energy (kJ mol^{-1}):** -266.860539824510
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.882013 1.273803 0.000000 1 -0.446243 1.763739 -0.872659 1 -1.961896 1.389470 0.000000 1 -0.446243 1.763737 0.872660 6 -0.521809 -0.181039 -0.000001 6 0.971192 -0.544801 0.000000 8 1.852626 0.271981 0.000000 1 1.154434 -1.635290 0.000001 8 -1.315661 -1.093160 0.000000	83.9092, 120.9176, 247.4205, 467.0722, 483.6734, 568.3116, 777.5089, 907.5434, 1011.4438, 1081.1489, 1240.6326, 1360.532, 1393.964, 1456.9239, 1461.6638, 1778.9799, 1798.1316, 2932.8523, 3039.5034, 3090.9298, 3148.8663

Compound: $(CH_3)_2CO$	**Energy (kJ mol^{-1}):** -192.924334709876
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.287796 -0.611342 0.000009 6 -0.000000 0.184263 0.000001 8 0.000000 1.394544 -0.000000 6 1.287796 -0.611342 -0.000008 1 2.142292 0.059795 -0.000458 1 1.329612 -1.261732 -0.876460 1 1.329998 -1.260974 0.876992 1 -2.142291 0.059795 0.000470 1 -1.330002 -1.260963 -0.876999 1 -1.329607 -1.261743 0.876452	27.6477, 131.5768, 380.6368, 490.9686, 535.2152, 782.9184, 886.7496, 887.4282, 1085.1731, 1120.8963, 1233.7118, 1387.5641, 1387.871, 1459.7874, 1465.7347, 1470.3334, 1488.1926, 1781.7479, 3025.4845, 3032.6623, 3076.7144, 3084.1624, 3137.7556, 3138.7532

Compound: CF_3CFO	**Energy (kJ mol^{-1}):** -550.398192942521
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -0.590884 0.016760 -0.000000 6 0.950258 0.161191 -0.000000 8 1.560686 1.164510 0.000000 9 1.511346 -1.053957 -0.000000 9 -0.986585 -0.656718 1.087722 9 -1.165035 1.213645 -0.000003 9 -0.986585 -0.656723 -1.087719	43.7845, 226.0109, 238.7949, 378.7825, 419.3861,1. 512.0808, 584.7772, 688.3344, 765.2522, 800.0823, 1086.2930, 1167.3575, 1222.6180, ,1305.3726, 1935.9581

Compound: CF_3CF_2CHO con 1	**Energy (kJ mol^{-1}):** -688.812957684290
Reaction Coordinates: 6 -0.422322 0.474806 -0.007111 6 -1.578544 -0.376488 0.578734 8 -2.411136 -0.878783 -0.111479 1 -1.564497 -0.448302 1.679382 9 -0.698082 0.855351 -1.264304 9 -0.294172 1.582858 0.773134 6 0.938571 -0.268521 -0.002943 9 1.226271 -0.667494 1.247370 9 0.872605 -1.348671 -0.787048 9 1.918640 0.522377 -0.435778	**Frequencies (cm^{-1}):** 51.5838, 63.0683, 193.5618, 211.5132, 256.0864, 305.4401, 356.7146, 378.5992, 447.2778, 535.8368, 576.8438, 597.3911, 723.1946, 791.5991, 919.2348, 1072.488, 1137.8257, 1184.1741, 1198.6606, 1237.1088, 1317.8364, 1396.8437, 1843.4596, 2961.9338

Compound: CF_3CF_2CHO con 2	**Energy (kJ mol^{-1}):** -688.812777288418
Reaction Coordinates: 6 -0.437650 0.570319 0.000000 6 -1.776191 -0.200583 0.000000 8 -1.870643 -1.390064 -0.000000 1 -2.642222 0.486317 0.000000 9 -0.424425 1.368847 -1.097860 9 -0.424425 1.368847 1.097860 6 0.851157 -0.287979 0.000000 9 0.893553 -1.059323 1.088778 9 0.893553 -1.059323 -1.088778 9 1.926575 0.508024 0.000000	**Frequencies (cm^{-1}):** 69.26, 76.1892, 150.7349, 212.3416, 273.9584, 302.4093, 345.8929, 419.3262, 424.4234, 511.1899, 581.8153, 587.6043, 688.2018, 767.8071, 974.4221, 1102.9404, 1137.7221, 1174.2323, 1204.6731, 1208.8089, 1317.4186, 1420.6831, 1843.9034, 2940.2234

Compound: CF_3CHO	**Energy (kJ mol^{-1}):** -451.199957828211
Reaction Coordinates: 6 0.015009 0.360282 0.000000 6 0.501814 -1.106406 -0.000000 8 -0.245475 -2.035870 -0.000000 1 1.601864 -1.198064 -0.000000 9 0.501814 0.987869 1.088491 9 0.501814 0.987869 -1.088491 9 -1.307962 0.464459 0.000000	**Frequencies (cm^{-1}):** 73.5798, 250.7650, 307.2813, 422.6928, 518.9491, 524.0490, 701.8523, 834.5377, 974.2730, 1150.4161, 1174.8562, 1288.1325, 1403.3576, 1849.8517, 2955.8187

Compound: ClCHO	**Energy (kJ mol^{-1}):** -573.573415675277
Reaction Coordinates: 6 0.000000 0.806099 0.000000 17 -0.473506 -0.921812 0.000000 1 -0.898423 1.430438 0.000000 8 1.118503 1.175472 -0.000000	**Frequencies (cm^{-1}):** 445.4726, 717.2277, 947.4225, 1321.5214, 1845.7994, 3051.6439

Compound: FCHO	**Energy (kJ mol^{-1}):** -213.595002968390
Reaction Coordinates: 6 0.000000 0.400194 0.000000 9 -0.967389 -0.541739 0.000000 1 -0.464528 1.390119 0.000000 8 1.146378 0.135546 -0.000000	**Frequencies (cm^{-1}):** 661.6044, 1029.8624, 1055.9306, 1362.001, 1882.619, 3084.6994

Compound: nPrCHO con 1	**Energy (kJ mol^{-1}):** -232.170419945897
Reaction Coordinates: 6 -0.097122 0.733975 0.000001 6 -1.565367 0.404295 -0.000000 8 -2.028030 -0.708387 -0.000001 1 -2.238126 1.287813 0.000000 1 0.081540 1.382468 -0.867462 1 0.081539 1.382470 0.867462 6 0.841647 -0.466402 0.000003 1 0.624032 -1.088297 0.870079 1 0.624027 -1.088304 -0.870067 6 2.314355 -0.061509 -0.000002 1 2.563923 0.533617 -0.880971 1 2.563927 0.533624 0.880961 1 2.962296 -0.938444 0.000000	**Frequencies (cm^{-1}):** 79.0249, 171.9653, 191.8132, 244.2293, 344.4104, 666.0703, 692.8205, 790.8347, 852.1237, 951.5362, 961.9475, 1043.9681, 1133.3022, 1156.6431, 1256.8694, 1317.3106, 1325.6864, 1395.4313, 1415.1439, 1419.5698, 1447.599, 1491.6665, 1501.7294, 1508.6961, 1799.3454, 2861.5282, 2989.48, 3006.1864, 3020.0669, 3039.5484, 3058.8197, 3083.8279, 3087.8297

Compound: nPrCHO con 2	**Energy (kJ mol^{-1}):** -232.170348997214
Reaction Coordinates: 6 0.199645 1.019758 0.141947 6 1.415581 0.135016 0.236253 8 1.523900 -0.957904 -0.259595 1 2.262649 0.575269 0.803554 1 -0.029844 1.367689 1.156366 1 0.531469 1.920463 -0.390414 6 -1.022395 0.397694 -0.529479 1 -1.724891 1.196104 -0.777518 1 -0.713996 -0.053718 -1.473928 6 -1.724791 -0.650424 0.334054 1 -1.059489 -1.481653 0.564841 1 -2.067959 -0.217559 1.276486 1 -2.597370 -1.055625 -0.179274	**Frequencies (cm^{-1}):** 99.5657, 162.1953, 195.5618, 274.8177, 362.6911, 656.9668, 703.4042, 786.5623, 844.3608, 936.0297, 969.4128, 1057.1531, 1115.6621, 1146.5275, 1253.2475, 1297.9877, 1376.1737, 1381.507, 1413.563, 1419.1272, 1443.705, 1486.4416, 1500.17, 1510.136, 1799.5379, 2861.6032, 2993.2277, 3013.3291, 3024.6457, 3033.6785, 3062.7094, 3084.3356, 3103.6045

Compound: nPrCHO con 3	**Energy (kJ mol^{-1}):** -232.169370024577
Reaction Coordinates: 6 0.118374 -0.465499 0.251195 6 1.458818 0.215512 0.288500 8 2.419405 -0.106593 -0.363825 1 1.521548 1.084936 0.978300 1 0.170448 -1.311078 -0.435125 1 -0.078575 -0.854737 1.257306 6 -1.009186 0.503603 -0.136768 1 -0.987093 1.370844 0.528866	**Frequencies (cm^{-1}):** 68.7684, 96.8771, 235.1684, 254.6435, 380.387, 515.9786, 746.7568, 805.7749, 901.2618, 953.5301, 1005.3719, 1041.2682, 1137.0209, 1165.6705, 1254.7152, 1290.5464, 1329.9931, 1379.6366, 1415.7718, 1421.7209, 1466.9131, 1494.153, 1500.1553, 1509.006,

1 -0.821525 0.883269 -1.143889 6 -2.389081 -0.148570 -0.081681 1 -2.616927 -0.504401 0.924822 1 -2.448282 -1.003756 -0.756908 1 -3.168382 0.557398 -0.370252	1799.3304, 2852.6102, 2998.645, 3017.4256, 3024.9442, 3044.3664, 3080.8028, 3088.5077, 3090.2776

Compound: nPrCHO con 4	**Energy (kJ mol^{-1}):** -232.169477639287
Reaction Coordinates: 6 -0.155968 0.842209 -0.360288 6 -1.228391 0.075748 0.366894 8 -2.074188 -0.605771 -0.154061 1 -1.202106 0.180973 1.473895 1 -0.219596 0.615075 -1.425055 1 -0.390638 1.904968 -0.228506 6 1.248991 0.566634 0.197494 1 1.943330 1.283618 -0.243997 1 1.253859 0.764684 1.273298 6 1.737771 -0.856377 -0.069868 1 1.770445 -1.064835 -1.140641 1 1.083177 -1.600367 0.387544 1 2.740619 -1.007240 0.330553	**Frequencies (cm^{-1}):** 68.4528, 118.7583, 216.731, 302.3159, 396.1621, 511.5794, 755.9297, 774.6293, 898.4108, 946.3573, 979.0731, 1056.5192, 1125.8027, 1160.8035, 1238.2905, 1281.6809, 1351.1196, 1376.0608, 1418.2633, 1422.1193, 1461.9924, 1492.0975, 1501.3307, 1505.2713, 1799.7486, 2845.5201, 3003.1553, 3017.902, 3026.1685, 3051.7702, 3079.617, 3086.974, 3091.144

Compound: nPrCHO con 5	**Energy (kJ mol^{-1}):** -232.167656622638
Reaction Coordinates: 6 -0.188305 0.723213 0.418471 6 -1.178795 -0.385544 0.184842 8 -2.274620 -0.231140 -0.295053 1 -0.847013 -1.401782 0.480098 1 -0.676292 1.665685 0.170991 1 0.055799 0.733347 1.486996 6 1.115237 0.558484 -0.389455 1 0.867846 0.473053 -1.450287 1 1.684892 1.483908 -0.285759 6 1.991488 -0.619543 0.038389 1 1.498318 -1.579572 -0.116221 1 2.256337 -0.549266 1.095310 1 2.919322 -0.635924 -0.534185	**Frequencies (cm^{-1}):** 32.5075, 106.1833, 230.6751, 282.4868, 401.4827, 502.8874, 750.1966, 820.4108, 872.2837, 955.4863, 982.8532, 1050.0988, 1137.8552, 1149.2595, 1249.7828, 1288.7109, 1342.9645, 1376.2946, 1419.3167, 1427.9824, 1469.4841, 1495.2402, 1503.2179, 1509.413, 1794.2093, 2876.4281, 3003.0939, 3025.2069, 3028.2935, 3053.6752, 3085.6866, 3087.6659, 3092.9057

6.2.3 Epoxide

Compound: MeCH(O)CH$_2$ epoxide	**Energy (kJ mol^{-1}):** -192.878663433749
Reaction Coordinates: 6 -1.508220 0.097295 -0.148746 6 -0.152958 -0.033618 0.484762 6 1.040045 0.616688 -0.061356 1 0.953858 1.210439 -0.965730 1 1.864601 0.879926 0.592659 8 0.828990 -0.789185 -0.238075 1 -0.153870 -0.247576 1.550743 1 -1.418683 0.319184 -1.211821 1 -2.074599 -0.828747 -0.037983 1 -2.076426 0.898071 0.328772	**Frequencies (cm^{-1}):** 206.9689, 367.2093, 410.1583, 770.2174, 842.076, 907.7501, 972.2655, 1042.6983, 1129.1516, 1156.8279, 1166.8292, 1189.2541, 1293.3958, 1406.7794, 1438.6459, 1483.164, 1496.9703, 1529.0015, 3027.8395, 3080.6169, 3084.617, 3087.9567, 3109.3484, 3163.9921

Compound: MVK epoxide 1	**Energy (kJ mol^{-1}):** -306.085253261747
Reaction Coordinates: 6 2.038053 -0.662345 0.054704 6 0.786358 0.178150 -0.014888 6 -0.509862 -0.589469 -0.125013 6 -1.672912 -0.147652 0.669190 1 -2.400258 -0.885087 0.991096 1 -1.563704 0.737727 1.285160 8 -1.610151 0.085568 -0.727499 1 -0.429169 -1.641442 -0.381104 8 0.799777 1.384927 0.028628 1 2.178921 -1.190621 -0.891664 1 1.946886 -1.424690 0.831905 1 2.900495 -0.031953 0.251609	**Frequencies (cm^{-1}):** 59.3766, 128.7536, 238.073, 266.2238, 374.635, 593.4428, 611.4556, 763.4566, 866.6265, 891.2063, 956.7035, 995.5147, 1058.3488, 1100.7998, 1161.1896, 1165.9146, 1197.2407, 1276.3587, 1384.3475, 1413.5506, 1463.6677, 1473.9134, 1508.1708, 1789.418, 3025.4932, 3076.2812, 3088.1766, 3116.7276, 3142.22, 3183.5725

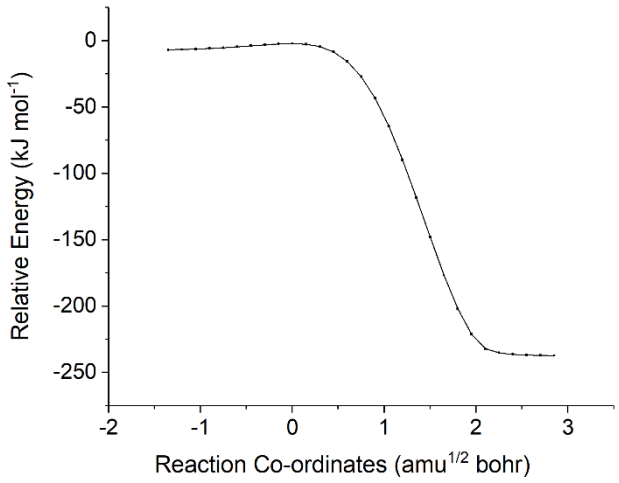
Compound: MVK epoxide 2	**Energy (kJ mol^{-1}):** -306.088513722259
Reaction Coordinates: 6 1.189939 1.271715 0.081328 6 0.866183 -0.196251 -0.021157 6 -0.566270 -0.592823 -0.248650 6 -1.635483 -0.142820 0.660098 1 -2.496959 -0.785349 0.802985 1 -1.398787 0.519029 1.486012 8 -1.497983 0.422872 -0.636579 1 -0.682880 -1.550471 -0.744110 8 1.706168 -1.065329 0.055880 1 0.517612 1.787253 0.767438 1 1.047793 1.737605 -0.896035 1 2.221528 1.392670 0.399584	**Frequencies (cm^{-1}):** 91.8198, 110.1739, 234.6262, 263.4874, 478.3598, 506.3708, 595.9417, 739.7356, 858.0709, 896.9919, 931.2284, 1011.6297, 1065.5649, 1097.0453, 1154.8359, 1165.8901, 1249.4673, 1272.1889, 1387.5027, 1393.4862, 1457.9142, 1469.6452, 1524.813, 1772.6261, 3040.1397, 3090.4468, 3094.1255, 3138.5166, 3144.7729, 3178.0915

6.2.4 Oxygen

Compound: O_2	**Energy (kJ mol^{-1}):** -150.147598743643
Reaction Coordinates: 8 0.000000 0.000000 0.602585 8 0.000000 0.000000 -0.602585	**Frequencies (cm^{-1}):** 1614.3238

6.3 Ozonolysis of Propene (Alkene 1)

Compound: $MeCHCH_2 + O_3$ PRC1	**Energy (kJ mol^{-1}):** -342.973340622844
Reaction Coordinates: 6 2.046171 -0.757081 0.514567 6 1.408907 0.107682 -0.521617 6 0.971533 1.353841 -0.316182 1 0.531213 1.938242 -1.112426 1 1.068868 1.835740 0.648039 1 1.323959 -0.317086 -1.516737 1 2.105661 -0.251830 1.477924 1 1.478727 -1.680958 0.645647 1 3.055910 -1.045358 0.210847 8 -1.512327 0.661928 0.752210 8 -1.842990 -0.098257 -0.199497 8 -1.160183 -1.151847 -0.354451	**Frequencies (cm^{-1}):** 38.8907, 70.1551, 90.066, 100.3661, 129.2045, 212.2132, 276.861, 427.6039, 602.623, 741.8813, 925.1872, 952.2453, 956.0315, 1008.9446, 1069.5981, 1163.1981, 1192.1138, 1196.8335, 1325.778, 1407.2116, 1449.5641, 1477.8939, 1493.0218, 1667.0177, 3019.2457, 3064.5642, 3098.9453, 3134.0848, 3139.2265, 3220.6033

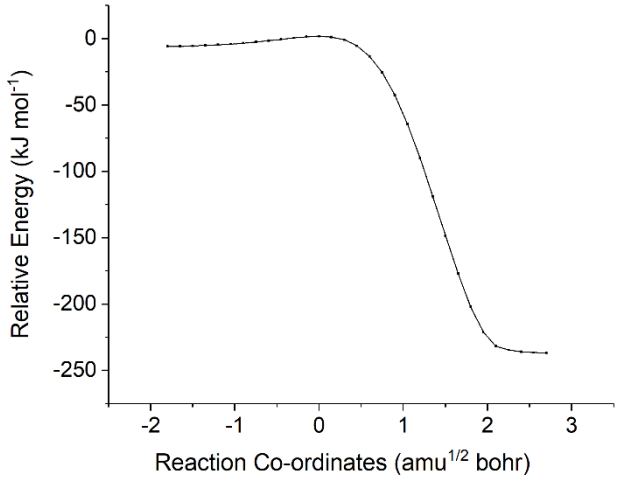
Compound: $MeCHCH_2 + O_3$ TS_{OZO} 1	**Energy (kJ mol^{-1}):** -342.964246608645
Reaction Coordinates: 6 -2.033369 -0.503898 -0.421156 6 -1.110850 0.185356 0.526972 6 -0.481983 1.364071 0.249512 1 0.044756 1.912973 1.015219 1 -0.647546 1.872572 -0.689368 1 -1.080407 -0.191077 1.541692 1 -1.849166 -1.578058 -0.436073 1 -1.924197 -0.119125 -1.434144 1 -3.071437 -0.358797 -0.108116 8 1.461418 0.617093 -0.613638 8 1.635810 -0.360818 0.205516 8 0.688422 -1.232732 0.155476	**Frequencies (cm^{-1}):** -195.1873, 83.5637, 131.979, 180.8475, 224.0039, 352.6094, 427.7067, 456.8352, 682.3138, 743.3604, 919.2146, 949.3388, 962.0258, 990.9226, 1054.6825, 1085.5173, 1117.2666, 1199.1591, 1300.8936, 1407.9286, 1445.1137, 1476.5941, 1492.8063, 1591.4831, 3019.9589, 3076.4735, 3109.7043, 3154.1064, 3165.2523, 3245.1805
IRC:  	

Compound: $MeCHCH_2 + O_3$ POZ1	**Energy (kJ mol^{-1}):** -343.063267068713
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -2.050387 0.025192 -0.245438 6 -0.701157 -0.038194 0.438893 6 0.246523 1.167424 0.181761 1 -0.151447 1.870719 -0.548496 1 0.491174 1.681784 1.113020 8 1.410517 0.590862 -0.404377 8 1.391085 -0.754568 0.128139 8 0.032978 -1.138922 -0.110778 1 -0.811837 -0.188223 1.515612 1 -1.931064 0.181911 -1.317147 1 -2.637065 0.846341 0.167823 1 -2.606274 -0.898030 -0.085981	75.1327, 229.9592, 316.7004, 364.9438, 462.5479, 667.3721, 717.3333, 743.3922, 839.0161, 906.0755, 933.0356, 962.7378, 994.9027, 1078.8553, 1146.0166, 1166.3657, 1235.2029, 1332.5979, 1351.3282, 1390.4342, 1416.348, 1486.5674, 1500.2498, 1512.1843, 3023.4868, 3037.8377, 3039.6458, 3100.108, 3104.1246, 3113.6936

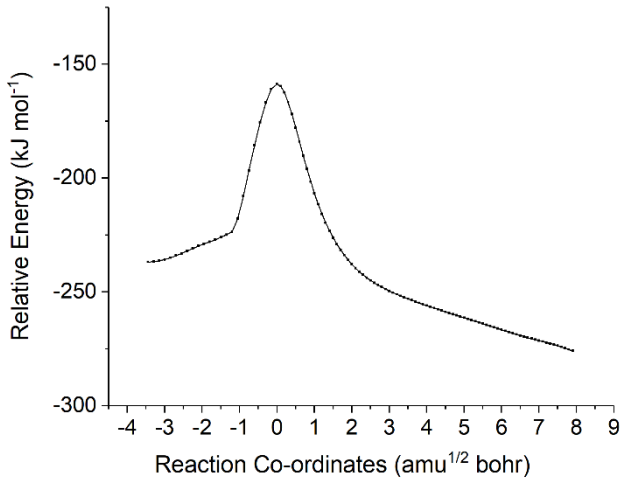
Compound: $MeCHCH_2 + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -342.973281732246
Reaction Coordinates: 6 2.122525 -0.742209 -0.531744 6 1.459586 0.116335 0.496454 6 0.975341 1.340484 0.275489 1 1.047800 1.810920 -0.697473 1 0.511754 1.915285 1.063783 1 1.389971 -0.298113 1.496664 1 3.146442 -0.982935 -0.233810 1 1.600609 -1.696077 -0.641658 1 2.155223 -0.253003 -1.505010 8 -1.736533 0.801348 -0.451900 8 -1.633209 -0.454117 -0.385960 8 -1.279821 -0.945198 0.722399	**Frequencies (cm^{-1}):** 35.9939, 49.1724, 78.4193, 94.9363, 117.9646, 211.3654, 257.3273, 427.3409, 603.4208, 742.7204, 924.135, 951.236, 959.3925, 1011.0515, 1069.5952, 1168.0601, 1194.718, 1197.6079, 1326.2731, 1408.371, 1451.0589, 1477.7041, 1494.3744, 1672.3857, 3015.9712, 3057.2143, 3094.5576, 3136.0295, 3141.2178, 3226.5704

Compound: $MeCHCH_2 + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -342.962560927001
Reaction Coordinates: 6 -1.926380 -0.562291 -0.477319 6 -1.129988 0.244089 0.497661 6 -0.475375 1.395306 0.162784 1 -0.050295 2.032662 0.921434 1 -0.529152 1.793872 -0.840672 1 -1.234267 -0.003310 1.545558 1 -1.872560 -1.626643 -0.255180 1 -1.589302 -0.398940 -1.501043 1 -2.980842 -0.273298 -0.426744 8 1.594726 0.664324 -0.303132 8 1.327607 -0.592512 -0.409856 8 0.758526 -1.070183 0.645224	**Frequencies (cm^{-1}):** -214.9837, 83.3289, 117.0989, 184.5561, 203.7508, 365.4669, 433.7475, 476.5627, 688.6408, 742.19, 916.1274, 952.9509, 955.9557, 989.4269, 1054.6929, 1079.7675, 1111.3577, 1196.1878, 1295.6607, 1406.6303, 1442.8075, 1479.0257, 1493.3283, 1586.1367, 3015.0671, 3074.3987, 3111.8664, 3155.4298, 3174.4678, 3251.3228
IRC:	



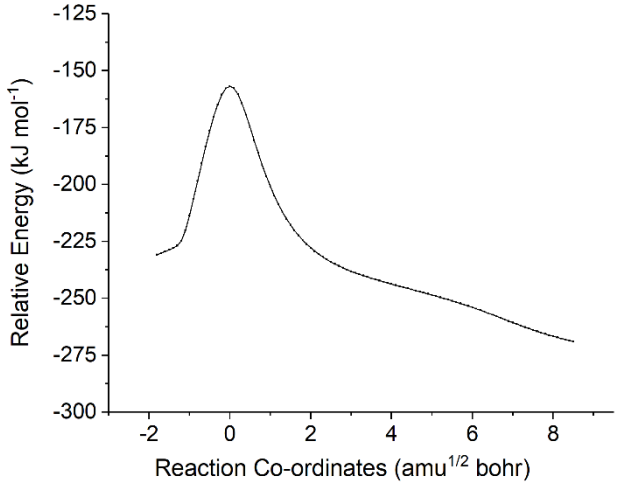
Compound: $MeCHCH_2 + O_3$ POZ 2	**Energy (kJ mol^{-1}):** -343.063413011835
Reaction Coordinates: 6 1.938333 0.041783 -0.397501 6 0.719003 0.104400 0.503272 6 -0.319630 1.177145 0.070401 1 -0.487873 1.944716 0.823288 1 -0.031970 1.631370 -0.880474 8 -1.539167 0.459373 -0.060512 8 -1.069230 -0.827669 -0.500997 8 -0.047318 -1.110899 0.476472 1 1.003755 0.228290 1.548449 1 2.474743 0.992813 -0.375366 1 1.641410 -0.162621 -1.426001 1 2.619423 -0.740974 -0.066630	**Frequencies (cm^{-1}):** 91.6591, 236.5009, 316.9286, 387.176, 478.9595, 671.8908, 711.1444, 742.0023, 835.0898, 904.9102, 934.1492, 954.7888, 1002.126, 1062.4926, 1110.8867, 1165.6292, 1241.2155, 1308.3908, 1345.076, 1380.989, 1411.275, 1486.8762, 1496.3555, 1506.9092, 3029.3811, 3033.4412, 3063.3112, 3095.2046, 3110.6938, 3116.8918

Compound: $MeCHCH_2 + O_3$ TS_{ANTI}	**Energy (kJ mol^{-1}):** -343.031950106195
Reaction Coordinates: 6 2.108980 0.187069 -0.056931 6 0.704892 -0.095474 0.369695 6 -0.497599 1.290475 -0.095848 1 -0.181191 1.950361 0.727608 1 -0.106096 1.573175 -1.084563 1 0.465767 -0.120182 1.427646 1 2.797103 -0.533157 0.389879 1 2.404011 1.180431 0.278889 1 2.204504 0.138218 -1.140033 8 -1.642531 0.750919 -0.019875 8 -1.134302 -1.261881 0.114900 8 0.091617 -1.049195 -0.332642	**Frequencies (cm^{-1}):** -435.5564, 159.8915, 162.7443, 243.3816, 337.013, 364.1606, 493.2648, 518.3261, 616.5203, 856.7676, 907.117, 994.0697, 1017.6363, 1120.2254, 1153.7143, 1182.835, 1220.6793, 1270.1363, 1389.7569, 1392.5438, 1423.9989, 1479.9475, 1492.2612, 1544.0705, 2907.356, 2969.0715, 3037.5842, 3097.7653, 3121.9158, 3139.4026
IRC:	



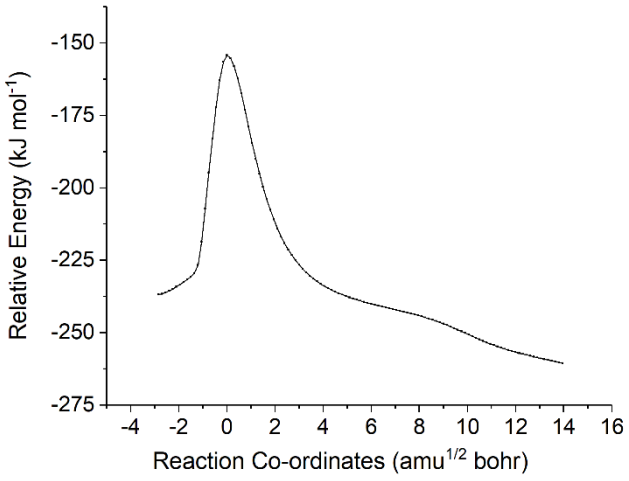
Compound: $MeCHCH_2 + O_3$ C_{ANTI}	**Energy (kJ mol^{-1}):** -343.070570907990
Reaction Coordinates: 6 2.197640 -0.529115 0.098610 6 0.958332 0.105026 -0.385106 1 0.536037 -0.090929 -1.361383 8 0.400476 0.976339 0.330402 8 -0.826700 1.434854 -0.130168 1 3.011534 -0.346947 -0.607012 1 2.037337 -1.608719 0.138469 1 2.469683 -0.163904 1.085429 6 -1.874516 -0.546271 0.078546 1 -2.271882 -0.198727 1.040808 1 -2.454921 -0.266176 -0.810583 8 -0.950841 -1.348998 0.020012	**Frequencies (cm^{-1}):** 62.1318, 97.2317, 140.2578, 151.4405, 304.1128, 314.8473, 337.3339, 380.8651, 561.4254, 573.6272, 866.8006, 897.8345, 973.5133, 1066.902, 1149.0758, 1168.9578, 1251.1705, 1351.7798, 1408.3246, 1454.1633, 1464.0759, 1508.2848, 1579.4701, 1689.4636, 2956.3467, 3020.7985, 3031.2656, 3081.6618, 3140.6488, 3197.8733

Compound: $MeCHCH_2 + O_3$ TS_{FO} 1	**Energy (kJ mol^{-1}):** -343.029736721201
Reaction Coordinates: 6 -1.863419 0.325251 -0.555472 6 -0.900294 -0.214589 0.490774 6 0.531012 0.992746 0.625922 1 0.176450 2.014223 0.558547 1 0.967698 0.645722 1.554058 1 -1.203517 -0.031654 1.537554 1 -2.730821 -0.335153 -0.601855 1 -2.213169 1.328091 -0.307063 1 -1.396042 0.333887 -1.538607 8 1.170957 0.617530 -0.477435 8 1.591772 -0.629740 -0.367051 8 -0.288279 -1.309736 0.273239	**Frequencies (cm^{-1}):** -441.1182, 130.408, 178.8658, 265.1302, 306.2098, 476.8837, 494.434, 566.6192, 606.6314, 848.6613, 897.3717, 947.7903, 1017.5617, 1051.8142, 1112.7448, 1170.13, 1222.4076, 1267.6481, 1317.82, 1398.6733, 1451.4804, 1477.7491, 1481.9663, 1499.9064, 2891.6285, 3032.5107, 3092.4971, 3106.4542, 3118.8222, 3224.4608
IRC:	



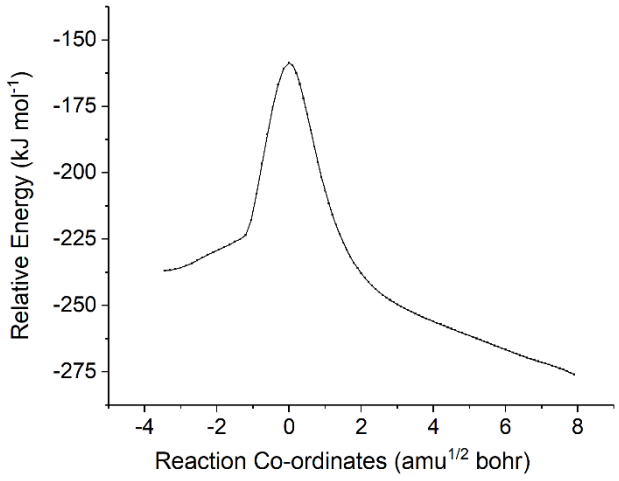
Compound: $MeCHCH_2 + O_3$ CPr_{FO} 1	**Energy (kJ mol^{-1}):** -343.066723044814
Reaction Coordinates: 6 -1.628628 1.178988 0.019416 6 -2.014980 -0.263196 0.043493 1 -3.099230 -0.463665 0.154371 8 -1.252698 -1.199519 -0.046059 1 -2.182262 1.678699 -0.780919 1 -1.959522 1.646138 0.951932 1 -0.555607 1.321104 -0.111564 6 1.459277 -1.055111 -0.183656 1 1.514456 -1.979499 0.373492 1 1.142293 -0.980298 -1.214471 8 1.809286 -0.028010 0.433852 8 1.724144 1.179208 -0.218837	**Frequencies (cm^{-1}):** 51.0945, 82.2432, 90.2483, 109.0794, 128.3928, 181.0936, 202.4777, 519.0435, 532.8399, 678.8141, 782.7034, 865.1322, 896.3788, 992.8464, 1143.6419, 1149.8444, 1235.5433, 1389.7419, 1413.674, 1423.7214, 1467.8134, 1478.4089, 1567.3742, 1779.2423, 2890.1717, 3004.4732, 3062.778, 3101.2363, 3132.8648, 3276.8435

Compound: $MeCHCH_2 + O_3$ TS_{FO} 2	**Energy (kJ mol^{-1}):** -343.028828640250
Reaction Coordinates: 6 -2.095277 0.231115 0.315259 6 -0.856701 -0.188307 -0.474101 6 0.400100 1.129165 0.043748 1 0.272014 2.028118 -0.546933 1 0.150824 1.152906 1.097425 1 -0.899090 0.060505 -1.547828 1 -1.950961 0.042396 1.377925 1 -2.938163 -0.371555 -0.025995 1 -2.345793 1.281110 0.155790 8 1.515835 0.486568 -0.264913 8 1.626155 -0.617773 0.450336 8 -0.264186 -1.271960 -0.162900	**Frequencies (cm^{-1}):** -447.2867, 92.3351, 208.7885, 274.9778, 337.672, 466.7115, 477.8343, 529.6582, 599.4037, 873.647, 884.7108, 988.5419, 989.6916, 1062.2058, 1090.5631, 1182.0517, 1229.8464, 1265.8517, 1351.3143, 1392.0788, 1451.3561, 1479.2682, 1483.454, 1501.2031, 2912.5449, 3028.9988, 3091.7495, 3104.8768, 3115.7515, 3224.0316
IRC	



Compound: $MeCHCH_2 + O_3$ CPr_{FO} 2	**Energy (kJ mol^{-1}):** -343.064735066772
Reaction Coordinates: 6 -2.019621 -1.247414 -0.000007 6 -2.440784 0.188467 0.000015 1 -3.534865 0.363110 0.000049 8 -1.686882 1.132770 -0.000001 1 -2.444380 -1.746527 -0.875108 1 -2.444331 -1.746540 0.875111 1 -0.937189 -1.348876 -0.000038 6 1.565528 1.042583 -0.000006 1 2.454020 1.663367 0.000053 1 0.539327 1.388502 -0.000047 8 1.702666 -0.203437 -0.000027 8 2.951301 -0.738689 0.000024	**Frequencies (cm^{-1}):** 28.4229, 38.0975, 54.7174, 62.5817, 92.6413, 123.3914, 164.5267, 515.2057, 531.0457, 712.471, 778.0505, 891.4224, 901.1816, 997.4803, 1137.4001, 1140.1854, 1255.8368, 1384.2757, 1409.2608, 1426.4191, 1461.2988, 1469.9073, 1544.7324, 1792.4954, 2893.9688, 3022.6592, 3072.2478, 3098.3098, 3137.99, 3251.0177

Compound: $MeCHCH_2 + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -343.031540552877
Reaction Coordinates: 6 1.547685 -0.613374 -0.584216 6 0.726375 -0.220193 0.609068 6 -0.947402 -1.023218 0.365839 1 -0.525956 -1.999100 0.078884 1 -1.371198 -0.992132 1.379130 1 1.095816 -0.499901 1.591394 1 0.965329 -0.573860 -1.499174 1 1.942306 -1.617141 -0.438116 1 2.387497 0.079938 -0.677500 8 -1.491250 -0.326126 -0.549136 8 -0.299553 1.391748 -0.474450 8 0.234086 1.027242 0.676240	**Frequencies (cm^{-1}):** -444.8601, 156.655, 188.4216, 296.5703, 306.3347, 344.3532, 527.3134, 563.6148, 702.2926, 871.6034, 883.8925, 939.2037, 1020.9308, 1086.1398, 1147.213, 1186.0746, 1222.8821, 1223.6026, 1375.6538, 1398.5207, 1429.4044, 1471.5763, 1495.3352, 1539.1968, 2919.339, 2983.6402, 3034.7282, 3105.2349, 3132.4762, 3154.7314
IRC	

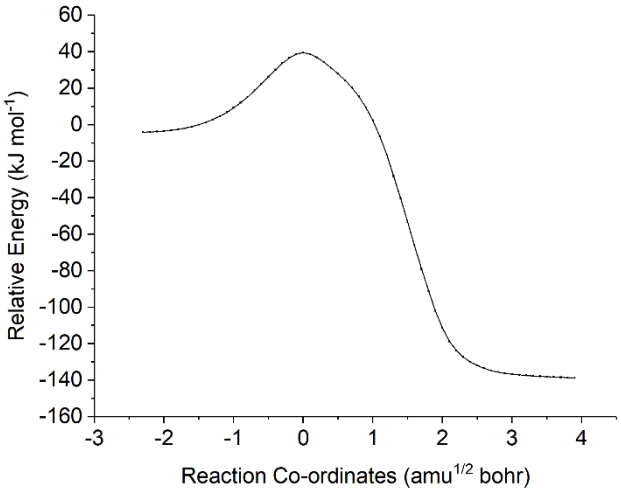


Compound: $MeCHCH_2 + O_3$ CPr_{SYN}	**Energy (kJ mol^{-1}):** -343.071168900871
Reaction Coordinates: 6 -1.491663 1.023885 -0.580865 6 -1.291439 0.196594 0.612757 1 -1.657196 0.454777 1.600228 8 -0.704673 -0.916383 0.595860 8 -0.164546 -1.328994 -0.604524 1 -0.524243 1.411419 -0.910582 1 -2.169283 1.847171 -0.372369 1 -1.860722 0.392913 -1.393197 6 2.029503 -0.043452 -0.167678 1 2.334801 -0.918443 0.427315 1 2.130582 -0.146991 -1.259248 8 1.652675 0.982500 0.348985	**Frequencies (cm^{-1}):** 77.6957, 91.1998, 96.0059, 126.0497, 167.3703, 210.1412, 301.7889, 345.5066, 454.0568, 670.0869, 770.7042, 884.7781, 980.147, 1062.5706, 1116.0221, 1173.9362, 1259.687, 1354.4061, 1396.7133, 1442.0159, 1468.6435, 1527.8804, 1576.3099, 1770.6073, 2929.3797, 2990.1892, 3027.6469, 3074.0465, 3139.4954, 3172.2283

Compound: $MeCHCH_2 + O_3$ TS_{POZ} 1	**Energy (kJ mol^{-1}):** -343.058289489220
Reaction Coordinates: 6 -1.770030 0.021830 -0.574846 1 -2.452965 0.862794 -0.443128 6 0.294413 1.112429 0.491275 1 -0.105029 2.071086 0.164575 1 0.824696 1.213039 1.441433 1 -1.216489 -0.057506 1.527534 1 -1.282974 0.115213 -1.544233 1 -2.354401 -0.897134 -0.567872 6 -0.743636 -0.003946 0.545064 8 1.155342 0.668945 -0.541954 8 0.106216 -1.149527 0.497977 8 1.226277 -0.780590 -0.374431	**Frequencies (cm^{-1}):** -148.4636, 205.8173, 210.8383, 355.8478, 435.069, 679.0243, 730.9869, 792.7407, 825.3244, 857.8566, 940.0433, 963.0335, 1010.6141, 1058.0101, 1108.7303, 1166.2742, 1238.0158, 1289.3759, 1346.913, 1371.4596, 1412.9007, 1485.8917, 1496.2793, 1499.0454, 3028.4694, 3038.0729, 3061.594, 3102.2062, 3113.0063, 3121.4633
IRC To low a barrier for IRC to be done	

Compound: $MeCHCH_2 + O_3$ TS_{POZ} 2	**Energy (kJ mol^{-1}):** -343.058489104847
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.106630 0.013743 0.107061 1 2.638281 0.896363 -0.249638 6 -0.219517 1.125932 0.180945 1 -0.061519 1.244385 1.257219 1 -0.133667 2.081572 -0.334133 1 0.636947 0.072052 -1.487915 1 2.136289 -0.003363 1.195784 1 2.625909 -0.866339 -0.268922 6 0.677520 0.040398 -0.394185 8 -1.511611 0.632049 -0.109715 8 0.018055 -1.131655 0.081309 8 -1.410199 -0.813532 0.093991	-156.0534, 207.4398, 217.9388, 304.7319, 474.3486, 588.3768, 687.9952, 796.7495, 854.3928, 882.1112, 929.957, 973.3332, 1026.6192, 1098.1578, 1154.8162, 1172.7298, 1231.7007, 1320.6615, 1350.6856, 1399.1551, 1415.5187, 1485.3536, 1489.7797, 1502.139, 3004.8346, 3019.348, 3042.6493, 3106.7355, 3109.9472, 3117.9724
IRC To low a barrier for IRC to be done	

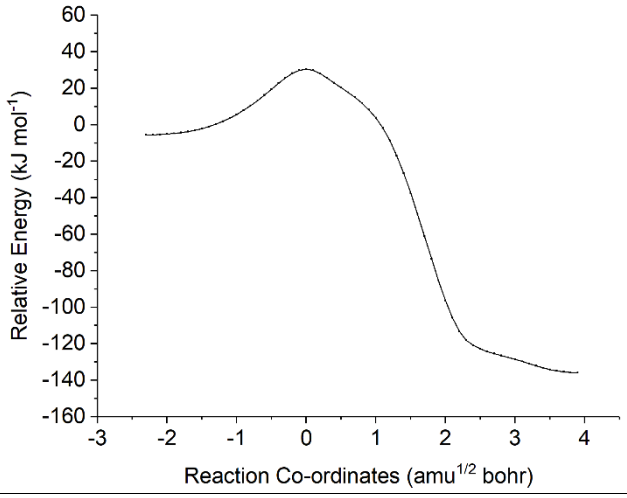
Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 1.1	**Energy (kJ mol^{-1}):** -342.948262646173
Reaction Coordinates: 6 -2.740752 0.144761 0.021832 6 -1.391132 -0.185457 -0.483571 6 -0.353293 -0.702617 0.286337 1 0.429019 -1.316895 -0.170983 1 -0.570496 -0.983558 1.309457 1 -1.167316 0.073903 -1.512007 1 -2.889008 -0.180268 1.050220 1 -2.919873 1.225437 -0.031890 1 -3.512534 -0.310908 -0.607440 8 0.604187 0.688710 0.497098 8 1.729170 0.590012 -0.273224 8 2.359302 -0.534701 -0.096993	**Frequencies (cm^{-1}):** -382.1614, 101.4164, 108.0224, 135.5877, 254.3742, 279.205, 398.7884, 482.7397, 690.1105, 757.4164, 829.2432, 914.079, 939.2783, 1025.804, 1082.0467, 1101.5531, 1173.6473, 1211.9429, 1282.641, 1395.4896, 1428.4528, 1461.2645, 1489.0598, 1554.2961, 2989.9711, 2995.3128, 3023.6044, 3105.4394, 3155.2867, 3173.0738
IRC  	

Compound: $MeCHCH_2 + O_3$ C_{EPOX} 1.1	**Energy (kJ mol^{-1}):** -343.028197768054
Reaction Coordinates: 6 2.468762 -0.455772 -0.212769 6 1.008149 -0.149538 -0.361990 6 0.417189 1.137867 0.005508 1 -0.495557 1.467169 -0.488777 1 1.034580 1.929810 0.415405	**Frequencies (cm^{-1}):** 44.7431, 88.8489, 110.1613, 139.1573, 204.1164, 226.2105, 388.693, 414.3471, 765.5782, 835.097, 898.2627, 975.6358, 1045.4723, 1127.4202, 1159.6756,

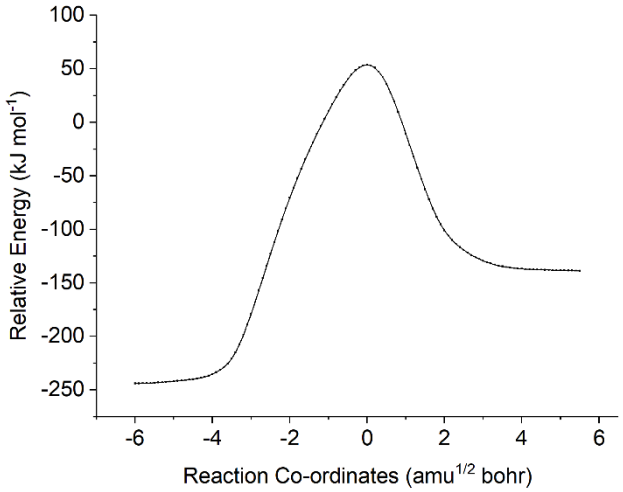
1 0.472611 -0.732859 -1.105092 1 2.923340 0.172896 0.552033 1 2.615225 -1.500105 0.065859 1 2.985959 -0.284690 -1.158719 8 0.255585 0.005407 0.860174 8 -1.992246 -0.669045 0.307241 8 -2.375935 0.132694 -0.525565	1167.79, 1189.7997, 1292.8954, 1408.9358, 1440.3971, 1482.727, 1496.9486, 1509.1175, 1532.2595, 3031.7441, 3055.2511, 3090.019, 3101.4133, 3121.2395, 3154.7858

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 1.2	**Energy (kJ mol^{-1}):** -342.951372446173
Reaction Coordinates: 6 -1.579663 -1.108916 -0.032929 6 -1.594030 0.357591 0.017869 6 -0.518118 1.052013 0.571927 1 0.050748 0.587741 1.375602 1 -0.545260 2.132299 0.592692 1 -2.357344 0.903858 -0.521367 1 -0.736611 -1.423102 -0.679896 1 -1.339462 -1.547748 0.940208 1 -2.497742 -1.537360 -0.426263 8 0.642833 0.816537 -0.688149 8 1.256242 -0.388099 -0.532121 8 1.797992 -0.543415 0.642497	**Frequencies (cm^{-1}):** -372.8165, 91.0412, 209.2279, 218.0342, 269.3696, 312.015, 417.7306, 459.9832, 661.5842, 734.0844, 823.6845, 937.4342, 976.3175, 1012.6483, 1070.9918, 1088.3252, 1155.4584, 1189.5664, 1274.4453, 1380.0642, 1435.6745, 1444.0909, 1482.1532, 1541.6648, 2879.1075, 3025.6445, 3074.3884, 3125.3923, 3171.6796, 3206.1311

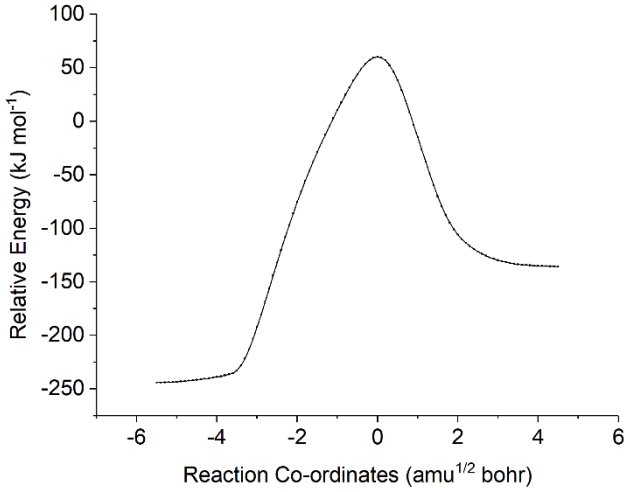
IRC



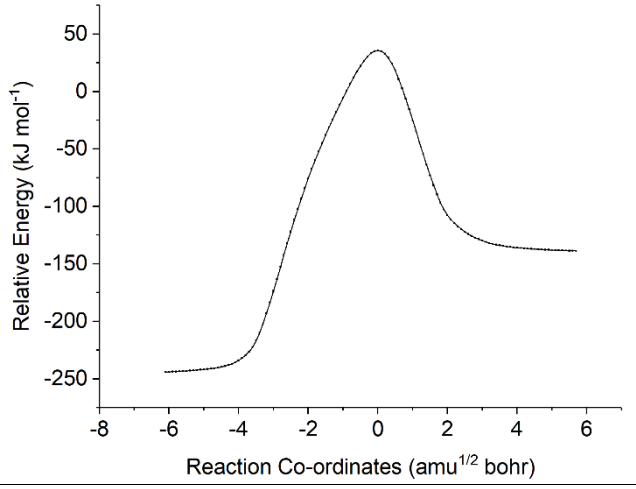
Compound: $MeCHCH_2 + O_3$ C_{EPOX} 1.2	**Energy (kJ mol^{-1}):** -343.029307044133
Reaction Coordinates: 6 1.376762 1.351779 0.177650 6 1.500104 -0.120290 -0.087224 6 0.669838 -1.120100 0.588975 1 -0.080770 -0.784239 1.302479 1 1.023592 -2.134735 0.734062 1 2.464399 -0.448757 -0.464688 1 2.123888 1.660795 0.911168 1 1.549837 1.919557 -0.737509 1 0.388328 1.603503 0.557108 8 0.401585 -0.764709 -0.767803 8 -1.828064 0.313752 -0.591601 8 -2.167209 0.140399 0.562027	**Frequencies (cm^{-1}):** 50.9066, 85.4481, 94.5183, 136.9927, 190.4257, 221.3491, 375.9241, 415.1245, 762.5352, 826.4749, 911.1214, 974.7285, 1045.134, 1127.4185, 1154.2868, 1172.3421, 1191.6762, 1293.661, 1410.1606, 1438.9188, 1484.0048, 1497.8489, 1520.1165, 1541.095, 3033.594, 3058.9607, 3088.6311, 3100.8575, 3124.0406, 3156.8632

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.1	**Energy (kJ mol^{-1}):** -342.928960564643
Reaction Coordinates: 6 2.307968 -0.223449 0.009537 6 0.849810 0.012745 0.359857 6 0.242926 1.285914 -0.020434 1 0.445718 1.664840 -1.011123 1 -0.455477 1.823400 0.599345 1 0.629809 -0.280291 1.386818 1 2.507648 0.054573 -1.024486 1 2.957659 0.359086 0.664014 1 2.536428 -1.280825 0.137433 8 -0.010822 -0.690193 -0.550564 8 -1.505744 -0.721235 0.291598 8 -2.111686 0.312422 -0.096755	**Frequencies (cm^{-1}):** -570.1874, 128.0702, 137.9225, 225.4772, 319.844, 334.1269, 368.2555, 458.78, 526.1414, 621.5262, 822.399, 861.2638, 916.7975, 948.0967, 1066.1151, 1163.5387, 1214.8922, 1229.5672, 1291.2611, 1367.1173, 1403.3944, 1481.5273, 1488.0138, 1501.7066, 3036.926, 3061.6297, 3105.6648, 3117.5296, 3173.9609, 3290.3376
IRC  	

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.2	**Energy (kJ mol^{-1}):** -342.925694536270
Reaction Coordinates: 6 1.682531 -0.794664 -0.476267 6 1.059805 0.340558 0.303264 6 0.304998 1.364428 -0.406042 1 -0.117171 1.199946 -1.385016 1 0.072890 2.288173 0.100559 1 1.764245 0.755207 1.028041 1 0.986512 -1.208694 -1.200915 1 2.563276 -0.425932 -1.004781 1 1.995727 -1.586447 0.203116 8 -0.127945 0.014087 1.084656 8 -1.150903 -0.845288 0.076444 8 -1.914837 0.020678 -0.444441	**Frequencies (cm^{-1}):** -598.1671, 102.2364, 146.5392, 213.2375, 280.9727, 319.1854, 392.2809, 484.7764, 541.5084, 590.46, 770.9612, 868.9008, 926.4686, 933.3537, 1072.1183, 1183.7133, 1194.7462, 1208.365, 1254.3455, 1384.9941, 1415.4801, 1481.0829, 1495.1666, 1507.3114, 3034.5635, 3042.9244, 3104.0708, 3136.5178, 3174.9153, 3286.5389
IRC	

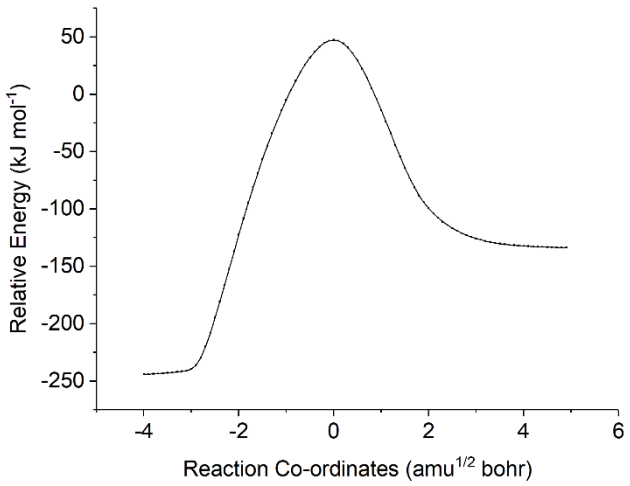


Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.3	**Energy (kJ mol^{-1}):** -342.931620239017
Reaction Coordinates: 6 1.947490 -0.728760 -0.290679 6 0.931486 -0.131639 0.584130 6 0.418762 1.227928 0.388197 1 1.172716 1.960499 0.085628 1 -0.183677 1.622359 1.205815 1 0.502315 -0.755781 1.354848 1 2.263195 -0.061581 -1.088696 1 2.815531 -0.997095 0.326883 1 1.585413 -1.666660 -0.718523 8 -0.369994 0.854890 -0.735818 8 -1.727811 0.035347 0.006916 8 -1.394935 -1.178601 0.071921	**Frequencies (cm^{-1}):** -543.7565, 115.8676, 145.0436, 170.7617, 255.7417, 306.5185, 372.0354, 402.9876, 493.3588, 776.0273, 869.0121, 930.3549, 941.6226, 1011.6996, 1133.6489, 1190.1843, 1224.7159, 1241.3858, 1309.7704, 1382.3611, 1413.7772, 1449.889, 1479.3643, 1502.6432, 2985.7553, 3014.4114, 3051.191, 3084.796, 3128.7091, 3209.2065
IRC	



Compound: $MeCHCH_2 + O_3$ C_{EPOX} 2.3	**Energy (kJ mol^{-1}):** -343.028240894697
Reaction Coordinates: 6 -2.203837 -0.830412 0.110700 6 -0.870121 -0.241187 -0.247402 6 -0.662937 1.176457 -0.546883	**Frequencies (cm^{-1}):** 49.8264, 85.1125, 94.1088, 145.019, 202.2485, 233.9425, 372.4427, 416.6181, 769.7162, 841.9186, 901.5127, 967.7652,

1 -1.495972 1.868095 -0.489852 1 0.159729 1.474456 -1.186470 1 -0.155688 -0.936753 -0.690347 1 -2.863513 -0.072392 0.531355 1 -2.676804 -1.253652 -0.777018 1 -2.083937 -1.630028 0.842587 8 -0.265318 0.622207 0.720320 8 2.081622 0.103362 0.447648 8 2.125890 -0.735429 -0.434062	1046.2344, 1129.1427, 1156.9692, 1169.5062, 1192.3677, 1295.4624, 1408.8841, 1438.239, 1483.4503, 1496.6679, 1515.101, 1531.9835, 3032.8811, 3048.3083, 3092.9898, 3094.901, 3110.0811, 3183.2719

Compound: $MeCHCH_2 + O_3$ TS_{EPOX} 2.4	**Energy (kJ mol^{-1}):** -342.928697425059
Reaction Coordinates: 6 -1.666830 -0.989808 0.197115 6 -1.098744 0.196731 -0.450311 6 -0.485261 1.314852 0.272052 1 -0.483094 1.193098 1.359517 1 -0.907821 2.295956 0.023029 1 -1.136147 0.298970 -1.526126 1 -1.137526 -1.237058 1.116400 1 -2.692684 -0.710039 0.499230 1 -1.727998 -1.856055 -0.454462 8 0.790343 1.169754 -0.297898 8 1.449696 -0.320871 0.486130 8 1.208745 -1.238324 -0.329571	**Frequencies (cm^{-1}):** -443.6144, 65.4392, 137.6475, 218.3967, 247.7296, 351.5253, 382.7625, 407.8247, 475.0785, 699.9707, 881.1373, 927.2014, 958.212, 1032.4886, 1122.6276, 1184.4346, 1238.1183, 1280.1881, 1297.0164, 1369.8806, 1418.1876, 1440.5792, 1458.7186, 1483.9871, 2917.021, 2979.2809, 3032.3658, 3075.2598, 3144.9878, 3202.5677
IRC  	

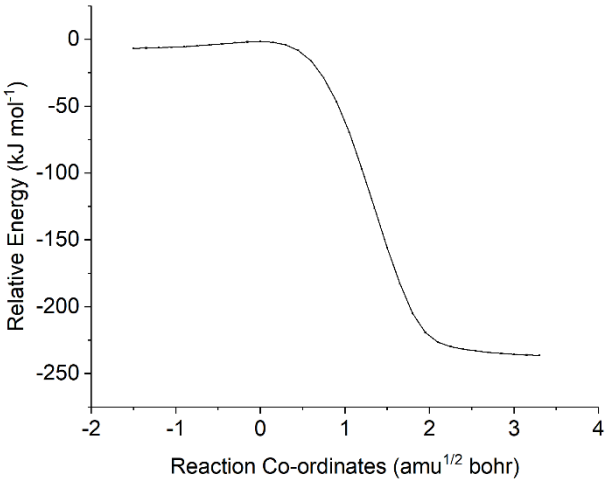
Compound: $MeCHCH_2 + O_3$ C_{EPOX} 2.4	**Energy (kJ mol^{-1}):** -343.029307044133
Reaction Coordinates: 6 1.433661 1.420098 0.157776 6 1.575944 0.003105 -0.316831 6 1.165124 -1.148303 0.489058 1 0.721361 -0.981024 1.464760 1 1.644825 -2.111088 0.351837 1 2.352034 -0.166597 -1.058609 1 0.630995 1.505919 0.888676 1 2.365153 1.759272 0.615041 1 1.208914 2.083680 -0.678487 8 0.363265 -0.711534 -0.616745	**Frequencies (cm^{-1}):** 17.8645, 47.078, 59.583, 85.3431, 148.5701, 207.7645, 368.7, 411.5208, 763.5696, 836.1884, 908.1741, 971.1267, 1043.617, 1127.3473, 1156.0878, 1168.4814, 1191.6137, 1292.7872, 1407.3048, 1437.8474, 1482.9579, 1498.0797, 1526.5915, 1576.3728, 3030.8861, 3086.7625, 3087.1007, 3094.0738, 3116.7155, 3171.8456

8 -1.866126 0.021292 0.488935 8 -2.743595 0.222797 -0.317594	

6.4 Ozonolysis of 1-butene (Alkene 2)

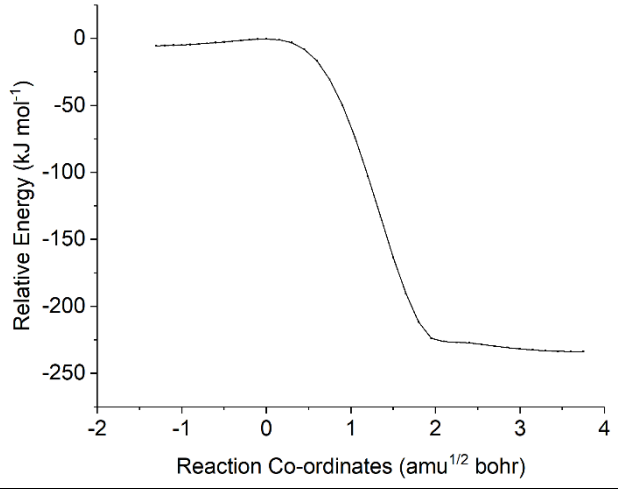
Compound: $EtCHCH_2 + O_3$ PRC1.1	**Energy (kJ mol^{-1}):** -382.230525502064
Reaction Coordinates: 6 -1.630533 -0.283798 -0.487614 6 -0.817910 0.450015 0.531206 6 -0.158363 1.591715 0.313309 1 0.397505 2.085402 1.098787 1 -0.177762 2.080236 -0.652450 1 -0.802016 0.018866 1.528307 1 -1.573144 0.236659 -1.445564 1 -1.186508 -1.271775 -0.640964 6 -3.095701 -0.455801 -0.065475 1 -3.587170 0.510387 0.054068 1 -3.172059 -0.988424 0.884063 1 -3.648243 -1.026577 -0.812353 8 2.158409 0.444344 -0.765220 8 2.348457 -0.356707 0.191122 8 1.488688 -1.269832 0.353793	**Frequencies (cm^{-1}):** 34.8339, 52.3655, 65.9584, 83.5563, 92.9886, 161.968, 227.1799, 266.4111, 335.1609, 436.6102, 656.9583, 741.9062, 795.9895, 859.8372, 957.6317, 991.829, 1012.5774, 1024.1559, 1093.5321, 1164.0568, 1193.1405, 1203.3832, 1288.523, 1321.5176, 1343.3053, 1410.0117, 1459.5007, 1484.6247, 1498.7092, 1507.23, 1663.4004, 3016.5505, 3026.5198, 3053.5385, 3088.1504, 3093.1286, 3123.3646, 3135.6188, 3218.3977

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -382.221047574187
Reaction Coordinates: 6 -1.538579 -0.373826 -0.433901 6 -0.569324 0.255682 0.514995 6 0.122688 1.400418 0.244280 1 0.674544 1.920171 1.012754 1 -0.011181 1.918302 -0.694751 1 -0.566953 -0.124072 1.529990 1 -1.361180 0.007638 -1.440851 1 -1.357647 -1.449767 -0.466709 6 -2.997624 -0.121693 -0.023701 1 -3.232361 0.943128 -0.027567 1 -3.197435 -0.504462 0.978389 1 -3.678318 -0.621194 -0.713484 8 2.033050 0.557152 -0.602040 8 2.143735 -0.434807 0.211468 8 1.151660 -1.253999 0.142095	**Frequencies (cm^{-1}):** -186.9921, 54.9005, 76.5792, 142.2443, 210.6562, 232.5778, 262.8272, 411.6885, 432.19, 478.1984, 714.0718, 747.067, 794.6543, 861.8132, 955.4058, 987.4069, 1002.5004, 1015.5685, 1082.7432, 1087.4429, 1114.8814, 1203.9886, 1284.0831, 1304.8381, 1339.2164, 1409.0095, 1455.9482, 1489.2505, 1498.4093, 1509.5707, 1586.0963, 3027.8581, 3034.8293, 3065.9934, 3092.126, 3096.2226, 3151.4553, 3155.197, 3243.0157
IRC:	



Compound: $EtCHCH_2 + O_3$ POZ1.1	**Energy (kJ mol^{-1}):** -382.319943476474
Reaction Coordinates: 6 -1.504470 -0.525361 -0.399433 6 -0.230572 -0.245440 0.381137 6 0.440859 1.133954 0.123839 1 0.533128 1.709240 1.046655 1 -0.069143 1.719758 -0.639727 8 1.723752 0.812806 -0.405419 8 1.992878 -0.467463 0.207223 8 0.771985 -1.172593 -0.052943 1 -0.396593 -0.373982 1.454649 1 -1.316340 -0.328687 -1.456880 1 -1.731671 -1.589510 -0.311050 6 -2.692381 0.297014 0.100263 1 -2.514752 1.369409 0.001653 1 -3.589153 0.060618 -0.471490 1 -2.905019 0.090152 1.150457	**Frequencies (cm^{-1}):** 68.6128, 108.3092, 198.6264, 238.6002, 373.725, 400.4181, 438.3137, 687.4325, 714.0783, 740.3368, 798.552, 849.5255, 926.8129, 963.3562, 980.875, 991.108, 1015.8819, 1066.249, 1146.141, 1176.6836, 1234.4693, 1289.8072, 1317.1576, 1350.708, 1365.2287, 1402.6174, 1420.9226, 1492.1014, 1503.5637, 1507.7334, 1512.2073, 3012.9544, 3027.309, 3034.9297, 3039.3954, 3064.1211, 3088.5102, 3098.2701, 3101.9917

Compound: $EtCHCH_2 + O_3$ PRC1.2	**Energy (kJ mol^{-1}):** -382.230906391601
Reaction Coordinates: 6 1.767471 -0.594112 -0.456608 6 0.846397 0.471600 -0.967277 6 0.427271 1.550464 -0.297606 1 -0.227650 2.275577 -0.760757 1 0.743788 1.760789 0.714088 1 0.519284 0.344256 -1.994507 1 1.256026 -1.556009 -0.564209 1 2.624080 -0.652528 -1.137801 6 2.256393 -0.430501 0.978654 1 1.423014 -0.419772 1.681525 1 2.818708 0.495485 1.108062 1 2.912644 -1.256634 1.252351 8 -1.702680 0.339272 1.064797 8 -2.222647 -0.160325 0.028660 8 -1.556559 -1.050931 -0.573674	**Frequencies (cm^{-1}):** 35.6908, 48.5383, 74.4002, 89.8883, 105.4143, 203.3659, 256.2881, 271.5581, 288.8633, 547.3533, 572.4638, 741.9925, 800.6366, 838.3618, 954.8439, 998.1469, 1019.4682, 1033.0241, 1107.0148, 1147.9657, 1163.3939, 1191.5189, 1294.2422, 1329.206, 1382.8584, 1412.5565, 1453.5151, 1469.1815, 1500.7741, 1510.7445, 1661.5009, 2998.8943, 3020.446, 3031.8002, 3089.8524, 3096.7225, 3130.3167, 3147.8487, 3227.611

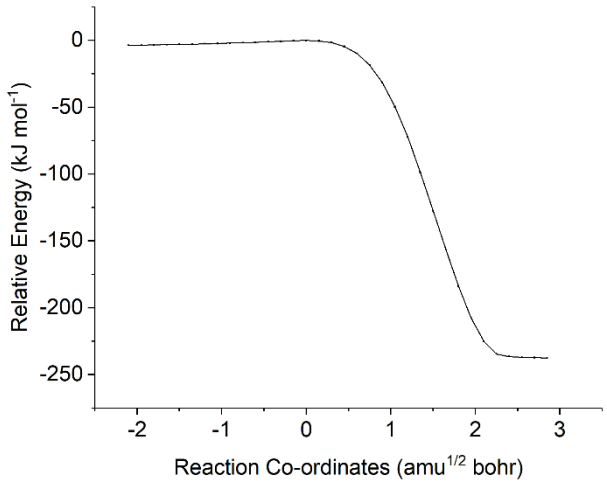
Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -382.221276651576
Reaction Coordinates: 6 -1.712962 -0.533934 0.383261 6 -0.536592 0.149186 1.011613 6 -0.001738 1.339207 0.605554 1 0.732251 1.849827 1.209861 1 -0.423885 1.896673 -0.216067 1 -0.208465 -0.259898 1.959088 1 -1.473913 -1.596028 0.288575 1 -2.539491 -0.490237 1.102413 6 -2.167224 0.015088 -0.965669 1 -1.357160 -0.014443 -1.694061 1 -2.517082 1.045457 -0.887553 1 -2.992067 -0.580889 -1.355624 8 1.600670 0.643595 -0.803980 8 1.996373 -0.365597 -0.106980 8 1.064320 -1.236466 0.084062	**Frequencies (cm^{-1}):** -201.5674, 68.1783, 75.7968, 171.7182, 217.2814, 264.1829, 282.1966, 360.9185, 454.9815, 549.9239, 662.3059, 741.6828, 799.7036, 836.2231, 956.5864, 991.1374, 1005.9099, 1030.4454, 1080.9974, 1097.9025, 1117.3764, 1149.1535, 1290.9145, 1306.2081, 1384.2254, 1412.8333, 1449.7188, 1467.687, 1502.4339, 1511.2094, 1584.0667, 2996.9013, 3033.3241, 3039.7643, 3091.504, 3103.3231, 3159.5234, 3166.6355, 3252.5972
IRC:  	

Compound: $EtCHCH_2 + O_3$ POZ1.2	**Energy (kJ mol^{-1}):** -382.319409856411
Reaction Coordinates: 6 -1.671383 -0.182012 0.556324 6 -0.164756 -0.219936 0.788165 6 0.628399 1.087394 0.502234 1 1.180480 1.407435 1.387717 1 0.007863 1.899676 0.129414 8 1.518475 0.741033 -0.552767 8 1.755705 -0.659398 -0.293450 8 0.418696 -1.154957 -0.128843 1 0.045874 -0.545944 1.809935 1 -2.067838 -1.172352 0.790852 1 -2.094352 0.494503 1.304166 6 -2.112007 0.230650 -0.847219 1 -1.715061 -0.448552 -1.599170 1 -3.199695 0.217004 -0.917000 1 -1.781807 1.238230 -1.102464	**Frequencies (cm^{-1}):** 65.1323, 98.7274, 200.7239, 263.5289, 320.1656, 390.3531, 544.6024, 677.8918, 725.6788, 741.3978, 780.5397, 818.4099, 925.8984, 942.846, 962.1285, 996.4387, 1010.3064, 1096.9266, 1126.9136, 1156.0492, 1228.1477, 1298.0739, 1338.4963, 1354.7237, 1366.2583, 1400.8007, 1425.8291, 1484.1072, 1495.1786, 1507.9826, 1514.3224, 3015.519, 3028.5272, 3038.9265, 3043.2625, 3054.2167, 3092.8109, 3111.6942, 3115.7622

Compound: $EtCHCH_2 + O_3$ PRC1.3	**Energy (kJ mol^{-1}):** -382.228599800530
Reaction Coordinates: 6 -2.130347 0.202561 -0.259217 6 -1.068762 0.848588 0.576226 6 -0.227477 1.795396 0.158017 1 0.493447 2.249035 0.824237 1 -0.253661 2.168164 -0.858187 1 -1.016379 0.523041 1.611897 1 -3.106984 0.538012 0.108359 1 -2.049004 0.554764 -1.289562 6 -2.094436 -1.329642 -0.217914 1 -2.196083 -1.696756 0.804883 1 -1.153952 -1.708552 -0.615361 1 -2.911121 -1.750322 -0.805266 8 2.052280 0.360976 -0.814691 8 2.222685 -0.342675 0.215684 8 1.390019 -1.265652 0.433548	**Frequencies (cm^{-1}):** 23.0789, 43.8839, 49.2668, 59.765, 84.0331, 149.3418, 213.395, 231.6386, 318.2882, 439.6973, 649.9411, 742.7602, 797.2015, 857.7105, 956.8765, 994.2985, 1016.1967, 1029.7659, 1095.4383, 1172.6715, 1202.4061, 1204.4995, 1291.3919, 1323.8675, 1344.3324, 1411.4945, 1459.5393, 1479.6798, 1498.2473, 1508.1073, 1672.1468, 2993.2549, 3030.2285, 3048.7193, 3087.9893, 3107.3691, 3118.4952, 3134.2576, 3216.6013

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -382.220877506051
Reaction Coordinates: 6 -1.649715 0.465644 -0.434184 6 -0.537339 0.773639 0.522467 6 0.496938 1.610163 0.236390 1 1.190992 1.926638 1.000131 1 0.557914 2.116167 -0.716831 1 -0.651302 0.421193 1.541098 1 -2.281738 1.357365 -0.517668 1 -1.224181 0.305159 -1.427546 6 -2.513638 -0.724773 -0.023055 1 -2.968880 -0.559415 0.955277 1 -1.922368 -1.637756 0.031829 1 -3.318922 -0.884845 -0.739860 8 2.037598 0.144752 -0.598616 8 1.819320 -0.825642 0.213165 8 0.623207 -1.293178 0.143433	**Frequencies (cm^{-1}):** -151.4348, 66.5451, 72.7259, 135.018, 184.6745, 231.8333, 299.451, 336.152, 443.7817, 466.5845, 641.355, 740.5878, 794.0563, 854.1417, 959.481, 986.8413, 1001.663, 1048.5826, 1093.4344, 1095.0729, 1120.7129, 1189.02, 1289.7741, 1307.1898, 1340.1493, 1417.2828, 1458.2862, 1462.7855, 1500.0279, 1506.4582, 1593.2837, 2995.0998, 3031.3143, 3044.8711, 3089.5667, 3108.3985, 3149.9663, 3153.2702, 3241.6098

IRC:



Compound: $EtCHCH_2 + O_3$ POZ1.3	**Energy (kJ mol^{-1}):** -382.320341440266
Reaction Coordinates: 6 -1.508790 0.629419 -0.257676 6 -0.221171 0.211465 0.431242 6 1.001698 1.137758 0.183797 1 1.361927 1.572940 1.117838 1 0.798603 1.919519 -0.546997 8 1.986854 0.287469 -0.397164 8 1.624374 -1.010790 0.128621 8 0.214659 -1.039123 -0.117651 1 -0.375765 0.090394 1.507336 1 -1.767424 1.626656 0.108450 1 -1.311502 0.724308 -1.327945 6 -2.671807 -0.330536 -0.011437 1 -2.884976 -0.425536 1.054865 1 -3.577316 0.027236 -0.501398 1 -2.450214 -1.324605 -0.398156	**Frequencies (cm^{-1}):** 65.2954, 115.3709, 199.6292, 237.2257, 358.9284, 388.1195, 460.5116, 671.0041, 727.5271, 748.2662, 780.3189, 850.9964, 928.8021, 952.2661, 985.2885, 999.3279, 1014.839, 1078.7281, 1134.1059, 1173.6122, 1230.9585, 1303.126, 1332.7172, 1338.3592, 1362.5094, 1408.7121, 1419.7459, 1478.2041, 1500.0585, 1507.1522, 1511.7475, 3012.9483, 3022.6369, 3031.6265, 3037.112, 3058.7669, 3091.3823, 3099.8501, 3105.2803

Compound: $EtCHCH_2 + O_3$ PRC 2.1	**Energy (kJ mol^{-1}):** -382.229766660375
Reaction Coordinates: 6 1.685301 -0.305632 -0.496591 6 0.861220 0.432571 0.512355 6 0.184925 1.559275 0.278125 1 0.196250 2.033770 -0.695621 1 -0.384317 2.049707 1.054293 1 0.846041 0.012981 1.513944 6 3.155354 -0.439892 -0.076511 1 3.718331 -1.012405 -0.814241 1 3.624553 0.539327 0.023644 1 3.244660 -0.952350 0.882759 1 1.268379 -1.309131 -0.631056 1 1.617010 0.195583 -1.464413 8 -2.399302 0.574651 -0.482150 8 -2.096428 -0.646445 -0.392639 8 -1.685734 -1.057633 0.728093	**Frequencies (cm^{-1}):** 30.6697, 43.3188, 54.7551, 77.1034, 86.5672, 155.6428, 227.1418, 249.883, 333.6375, 435.6802, 659.5907, 742.7863, 797.815, 859.5351, 960.8561, 992.822, 1013.1985, 1024.2658, 1093.0287, 1168.7283, 1198.3471, 1202.9182, 1291.6098, 1321.6709, 1344.4412, 1409.6733, 1459.7266, 1483.9957, 1498.3309, 1506.7607, 1668.6475, 3005.0352, 3027.4241, 3048.3987, 3089.2462, 3094.1611, 3128.4813, 3135.03, 3224.5733

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -382.219503800034
Reaction Coordinates: 6 -1.462939 -0.494091 -0.325934 6 -0.566078 0.285518 0.586995 6 0.100146 1.414625 0.201979 1 0.588999 2.047408 0.925351 1 -0.002763 1.804812 -0.801195 1 -0.615149 0.049662 1.642512 1 -1.151867 -0.341502 -1.361697 1 -1.362830 -1.558946 -0.113835 6 -2.937108 -0.086645 -0.166508 1 -3.086262 0.963423 -0.419242 1 -3.277366 -0.235338 0.859314 1 -3.570312 -0.687515 -0.819889 8 2.120045 0.621501 -0.367062	**Frequencies (cm^{-1}):** -204.3484, 54.9709, 76.6521, 138.6429, 201.8572, 231.9775, 269.5435, 420.3311, 438.2748, 497.5519, 724.8427, 743.4985, 797.3091, 860.6013, 953.6243, 982.6006, 1003.3736, 1012.3355, 1078.8743, 1084.6019, 1109.3998, 1202.4471, 1282.6618, 1303.051, 1341.1662, 1407.4473, 1451.4457, 1491.5665, 1497.3453, 1510.6323, 1581.3824, 3028.0308, 3032.9149, 3069.6986, 3092.601, 3098.1658, 3153.276, 3164.6213, 3249.0501

8 1.808891 -0.626026 -0.462951 8 1.280243 -1.090280 0.618698	

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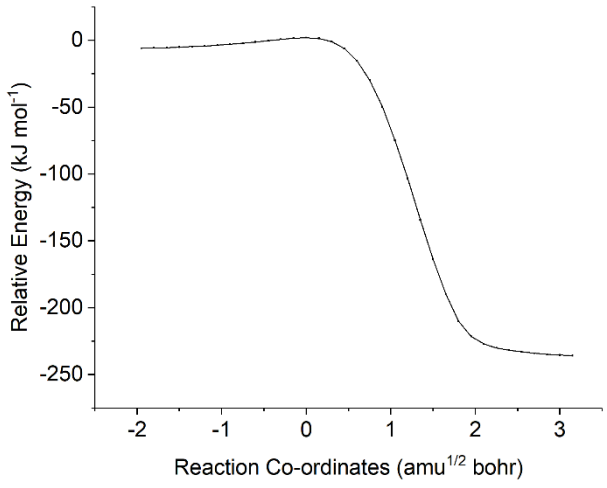
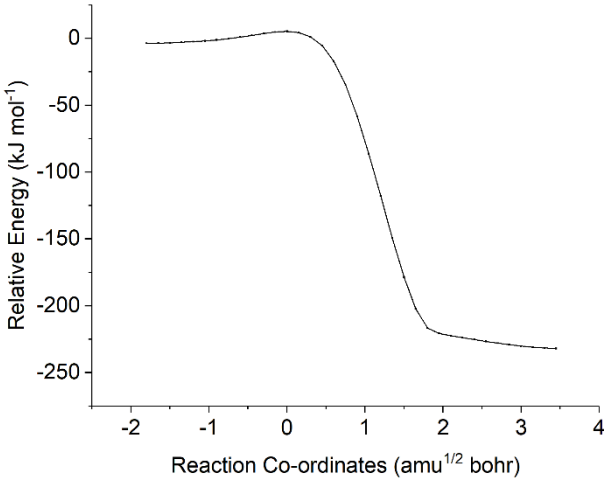


Compound: $EtCHCH_2 + O_3$ POZ 2.1	**Energy (kJ mol^{-1}):** -382.320300568466
Reaction Coordinates: 6 -1.434055 -0.592551 -0.314644 6 -0.231647 -0.199059 0.532914 6 0.432006 1.142453 0.112456 1 0.004090 1.510330 -0.822798 1 0.384944 1.911811 0.880344 8 1.805368 0.819846 -0.057236 8 1.721955 -0.527475 -0.551667 8 0.849333 -1.139157 0.421901 1 -0.490778 -0.195338 1.593421 1 -1.704203 -1.618325 -0.058681 1 -1.136431 -0.594912 -1.365442 6 -2.635931 0.327860 -0.097814 1 -2.953581 0.324298 0.946782 1 -3.483486 0.003596 -0.700886 1 -2.416036 1.360614 -0.374202	**Frequencies (cm^{-1}):** 82.5702, 118.0096, 203.5935, 237.0846, 358.3483, 418.328, 468.0392, 674.8196, 716.5394, 751.948, 795.5835, 847.7329, 918.1178, 950.7069, 979.6512, 990.3533, 1012.1364, 1057.8407, 1125.6752, 1176.028, 1238.8846, 1279.2342, 1312.0312, 1343.0749, 1356.7101, 1393.5814, 1419.1277, 1490.7329, 1503.3503, 1505.3105, 1509.5686, 3024.9742, 3031.4673, 3034.1999, 3048.4558, 3066.0854, 3087.8796, 3096.0377, 3114.5574

Compound: $EtCHCH_2 + O_3$ PRC 2.2	**Energy (kJ mol^{-1}):** -382.229362194436
Reaction Coordinates: 6 -1.854147 -0.561921 0.487839 6 -0.896901 0.510766 0.916176 6 -0.446851 1.522350 0.169942 1 0.239654 2.250643 0.575869 1 -0.759969 1.668612 -0.854877 1 -0.561703 0.443682 1.946111 1 -1.373886 -1.532644 0.653537 1 -2.701616 -0.552449 1.182586 6 -2.365624 -0.478324 -0.946845 1 -1.549527 -0.536688 -1.668271 1 -2.902263 0.454360 -1.125737 1 -3.050568 -1.300214 -1.155002	**Frequencies (cm^{-1}):** 30.9161, 36.703, 68.0854, 73.3323, 92.3649, 195.1418, 241.5331, 265.5029, 279.191, 547.9026, 574.4011, 742.4574, 801.4713, 837.1697, 957.7929, 999.0433, 1022.663, 1032.4371, 1106.6463, 1147.2995, 1169.2825, 1198.5046, 1291.7927, 1330.4384, 1381.0894, 1414.1438, 1455.4124, 1472.9456, 1500.424, 1509.1558, 1668.3891, 2997.8741, 3010.6237, 3031.0017,

8 2.008382 0.479814 -0.921559 8 1.912518 -0.653404 -0.376326 8 1.834228 -0.682977 0.883274	3089.0505, 3094.0824, 3135.1185, 3149.6993

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -382.218900812696
Reaction Coordinates: 6 -1.700854 -0.267542 0.541592 6 -0.537533 0.628918 0.857918 6 0.052496 1.499472 -0.019713 1 0.744061 2.245718 0.336053 1 -0.301979 1.607511 -1.033395 1 -0.295233 0.728926 1.907732 1 -1.525354 -1.239065 1.007379 1 -2.572874 0.144704 1.063725 6 -2.032566 -0.449937 -0.937745 1 -1.184956 -0.852350 -1.492778 1 -2.326632 0.490000 -1.406418 1 -2.863355 -1.145779 -1.052250 8 1.812373 0.368266 -0.757857 8 1.451309 -0.811979 -0.377848 8 1.190951 -0.861929 0.887911	**Frequencies (cm^{-1}):** -235.593, 55.1677, 79.6926, 172.9339, 203.8574, 257.8951, 284.5879, 383.6153, 471.2708, 557.969, 680.7842, 741.3744, 800.658, 831.2277, 952.4826, 987.3973, 1010.9764, 1029.0652, 1072.7843, 1094.9067, 1113.4809, 1148.7725, 1288.3515, 1301.8287, 1381.368, 1414.1937, 1447.0297, 1471.9504, 1503.1831, 1508.9876, 1576.4679, 2992.2243, 3034.4174, 3050.2089, 3093.6289, 3099.8519, 3167.942, 3170.4636, 3258.7538
IRC:  	

Compound: $EtCHCH_2 + O_3$ POZ 2.2	**Energy (kJ mol^{-1}):** -382.319190983776
Reaction Coordinates: 6 1.636123 0.462232 0.356338 6 0.151317 0.554586 0.703371 6 -0.758631 1.089353 -0.434513 1 -0.218881 1.147799 -1.381044 1 -1.211852 2.050003 -0.198233 8 -1.819804 0.147330 -0.513469 8 -1.139392 -1.077104 -0.193864 8 -0.439136 -0.718170 1.019424 1 0.020095 1.150096 1.607856 1 1.973745 1.471127 0.096330 1 2.172025 0.190794 1.268171 6 1.997444 -0.522261 -0.754937 1 1.546792 -0.255221 -1.710826	**Frequencies (cm^{-1}):** 84.6723, 107.9295, 209.6912, 261.2108, 320.3458, 403.9985, 555.3593, 665.3836, 714.7415, 749.1073, 789.2843, 816.6065, 915.1655, 941.9277, 958.0387, 1003.6401, 1013.0747, 1090.8281, 1117.156, 1150.3434, 1233.0562, 1280.2428, 1335.004, 1342.314, 1360.5873, 1398.1213, 1424.6931, 1482.7604, 1495.8028, 1506.0249, 1512.4485, 3009.8762, 3038.9152, 3044.8776, 3049.2336, 3059.6143, 3095.1818, 3110.9134, 3114.273

1 3.078082 -0.544915 -0.896658 1 1.669138 -1.529590 -0.503886	

Compound: $EtCHCH_2 + O_3$ PRC 2.3	**Energy (kJ mol^{-1}):** -382.228988543684
Reaction Coordinates: 6 -2.131443 0.231655 -0.280235 6 -1.049453 0.870700 0.534898 6 -0.185370 1.785553 0.092271 1 0.553197 2.228362 0.744144 1 -0.207099 2.135666 -0.932855 1 -0.998164 0.567888 1.576912 1 -3.098605 0.588003 0.092141 1 -2.056910 0.566625 -1.317073 6 -2.123682 -1.300570 -0.214677 1 -2.216344 -1.649370 0.815015 1 -1.197151 -1.708807 -0.618202 1 -2.955083 -1.716447 -0.784484 8 2.354289 0.442990 -0.468242 8 1.899856 -0.726071 -0.343496 8 1.385335 -1.033911 0.765595	**Frequencies (cm^{-1}):** 22.6626, 35.4936, 53.5445, 64.8888, 88.374, 149.874, 218.031, 228.4202, 321.2589, 439.4355, 651.1886, 742.4998, 796.6083, 857.3987, 959.5339, 993.9451, 1016.2569, 1029.1111, 1094.0636, 1173.2198, 1201.7851, 1204.4696, 1290.3604, 1323.7089, 1343.7175, 1412.3911, 1460.481, 1480.1734, 1499.0118, 1504.5769, 1671.9808, 2995.1495, 3030.171, 3045.9941, 3090.4018, 3098.006, 3125.2871, 3133.9174, 3225.082

Compound: $EtCHCH_2 + O_3$ TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -382.220139501245
Reaction Coordinates: 6 -1.534308 0.433568 -0.513878 6 -0.507377 0.858345 0.492953 6 0.577161 1.620722 0.180637 1 1.224681 2.008935 0.950634 1 0.724259 2.000392 -0.821133 1 -0.722783 0.666394 1.536637 1 -2.116223 1.317975 -0.799207 1 -1.024252 0.116216 -1.428897 6 -2.480144 -0.659891 -0.024807 1 -3.018908 -0.340810 0.869317 1 -1.928168 -1.566415 0.221028 1 -3.219255 -0.904402 -0.787543 8 2.149087 0.055625 -0.316026 8 1.378618 -0.970535 -0.410096 8 0.690877 -1.186934 0.657339	**Frequencies (cm^{-1}):** -168.2698, 58.7495, 76.7611, 136.5375, 185.055, 236.4693, 290.742, 358.0783, 461.7294, 477.0377, 647.9795, 739.97, 794.9847, 854.4728, 955.3336, 984.3293, 1001.6007, 1049.8064, 1086.0975, 1093.3256, 1113.4519, 1189.4787, 1285.358, 1299.7608, 1338.7952, 1416.4246, 1455.5804, 1465.169, 1498.3143, 1508.3509, 1589.0042, 2991.8327, 3020.5171, 3031.9198, 3089.5066, 3106.1029, 3152.9313, 3162.6447, 3248.0556
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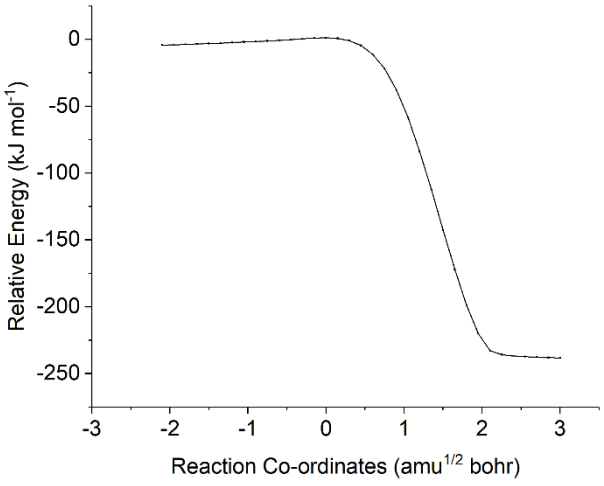

Compound: $EtCHCH_2 + O_3$ POZ 2.3	**Energy (kJ mol^{-1}):** -382.320843504655
Reaction Coordinates: 6 1.408035 0.534175 -0.433196 6 0.217196 0.312940 0.488041 6 -1.039479 1.131011 0.081841 1 -0.873489 1.648517 -0.865698 1 -1.363769 1.833508 0.847062 8 -2.071410 0.161535 -0.045729 8 -1.333186 -0.987149 -0.501395 8 -0.262413 -1.042222 0.462805 1 0.489293 0.488747 1.530378 1 1.111022 0.256084 -1.447162 1 1.622627 1.607498 -0.453342 6 2.652953 -0.240665 -0.009066 1 2.456984 -1.312432 0.009838 1 3.476830 -0.061680 -0.699891 1 2.984349 0.057675 0.987653	**Frequencies (cm^{-1}):** 77.9942, 120.7532, 201.9758, 243.3015, 357.8386, 389.9929, 493.3642, 683.9226, 709.8102, 736.2562, 798.7846, 845.2126, 917.3025, 951.4054, 969.1676, 1008.2779, 1014.6077, 1067.6618, 1114.4308, 1171.2805, 1238.0894, 1288.0406, 1300.1652, 1342.4949, 1360.94, 1399.2376, 1417.3, 1477.7868, 1499.8086, 1505.8782, 1508.0937, 3011.6614, 3028.7019, 3032.2436, 3044.6618, 3061.7501, 3088.8055, 3102.6517, 3112.0209

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -382.288435179066
Reaction Coordinates: 6 1.587555 -0.637953 -0.270134 6 0.212007 -0.388776 0.277428 6 -0.517248 1.298246 -0.207860 1 -0.154166 1.380884 -1.243624 1 0.071282 1.862109 0.531919 1 0.086226 -0.273544 1.350028 1 1.898083 -1.634092 0.060435 1 1.537484 -0.670872 -1.359333 6 2.617885 0.391514 0.196232 1 2.658544 0.448510 1.284864 1 3.609766 0.113804 -0.157132 1 2.396951 1.387143 -0.186792 8 -1.761525 1.170027 -0.001130 8 -1.927157 -0.880085 0.263091 8 -0.749489 -1.113958 -0.293756	**Frequencies (cm^{-1}):** -434.0304, 75.6953, 147.5764, 183.594, 224.0216, 292.1293, 353.3707, 419.8875, 490.1163, 523.8618, 605.4591, 783.5479, 852.3054, 927.0852, 1003.563, 1029.483, 1055.1412, 1116.9828, 1161.7934, 1181.4548, 1224.4051, 1252.5473, 1302.1954, 1332.5051, 1393.2667, 1414.6061, 1427.3964, 1481.6291, 1504.2286, 1508.2415, 1543.6663, 2910.6113, 2972.0186, 3015.5485, 3038.2162, 3067.72, 3100.3525, 3108.6845, 3124.3699

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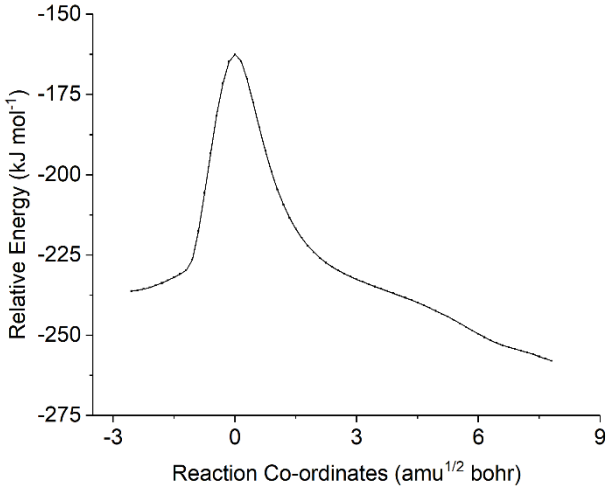

Compound: $EtCHCH_2 + O_3$ C_{ANTI} 1	**Energy (kJ mol^{-1}):** -382.327414870490
Reaction Coordinates: 6 1.843116 -0.591495 -0.106239 6 0.444781 -0.643042 0.373716 1 0.139883 -0.271908 1.344490 8 -0.425720 -1.210164 -0.333197 8 -1.729254 -1.160568 0.144151 1 2.424929 -1.275924 0.522807 1 1.883765 -0.969697 -1.127010 6 2.439931 0.820739 -0.002034 1 2.412401 1.185460 1.024438 1 3.478628 0.802260 -0.328420 1 1.883143 1.520213 -0.620722 6 -1.963460 1.088778 -0.082899 1 -2.610212 1.038337 0.803492 1 -2.453896 0.898097 -1.046584 8 -0.813132 1.498643 -0.019425	**Frequencies (cm^{-1}):** 53.1664, 78.9036, 95.3849, 127.9186, 199.3209, 225.5953, 301.9227, 329.7278, 355.6831, 435.7429, 541.6656, 557.1088, 779.185, 916.4365, 922.6306, 936.7791, 1024.1576, 1095.0425, 1151.2462, 1184.8295, 1252.3289, 1274.1252, 1326.8585, 1372.4759, 1420.4265, 1466.6476, 1496.2997, 1505.7345, 1511.6516, 1570.3404, 1699.5236, 2953.0824, 2998.9893, 3016.5501, 3047.2738, 3088.2774, 3111.2552, 3132.6541, 3182.4676

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -382.288487214481
Reaction Coordinates: 6 1.659253 0.181981 0.651277 6 0.182166 -0.094199 0.672300 6 -0.864046 1.292519 -0.066820 1 -0.231108 1.605286 -0.909508 1 -0.796177 1.940074 0.821030 1 -0.318812 -0.118208 1.634803 1 1.801261 1.196201 1.031760 1 2.129537 -0.477073 1.388228 6 2.341100 0.017274 -0.706474 1 1.897220 0.666523 -1.460604 1 3.396781 0.272644 -0.623856 1 2.268595 -1.007603 -1.066062 8 -1.982312 0.743625 -0.318351 8 -1.539077 -1.250146 -0.038180	**Frequencies (cm^{-1}):** -437.1696, 87.1471, 131.7377, 194.8405, 220.1672, 268.7754, 364.1744, 419.2462, 512.0625, 555.544, 642.733, 780.7455, 859.0935, 906.5766, 985.9784, 1037.189, 1059.6134, 1110.0781, 1139.7597, 1183.368, 1219.7462, 1262.7138, 1293.3588, 1377.5272, 1386.2681, 1398.4668, 1430.0063, 1478.4616, 1500.0669, 1507.1304, 1543.9012, 2914.596, 2977.6132, 3013.7009, 3045.7768, 3050.3427, 3106.0962, 3115.1249, 3129.1534

8 -0.235878 -1.051391 -0.158154	

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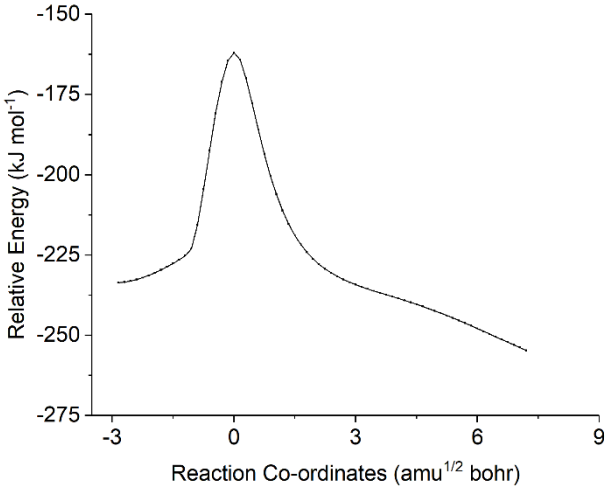

Compound: $EtCHCH_2 + O_3$ C_{ANTI} 2	**Energy (kJ mol^{-1}):** -382.328011970473
Reaction Coordinates: 6 -1.755577 -0.445704 0.572883 6 -0.420233 0.171306 0.724077 1 0.202463 -0.003937 1.591673 8 -0.007795 0.991083 -0.134147 8 1.303864 1.426479 0.030106 1 -1.593733 -1.523630 0.678597 1 -2.342470 -0.159618 1.454188 6 -2.496093 -0.121325 -0.719737 1 -1.922202 -0.441577 -1.587747 1 -3.455146 -0.636532 -0.734751 1 -2.682059 0.947404 -0.815607 6 2.234231 -0.597799 -0.325639 1 3.000035 -0.305728 0.405386 1 2.419669 -0.291318 -1.363267 8 1.328865 -1.370554 -0.038206	**Frequencies (cm^{-1}):** 50.0336, 82.8265, 98.5641, 139.8074, 195.5855, 219.4728, 312.8821, 322.6917, 353.1724, 447.2378, 565.8749, 626.9306, 739.932, 897.8154, 928.2548, 931.7204, 1027.8774, 1105.2947, 1125.4762, 1151.0374, 1251.5156, 1278.9729, 1350.4671, 1392.6685, 1423.7201, 1440.7971, 1499.9997, 1504.8281, 1509.239, 1572.3312, 1692.315, 2954.8476, 3002.3246, 3018.4074, 3031.757, 3049.2372, 3113.5535, 3117.2996, 3190.2494

Compound: $EtCHCH_2 + O_3$ TS_{ANTI} 3	**Energy (kJ mol^{-1}):** -382.289183739601
Reaction Coordinates: 6 -1.545335 -0.609861 -0.286742 6 -0.255296 -0.069809 0.251718 6 1.212363 -1.226087 -0.030727 1 0.976700 -1.609793 -1.034609 1 0.942455 -1.905010 0.793582 1 -0.135030 0.032524 1.326185 1 -1.502398 -0.601549 -1.376635 1 -1.624653 -1.653921 0.022398 6 -2.768403 0.172136 0.209604 1 -2.728957 1.210393 -0.118345 1 -3.683810 -0.272204 -0.180487 1 -2.829451 0.163127 1.298494 8 2.231101 -0.484774 0.118844	**Frequencies (cm^{-1}):** -426.1407, 72.9101, 138.5843, 183.0661, 219.8746, 268.0899, 346.7494, 459.651, 508.2332, 523.3521, 608.4241, 777.8767, 857.5223, 922.2455, 989.5744, 1023.7985, 1053.4144, 1129.407, 1159.8942, 1175.5114, 1220.2794, 1247.9129, 1308.0359, 1345.6354, 1391.6902, 1409.0356, 1427.4596, 1478.9227, 1499.4702, 1506.0657, 1543.4644, 2908.3518, 2969.9697, 3035.1435,

8 1.363557 1.404732 0.115508 8 0.245988 0.959812 -0.433565	3042.1514, 3076.1155, 3099.8787, 3107.8007, 3125.5084

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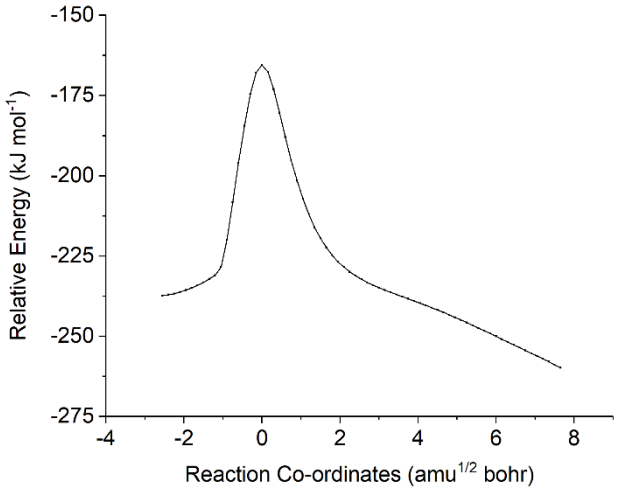
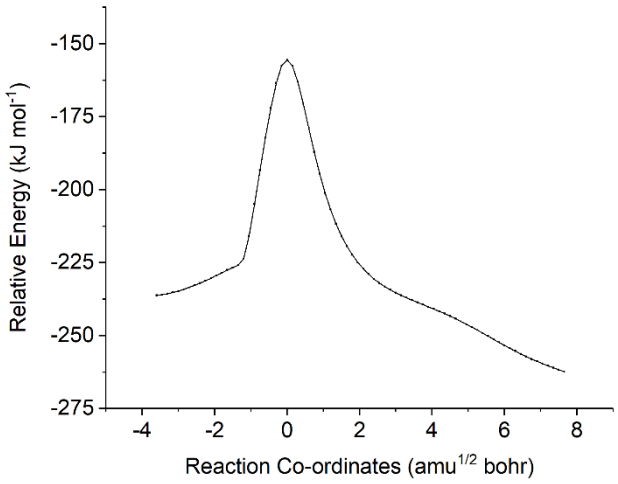


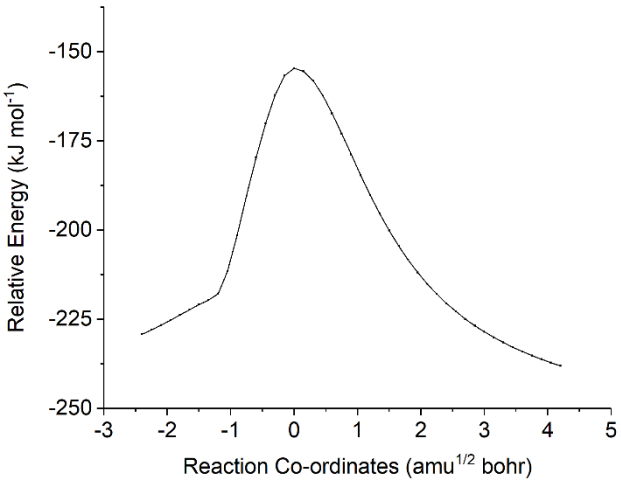
Compound: $EtCHCH_2 + O_3$ C_{ANTI} 3	**Energy (kJ mol^{-1}):** -382.326871850469
Reaction Coordinates: 6 1.682958 -0.376258 0.480233 6 0.478414 0.168596 -0.181204 1 0.202695 -0.081213 -1.197907 8 -0.218075 1.026178 0.419951 8 -1.395417 1.400440 -0.215688 1 1.766417 0.049307 1.479484 1 1.508398 -1.450676 0.592772 6 2.958300 -0.143078 -0.344184 1 3.173608 0.919880 -0.447576 1 3.807066 -0.614721 0.148639 1 2.869657 -0.572464 -1.342310 6 -2.363237 -0.631119 -0.075880 1 -2.836350 -0.404181 -1.040674 1 -2.897077 -0.277371 0.815657 8 -1.403136 -1.386295 0.010503	**Frequencies (cm^{-1}):** 51.1515, 66.648, 92.4584, 130.9317, 194.017, 208.92, 301.0918, 341.8677, 380.6756, 450.7932, 551.7221, 568.1698, 771.8888, 904.0266, 922.2135, 945.5875, 1022.4017, 1090.9935, 1150.018, 1184.417, 1251.413, 1272.135, 1327.7774, 1372.5887, 1418.121, 1468.3447, 1501.0234, 1505.4013, 1509.1729, 1568.4794, 1691.7973, 2954.917, 3018.8271, 3028.4212, 3040.1328, 3089.064, 3109.3343, 3111.5661, 3186.394

Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.1	**Energy (kJ mol^{-1}):** -382.286715066888
Reaction Coordinates: 6 1.430273 0.428141 -0.530970 6 0.313174 0.606204 0.496953 6 -0.634902 -1.014463 0.644438 1 0.035500 -1.863800 0.607104 1 -1.176311 -0.810951 1.559690 1 0.645912 0.547928 1.551081 1 0.998266 0.069531 -1.466329 1 1.805312 1.433304 -0.737928 6 2.578517 -0.464086 -0.067641 1 2.988791 -0.119827 0.884153	**Frequencies (cm^{-1}):** -439.9642, 73.5107, 123.9199, 197.9683, 238.1236, 296.9909, 335.888, 478.116, 506.3905, 581.9165, 606.1546, 780.8548, 842.1224, 893.1091, 953.5894, 1027.9135, 1048.2043, 1070.4783, 1124.7923, 1168.9999, 1222.7028, 1265.3405, 1283.8069, 1314.4639, 1346.4603, 1419.469, 1461.539, 1478.6197, 1481.5675, 1501.4491, 1504.7972,

1 3.390562 -0.457095 -0.794199 1 2.272042 -1.503845 0.060999 8 -1.342866 -0.893243 -0.473810 8 -2.159319 0.142811 -0.396169 8 -0.633122 1.421680 0.254823	2873.6851, 3024.9481, 3036.4129, 3064.2374, 3085.6938, 3094.9348, 3112.2787, 3230.1392
IRC:  	

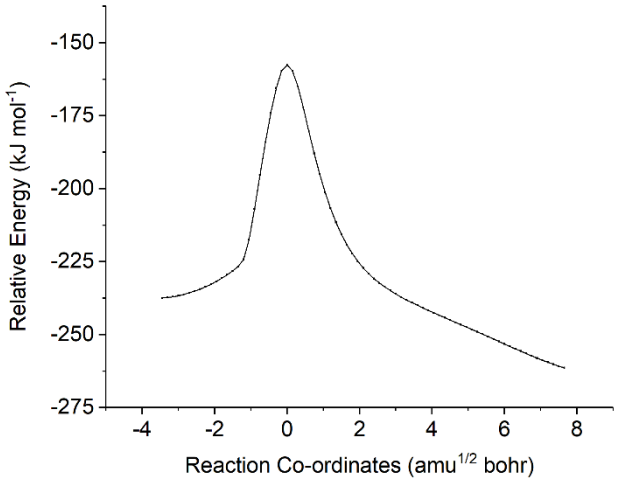
Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (kJ mol^{-1}):** -382.322960896800
Reaction Coordinates: 6 1.494273 -0.344190 -0.523841 6 1.422253 1.097645 -0.123270 1 2.404034 1.595192 0.019096 8 0.409876 1.737145 0.055801 1 1.983726 -0.368340 -1.505034 1 0.489418 -0.755936 -0.630550 6 2.332601 -1.162023 0.469615 1 1.850120 -1.202299 1.446027 1 2.443377 -2.183987 0.111109 1 3.331545 -0.741677 0.599234 6 -2.119883 0.748437 0.053993 1 -2.363421 1.499628 0.791643 1 -1.945866 0.953429 -0.993139 8 -2.060711 -0.425791 0.474275 8 -1.720215 -1.415757 -0.417246	**Frequencies (cm^{-1}):** 34.4786, 46.0728, 85.1184, 93.0153, 104.2227, 118.4669, 195.5732, 213.3356, 335.6695, 518.6634, 525.2046, 678.9695, 772.7089, 864.2354, 882.4815, 926.1092, 992.1537, 1005.1802, 1135.3161, 1171.588, 1235.5085, 1281.3139, 1348.2432, 1410.5303, 1413.6336, 1426.4816, 1479.1031, 1501.1103, 1505.8132, 1566.9118, 1773.7664, 2874.6532, 2995.7611, 3032.0021, 3066.2573, 3094.3015, 3109.391, 3132.972, 3276.9654

Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.2	**Energy (kJ mol^{-1}):** -382.286633762054
Reaction Coordinates: 6 -1.669419 -0.390400 0.329076 6 -0.327425 -1.002909 -0.084376 6 1.001530 -0.411284 1.082840 1 0.609067 -0.304648 2.087097 1 1.750780 -1.169851 0.892977 1 -0.210568 -2.052340 0.245868 1 -1.804013 -0.507487 1.407643 1 -2.432180 -1.023162 -0.136648	**Frequencies (cm^{-1}):** -431.625, 72.6385, 113.6497, 197.6924, 245.8676, 283.2265, 333.528, 494.8075, 519.3491, 599.6621, 675.4146, 789.6207, 798.1682, 904.8531, 958.3955, 1023.7223, 1046.5755, 1071.4018, 1104.8068, 1178.6738, 1220.4895, 1268.8971, 1291.6494, 1316.9868, 1349.2776,

6 -1.878597 1.057735 -0.101288 1 -1.192284 1.733355 0.408864 1 -2.895563 1.378306 0.125182 1 -1.713752 1.167345 -1.171700 8 1.243552 0.770668 0.519786 8 1.715580 0.608773 -0.702705 8 0.182366 -0.721986 -1.219180	1412.0758, 1462.3548, 1479.2253, 1488.4552, 1496.3595, 1508.5396, 2874.8741, 3008.9864, 3037.5066, 3042.1086, 3098.02, 3105.0916, 3114.9436, 3221.3521
IRC:  	

Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (kJ mol^{-1}):** -382.323347312587
Reaction Coordinates: 6 -2.143370 0.450045 0.362502 6 -1.676271 -0.975116 0.392088 1 -2.228098 -1.628750 1.097833 8 -0.781336 -1.439385 -0.275327 1 -2.076685 0.816305 1.394341 1 -3.220804 0.412340 0.157199 6 -1.409309 1.366318 -0.605344 1 -1.477623 0.989585 -1.626070 1 -1.846835 2.364064 -0.584346 1 -0.354608 1.453491 -0.343643 6 1.927570 -0.812155 -0.549178 1 2.088213 -1.873144 -0.423573 1 1.541445 -0.351449 -1.448276 8 2.206846 -0.102471 0.440087 8 1.997400 1.247232 0.357256	**Frequencies (cm^{-1}):** 27.7695, 46.0962, 56.3463, 84.5413, 97.9148, 139.1692, 167.3712, 247.6305, 261.9927, 521.5857, 662.647, 671.4475, 675.0085, 848.2526, 876.4525, 913.0698, 987.0925, 1009.638, 1115.4177, 1150.9914, 1238.9928, 1284.4164, 1369.5373, 1413.9423, 1415.5243, 1427.4129, 1444.7288, 1500.2482, 1516.5709, 1564.1745, 1783.0075, 2880.5873, 2995.9452, 3013.5071, 3032.9964, 3098.8361, 3101.6314, 3131.6207, 3276.7604

Compound: $EtCHCH_2 + O_3$ TS_{FO} 1.3	**Energy (kJ mol^{-1}):** -382.286982119882
Reaction Coordinates: 6 -1.384973 0.562988 -0.352627 6 -0.377448 -0.032768 0.625844 6 1.192010 0.993598 0.525410 1 0.953416 2.043977 0.410791 1 1.676826 0.658206 1.433644 1 -0.545509 0.245664 1.683675 1 -0.995771 0.447263 -1.364893	**Frequencies (cm^{-1}):** -424.932, 77.4893, 119.7766, 191.7724, 237.2637, 298.5403, 322.8331, 489.0463, 505.4911, 580.9748, 633.1193, 788.9526, 838.7947, 897.2929, 957.1657, 1009.0628, 1048.0401, 1076.4676, 1134.5701, 1165.2999, 1223.5572, 1267.8332,

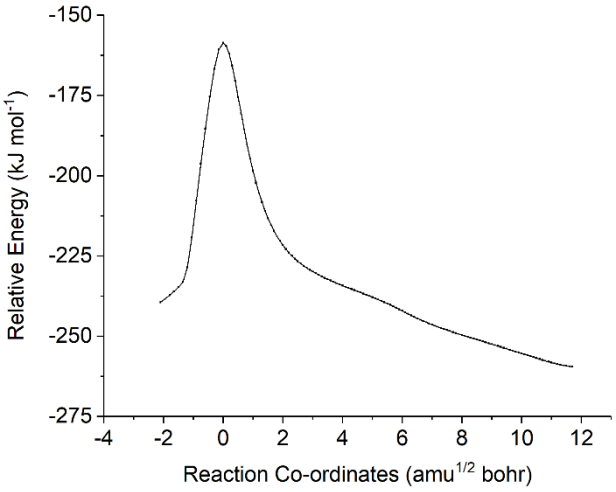
1 -1.500774 1.632356 -0.157284 6 -2.740661 -0.138092 -0.230040 1 -3.152188 -0.033546 0.775867 1 -3.460668 0.286794 -0.929765 1 -2.641004 -1.201781 -0.443789 8 1.668326 0.468690 -0.598820 8 1.951950 -0.810120 -0.430387 8 0.071236 -1.207732 0.426736	1288.9107, 1311.1114, 1355.2908, 1408.5138, 1467.9994, 1477.9073, 1481.9822, 1498.0798, 1505.6619, 2875.1948, 3022.0107, 3027.4968, 3071.0723, 3089.9051, 3105.1015, 3107.5291, 3225.5746
IRC:  	

Compound: $EtCHCH_2 + O_3$ CPr_{FO} 1.3	**Energy (kJ mol^{-1}):** -382.324741015052
Reaction Coordinates: 6 1.690299 -0.271686 -0.499951 6 0.717208 0.406541 0.422288 1 0.658832 -0.023362 1.438769 8 0.074983 1.399255 0.144480 1 1.639784 0.205032 -1.478686 1 1.367481 -1.309750 -0.605386 6 3.115162 -0.228054 0.069823 1 3.159076 -0.679739 1.062176 1 3.799203 -0.779180 -0.574592 1 3.479119 0.796760 0.149273 6 -2.412001 0.558882 -0.414034 1 -3.165813 1.266421 -0.096921 1 -1.817787 0.654924 -1.311459 8 -2.260816 -0.429976 0.335637 8 -1.287156 -1.334929 0.013392	**Frequencies (cm^{-1}):** 30.1604, 45.954, 81.5336, 95.3035, 147.8648, 188.3603, 214.9774, 217.4755, 363.5651, 509.4182, 524.9259, 676.2711, 776.3402, 876.5636, 889.8252, 921.666, 990.6525, 1002.4105, 1123.8642, 1162.4648, 1241.0283, 1270.7939, 1326.749, 1409.0759, 1415.1813, 1426.0621, 1473.3976, 1501.6345, 1505.7828, 1565.3267, 1751.1933, 2921.5946, 3030.7455, 3040.648, 3080.0986, 3099.3125, 3101.7129, 3132.2871, 3277.322

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.1	**Energy (kJ mol^{-1}):** -382.285727858044
Reaction Coordinates: 6 -1.618514 0.557145 -0.349981 6 -0.316079 0.542469 0.462769 6 0.505089 -1.097080 -0.057941 1 0.123052 -1.926393 0.523542 1 0.263850 -1.036333 -1.112195 1 -0.456725 0.295517 1.530484	**Frequencies (cm^{-1}):** -448.8384, 78.4755, 95.2102, 209.1631, 230.6325, 301.357, 379.0108, 463.2562, 495.4682, 541.6127, 599.2368, 770.3083, 863.1983, 886.8491, 973.744, 1022.3731, 1043.7217, 1062.7042, 1109.8577,

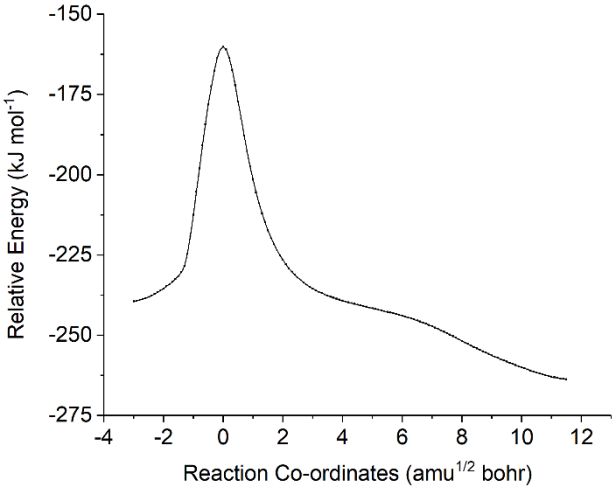
1 -2.080925 1.524470 -0.138895 1 -1.370482 0.564587 -1.412577 6 -2.598471 -0.560825 -0.004392 1 -2.791455 -0.598416 1.069596 1 -3.554966 -0.400594 -0.501329 1 -2.236929 -1.543321 -0.312432 8 1.756841 -0.809148 0.259922 8 2.190552 0.221640 -0.441849 8 0.586661 1.396287 0.188311	1180.2242, 1234.2499, 1264.8443, 1282.1637, 1332.1159, 1358.1025, 1418.3983, 1458.126, 1482.4169, 1485.6258, 1502.4556, 1506.1168, 2893.5197, 3026.2583, 3031.9729, 3062.6604, 3086.0261, 3094.0449, 3105.9157, 3227.6936

IRC:



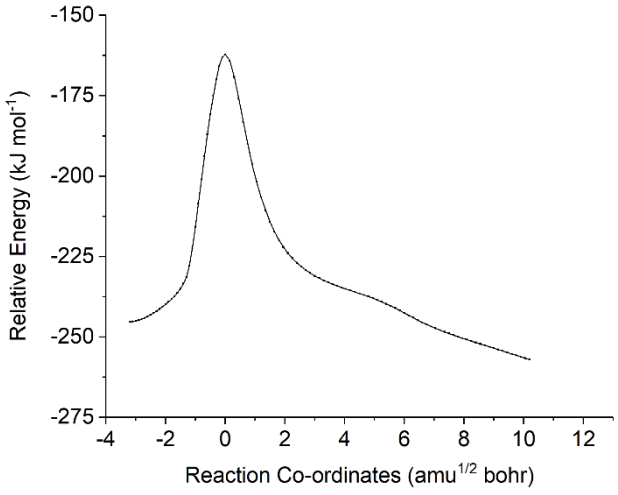
Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.1	**Energy (kJ mol^{-1}):** -382.319882014753
Reaction Coordinates: 6 3.100135 0.334385 -0.321039 6 1.626375 0.050355 -0.328125 1 1.339533 -0.938687 -0.740989 8 0.773504 0.803979 0.077677 1 3.417142 0.387282 -1.368841 1 3.269702 1.310668 0.131445 6 3.891702 -0.771625 0.389330 1 3.694880 -1.749138 -0.053250 1 3.633856 -0.821695 1.447183 1 4.961152 -0.581744 0.312327 6 -2.499820 0.672071 0.291620 1 -1.420404 0.748633 0.232645 1 -3.170302 1.439262 0.662170 8 -2.990701 -0.408999 -0.110362 8 -4.337292 -0.583192 -0.068991	**Frequencies (cm^{-1}):** 8.574, 14.6458, 29.6453, 57.9778, 68.5375, 91.1792, 100.5617, 212.5462, 329.69, 513.4695, 534.6844, 716.2997, 761.5634, 876.8402, 901.0774, 925.3868, 1000.3357, 1006.8919, 1136.6527, 1164.0504, 1252.4723, 1273.8152, 1329.2202, 1412.5385, 1416.8349, 1428.0329, 1466.8784, 1501.7927, 1506.0223, 1554.0107, 1788.3676, 2880.2464, 3008.2946, 3035.4159, 3084.2167, 3090.1533, 3102.8332, 3107.5848, 3241.9038

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.2	**Energy (kJ mol^{-1}):** -382.286060556534
Reaction Coordinates: 6 -1.724202 0.481397 -0.356216 6 -0.314432 0.124543 -0.865086 6 0.798931 1.085288 0.300072 1 0.883801 2.114736 -0.026101 1 0.272036 0.871095 1.221654	**Frequencies (cm^{-1}):** -439.3855, 81.5282, 103.8601, 185.656, 249.9298, 291.3336, 352.1234, 465.8166, 519.5706, 596.2634, 628.1544, 786.5274, 822.6682, 901.607, 974.009, 1019.9214, 1042.4958, 1068.4654, 1098.145,

1 -0.042473 0.650639 -1.796374 1 -1.781128 1.554233 -0.151653 1 -2.389409 0.304097 -1.206541 6 -2.192805 -0.338010 0.839238 1 -1.572489 -0.173978 1.722045 1 -2.157064 -1.402075 0.614987 1 -3.216043 -0.070814 1.103436 8 1.929386 0.416122 0.122558 8 1.784203 -0.841753 0.497432 8 0.111138 -1.070274 -0.743678	1180.6734, 1229.7018, 1264.0493, 1288.2701, 1329.2497, 1351.6901, 1414.9754, 1465.6484, 1479.2756, 1491.4379, 1495.3083, 1502.3192, 2903.0416, 3013.7327, 3033.7897, 3041.2551, 3088.0703, 3105.446, 3118.2012, 3222.6824
IRC:  	

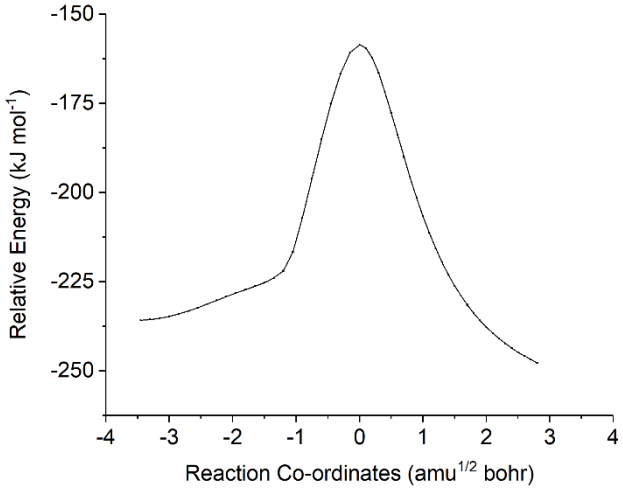
Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.2	**Energy (kJ mol^{-1}):** -382.322073512602
Reaction Coordinates: 6 2.633058 0.616289 -0.148968 6 2.342748 -0.856848 -0.175731 1 3.203424 -1.496240 -0.458344 8 1.277338 -1.363825 0.079930 1 3.005686 0.877513 -1.147139 1 3.500133 0.751900 0.508843 6 1.465181 1.499497 0.265979 1 1.758797 2.548438 0.262072 1 0.619458 1.382485 -0.410106 1 1.120852 1.247634 1.268438 6 -1.972442 -0.946911 0.241183 1 -2.781141 -1.620219 0.500213 1 -0.915803 -1.179874 0.266588 8 -2.261166 0.218933 -0.126858 8 -3.556507 0.596918 -0.188739	**Frequencies (cm^{-1}):** 17.4864, 24.5871, 38.4025, 52.8191, 79.9849, 109.927, 154.131, 235.7045, 254.1316, 537.152, 665.3932, 673.6723, 712.6024, 849.8849, 908.0474, 921.9476, 976.6018, 1007.0634, 1111.6093, 1149.4799, 1252.8649, 1283.2775, 1369.5684, 1409.9663, 1415.4914, 1427.9099, 1448.2734, 1498.4471, 1504.5696, 1544.9548, 1798.5572, 2886.0564, 3002.6774, 3019.1633, 3047.959, 3103.8004, 3110.2835, 3114.4077, 3259.3132

Compound: $EtCHCH_2 + O_3$ TS_{FO} 2.3	**Energy (kJ mol^{-1}):** -382.286281629323
Reaction Coordinates: 6 -1.550578 0.506450 0.377655 6 -0.378433 -0.064813 -0.429539 6 1.019875 1.115235 0.039352 1 0.962627 2.019681 -0.553893	**Frequencies (cm^{-1}):** -427.6269, 76.2639, 104.8845, 195.3002, 234.7553, 311.1044, 339.9104, 467.8435, 488.8197, 562.6578, 598.8786, 789.7228, 864.3865, 897.2137, 983.946, 1006.6296,

1 0.811665 1.167467 1.100901 1 -0.424881 0.166520 -1.508926 1 -1.356405 0.326843 1.436055 1 -1.619062 1.586881 0.222499 6 -2.863586 -0.160003 -0.038879 1 -2.828558 -1.231588 0.154590 1 -3.061167 -0.015177 -1.102511 1 -3.701968 0.263051 0.515418 8 2.052595 0.361364 -0.303770 8 2.082635 -0.743032 0.418888 8 0.096530 -1.201443 -0.109577	1054.1284, 1070.5482, 1120.9523, 1171.0366, 1231.0101, 1265.9809, 1290.7426, 1334.0374, 1362.9572, 1409.4332, 1459.9018, 1477.9161, 1483.4163, 1496.147, 1503.807, 2894.3577, 3016.0586, 3029.0684, 3068.197, 3089.5138, 3104.7318, 3105.673, 3224.62
IRC:  	

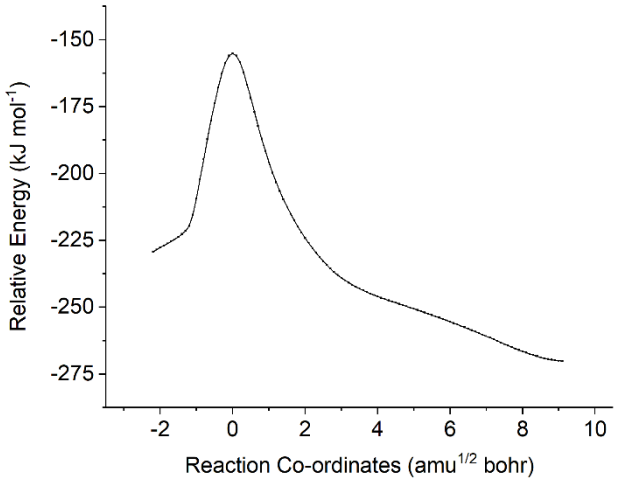
Compound: $EtCHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (kJ mol^{-1}):** -382.319253491307
Reaction Coordinates: 6 3.103895 -0.666554 0.000001 6 1.603232 -0.690025 -0.000060 1 1.150470 -1.701332 -0.000125 8 0.895512 0.289627 -0.000049 1 3.424521 -1.257896 -0.866269 1 3.424447 -1.257951 0.866260 6 3.728040 0.721365 0.000072 1 4.815026 0.651035 0.000117 1 3.421694 1.288371 -0.877987 1 3.421618 1.288315 0.878142 6 -2.352945 0.755007 -0.000071 1 -2.884957 1.699684 -0.000159 1 -1.275884 0.634474 -0.000052 8 -3.018767 -0.307060 0.000050 8 -4.375528 -0.240499 0.000052	**Frequencies (cm^{-1}):** 37.3724, 54.0953, 76.03, 86.588, 103.4856, 117.3332, 197.9561, 210.566, 335.3409, 518.5461, 522.1436, 677.9979, 759.5761, 865.3737, 882.7833, 925.194, 991.7934, 1008.9756, 1135.769, 1168.654, 1235.3345, 1282.2624, 1355.5913, 1411.607, 1413.5132, 1427.5967, 1472.7195, 1500.9884, 1506.0778, 1566.9298, 1773.9166, 2873.5664, 2994.791, 3031.4022, 3064.6244, 3092.3966, 3107.6809, 3133.3849, 3277.3626

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 1	**Energy (kJ mol^{-1}):** -382.288517541471
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.212418 -0.416797 -0.456320 6 -0.214385 -0.290017 0.668319 6 0.684875 1.321298 0.402284 1 -0.233412 1.897168 0.208361 1 1.133265 1.505873 1.388296 1 -0.603923 -0.295303 1.683584 1 -0.797639 0.010420 -1.366138 1 -1.323258 -1.489798 -0.645931 6 -2.563646 0.203725 -0.112345 1 -3.002224 -0.251537 0.777236 1 -2.483662 1.277510 0.064459 1 -3.262638 0.062516 -0.935736 8 1.450887 1.087897 -0.587106 8 1.449732 -1.003507 -0.568325 8 0.900248 -1.037652 0.632211	-440.1427, 89.2366, 158.5907, 198.5178, 239.5251, 291.054, 343.1318, 383.717, 523.8873, 567.0281, 708.8541, 786.3762, 871.0614, 905.1493, 950.24, 1021.9987, 1068.6957, 1080.919, 1150.3101, 1185.3924, 1214.2464, 1223.5968, 1283.3211, 1333.3493, 1378.3889, 1420.1614, 1431.9697, 1481.527, 1503.2818, 1504.4665, 1537.9293, 2919.6449, 2983.2082, 3016.75, 3029.4161, 3080.6706, 3100.0278, 3109.4595, 3122.3869
IRC  	

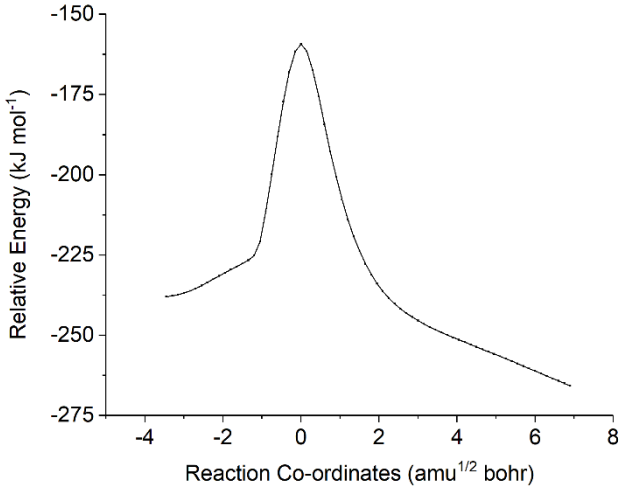
Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -382.327479598047
Reaction Coordinates: 6 -1.366405 0.090136 -0.469928 6 -0.726726 -0.590966 0.664619 1 -1.118208 -0.569233 1.677127 8 0.309198 -1.297525 0.566207 8 0.910221 -1.367103 -0.675054 1 -1.472711 -0.656888 -1.265588 1 -0.635787 0.801151 -0.867360 6 -2.685367 0.767733 -0.109194 1 -2.540772 1.536816 0.649970 1 -3.113514 1.247834 -0.987415 1 -3.417293 0.051275 0.265856 6 2.290668 0.765309 -0.203290 1 2.984526 0.095552 0.328432 1 2.380067 0.774490 -1.300849 8 1.513166 1.480344 0.384670	**Frequencies (cm^{-1}):** 51.2029, 74.5323, 90.7015, 93.9644, 138.2429, 201.8235, 207.701, 228.4531, 345.0508, 360.9387, 457.2332, 683.5288, 703.9688, 853.768, 876.7399, 936.3311, 1046.6932, 1107.6506, 1140.6115, 1173.3573, 1258.7894, 1259.6906, 1326.5811, 1378.6696, 1424.2028, 1426.1182, 1503.612, 1506.1109, 1527.7859, 1576.3443, 1770.4676, 2928.9124, 2989.5063, 3009.8623, 3036.4438, 3041.6298, 3095.7188, 3109.9274, 3154.0723

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 2	**Energy (kJ mol^{-1}):** -382.284033260298
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.463028 -0.418751 0.461912 6 -0.012774 -0.611109 0.860403 6 0.880302 1.042595 0.789515 1 0.037766 1.613062 1.213075 1 1.704849 0.863277 1.493561 1 0.135755 -1.005138 1.862567 1 -1.993303 -0.197948 1.390964 1 -1.798326 -1.414906 0.148796 6 -1.856807 0.601481 -0.605375 1 -1.392434 0.378302 -1.559994 1 -2.940828 0.581779 -0.724686 1 -1.573083 1.613913 -0.322723 8 1.150850 1.207571 -0.440199 8 0.817054 -0.737034 -1.174707 8 0.848777 -1.235242 0.047370	-429.0211, 57.4673, 168.6678, 231.4167, 257.9251, 267.8266, 312.4284, 416.121, 525.4244, 557.9337, 728.7221, 768.1373, 850.7435, 881.7869, 945.6776, 1011.9977, 1058.2694, 1111.4014, 1132.2061, 1177.0797, 1223.3155, 1233.8927, 1308.7506, 1372.9293, 1388.0543, 1417.0395, 1436.8388, 1462.5505, 1494.2816, 1501.1403, 1544.8087, 2909.8646, 2975.6213, 2998.2539, 3045.2036, 3051.5429, 3101.6442, 3123.1774, 3152.6663
IRC  	

Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -382.323026652093
Reaction Coordinates: 6 -2.016923 0.354860 0.074549 6 -1.121475 -0.483278 0.889383 1 -1.102244 -0.471635 1.973869 8 -0.286670 -1.292411 0.407348 8 -0.186366 -1.389047 -0.963281 1 -2.861941 0.659539 0.692118 1 -2.368595 -0.261301 -0.755869 6 -1.298244 1.598465 -0.496807 1 -2.004980 2.172619 -1.094329 1 -0.918953 2.237271 0.298997 1 -0.467315 1.296316 -1.127522 6 2.713775 0.100237 -0.251127 1 2.082873 -0.610473 -0.809624 1 3.801216 0.084397 -0.457502 8 2.245178 0.865404 0.553917	**Frequencies (cm^{-1}):** 25.67, 35.5123, 54.897, 64.6087, 102.8399, 120.797, 143.9543, 189.5781, 241.717, 322.8617, 535.5147, 648.8954, 811.6442, 846.5712, 875.0535, 906.311, 1008.992, 1084.7894, 1149.0123, 1223.5346, 1281.7979, 1289.4245, 1330.4292, 1374.8344, 1405.1727, 1462.3773, 1493.8901, 1506.6287, 1536.2747, 1570.837, 1789.1101, 2878.2978, 2980.1146, 3035.9277, 3050.436, 3088.4127, 3113.4934, 3143.8816, 3163.6244

Compound: $EtCHCH_2 + O_3$ TS_{SYN} 3	**Energy (kJ mol^{-1}):** -382.288986821508
Reaction Coordinates:	**Frequencies (cm^{-1}):**

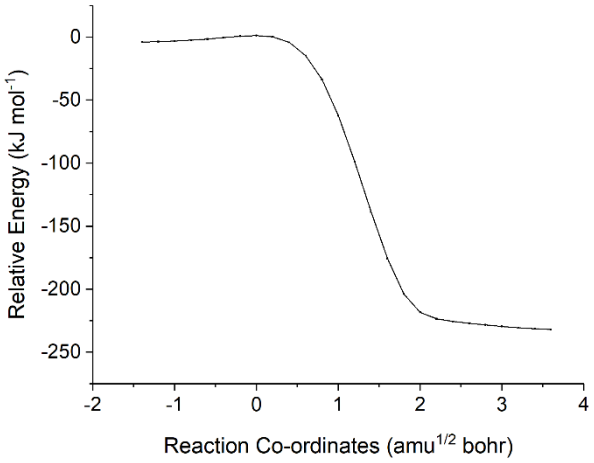
6 1.139313 -0.745949 -0.329732 6 0.172070 -0.295269 0.735179 6 -1.504407 -0.968989 0.223426 1 -1.113331 -1.962499 -0.044429 1 -2.058965 -0.938720 1.171780 1 0.370240 -0.614656 1.755274 1 1.289484 -1.818239 -0.196371 1 0.696430 -0.588587 -1.309695 6 2.479814 -0.008289 -0.220679 1 2.351457 1.062006 -0.374359 1 2.946394 -0.162551 0.753285 1 3.165822 -0.377177 -0.982965 8 -1.870266 -0.204811 -0.725008 8 -0.569809 1.409392 -0.440604 8 -0.230959 0.984343 0.762901	-435.4487, 81.4339, 152.4647, 200.2964, 228.8993, 290.6216, 342.778, 398.4184, 534.4638, 588.1708, 675.5289, 798.6774, 864.0052, 892.7892, 949.2167, 990.8005, 1058.7695, 1092.8118, 1149.2529, 1183.6557, 1216.0403, 1222.2684, 1305.3248, 1348.4056, 1382.9338, 1408.586, 1436.0844, 1482.362, 1498.3042, 1505.8137, 1540.0255, 2919.412, 2982.1101, 3035.0546, 3053.7511, 3091.8497, 3109.9608, 3118.1835, 3131.0544
IRC  	

Compound: $EtCHCH_2 + O_3$ CPr_{SYN} 3	**Energy (kJ mol^{-1}):** -382.326620083051
Reaction Coordinates: 6 1.240436 -0.873423 0.020622 6 0.647868 0.047219 1.006383 1 0.781998 -0.058283 2.078085 8 -0.011375 1.079072 0.715751 8 -0.282347 1.323265 -0.615623 1 1.456734 -1.817970 0.518154 1 0.506553 -1.042357 -0.764945 6 2.526805 -0.276690 -0.594626 1 2.305978 0.663203 -1.094832 1 3.290437 -0.105371 0.163736 1 2.927957 -0.975581 -1.327084 6 -2.363545 -0.185175 -0.509072 1 -2.878130 0.713776 -0.135671 1 -2.227962 -0.240608 -1.600904 8 -2.015396 -1.078386 0.227824	**Frequencies (cm^{-1}):** 56.3724, 73.1273, 74.5611, 101.6324, 133.5406, 198.5728, 216.2526, 257.3288, 323.2996, 357.0709, 529.8793, 649.6167, 808.4707, 863.1902, 874.6502, 907.0196, 1002.4159, 1083.5403, 1153.3104, 1171.6386, 1259.2095, 1281.1752, 1327.9208, 1377.8934, 1403.7791, 1470.1403, 1496.2481, 1510.2691, 1527.5009, 1573.782, 1768.4684, 2927.9084, 2988.0762, 3044.3065, 3065.7932, 3103.6046, 3119.7448, 3133.2652, 3161.4318

6.5 Ozonolysis of 3-methyl-1-butene (Alkene 3)

Compound: $iPrCHCH_2 + O_3$ PRC1.1	**Energy (kJ mol^{-1}):** -421.489482849833
Reaction Coordinates: 6 -1.464524 -0.250101 -0.288012 6 -0.543113 -0.161743 0.896637 6 0.084766 0.927362 1.351486 1 0.709616 0.883281 2.233069 1 -0.023164 1.895646 0.884024 1 -0.416960 -1.091856 1.443445 6 -1.623909 1.058531 -1.059926 1 -2.264037 0.907006 -1.929654 1 -0.663617 1.434471 -1.412564 1 -2.086010 1.830781 -0.441284 1 -1.016377 -0.986134 -0.965576 6 -2.827884 -0.813797 0.149671 1 -3.337708 -0.119516 0.820236 1 -2.717008 -1.764800 0.672722 1 -3.469632 -0.980115 -0.716525 8 2.324840 0.819733 -0.337556 8 2.600682 -0.383656 -0.075361 8 1.766089 -1.257362 -0.447961	**Frequencies (cm^{-1}):** 31.8282, 40.3334, 59.0657, 79.6143, 90.6047, 168.1063, 234.1535, 259.437, 265.9682, 295.3763, 359.1346, 389.732, 541.3701, 675.5503, 742.1642, 782.7728, 922.8119, 933.3482, 957.4492, 969.8111, 1021.1703, 1037.3617, 1115.7058, 1155.0823, 1164.0818, 1192.662, 1208.7715, 1312.9152, 1335.6855, 1370.9888, 1400.7006, 1416.6564, 1457.0657, 1491.1988, 1494.4483, 1504.9377, 1515.5425, 1658.5015, 2990.882, 3021.3132, 3026.5971, 3081.4837, 3085.2655, 3088.6269, 3097.0735, 3122.1312, 3147.1755, 3227.1471

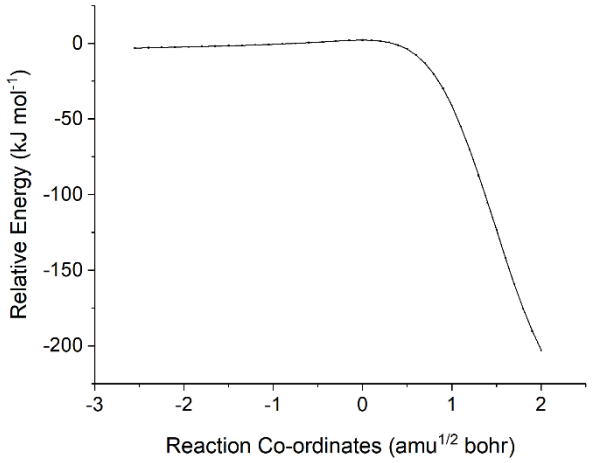
Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -421.480904807623
Reaction Coordinates: 6 1.395496 -0.224617 -0.309478 6 0.306054 -0.376163 0.716460 6 -0.379908 0.644519 1.311611 1 -1.011382 0.460564 2.167365 1 -0.172852 1.677178 1.077564 1 0.201415 -1.369883 1.135674 6 1.463594 1.160607 -0.951080 1 2.206610 1.166038 -1.749002 1 1.757875 1.924058 -0.227828 1 0.504127 1.446575 -1.380744 1 1.176074 -0.949591 -1.098764 6 2.746701 -0.626864 0.310450 1 3.034858 0.065581 1.103359 1 3.529001 -0.614223 -0.449503 1 2.709158 -1.630348 0.736616 8 -2.187929 0.795484 -0.013669 8 -2.356716 -0.469075 -0.194481 8 -1.346169 -1.031516 -0.764664	**Frequencies (cm^{-1}):** -191.7729, 49.3077, 72.7606, 131.1261, 211.5504, 232.2945, 257.3244, 270.3991, 297.5703, 371.878, 425.2393, 493.2796, 553.5254, 715.1305, 748.2884, 785.4731, 916.636, 935.7704, 957.7554, 969.3069, 1003.2055, 1036.1649, 1082.1979, 1108.9408, 1117.1182, 1151.7946, 1208.3295, 1299.2855, 1326.6037, 1374.6047, 1401.6084, 1415.1188, 1453.35, 1490.8505, 1495.5015, 1505.3806, 1515.3757, 1580.6629, 3013.2154, 3022.5412, 3028.1943, 3082.3569, 3087.4696, 3090.2022, 3103.6931, 3152.5397, 3165.2434, 3251.58
IRC:	



Compound: $iPrCHCH_2 + O_3$ POZ1.1	**Energy (kJ mol^{-1}):** -421.578518282609
Reaction Coordinates: 6 -1.373590 -0.294526 -0.338568 6 0.022147 0.279030 -0.604937 6 0.712833 1.061071 0.549343 1 0.997808 2.063216 0.224943 1 0.118949 1.113812 1.459153 8 1.863488 0.285214 0.864043 8 2.194230 -0.285855 -0.418350 8 0.924485 -0.810179 -0.839074 1 -0.006938 0.913115 -1.495319 6 -1.442787 -1.185493 0.903538 1 -2.425834 -1.652824 0.971136 1 -1.292767 -0.614742 1.821971 1 -0.692771 -1.973223 0.869670 1 -1.604156 -0.915792 -1.209279 6 -2.405779 0.836861 -0.288955 1 -2.234398 1.497455 0.564091 1 -3.411478 0.428946 -0.187063 1 -2.382979 1.444930 -1.194787	**Frequencies (cm^{-1}):** 64.6972, 83.1839, 204.8846, 212.2893, 240.7958, 274.7452, 342.4752, 391.9514, 444.1586, 542.0804, 688.6748, 731.5728, 735.8208, 802.8704, 890.2946, 926.1251, 937.3681, 965.1475, 983.2844, 991.0528, 1030.0028, 1036.6958, 1141.2549, 1166.0392, 1208.5972, 1234.4773, 1314.2187, 1347.5183, 1353.0846, 1365.8611, 1400.4929, 1407.5437, 1430.06, 1490.5894, 1492.6218, 1504.3786, 1512.5968, 1514.603, 3008.9786, 3018.5681, 3021.6055, 3032.3006, 3043.8503, 3077.7207, 3084.7376, 3093.2585, 3114.4672, 3116.0706

Compound: $iPrCHCH_2 + O_3$ PRC1.2	**Energy (kJ mol^{-1}):** -421.487640851647
Reaction Coordinates: 6 1.709232 0.043070 0.339030 6 0.716612 -0.705227 -0.503268 6 -0.045677 -1.715989 -0.085947 1 -0.005051 -2.072478 0.935787 1 -0.715903 -2.236939 -0.756136 1 0.657578 -0.397324 -1.544796 6 1.424593 1.551735 0.328983 1 2.147577 2.081189 0.951582 1 0.424313 1.768029 0.700564 1 1.499905 1.953904 -0.683958 1 1.618127 -0.318440 1.367236 6 3.140419 -0.243750 -0.145424 1 3.273782 0.081845 -1.179564 1 3.370043 -1.308259 -0.096533 1 3.866731 0.291806 0.468225	**Frequencies (cm^{-1}):** 24.0644, 29.3215, 42.8574, 51.9733, 73.3551, 137.7397, 203.5513, 223.3737, 241.1009, 316.3551, 332.7771, 348.8893, 503.7519, 701.5887, 742.9039, 801.7848, 929.4988, 934.9146, 956.9629, 965.0306, 1007.7716, 1025.228, 1110.6505, 1174.1137, 1184.7875, 1207.1399, 1219.8865, 1321.8451, 1335.5437, 1340.6646, 1397.5499, 1416.7347, 1461.5641, 1489.3117, 1490.0097, 1501.8104, 1511.8733, 1672.3498, 3013.9647, 3018.8397, 3024.1292, 3075.7117, 3082.1764, 3092.6219,

8 -2.467492 -0.440328 0.842535 8 -2.734464 0.135847 -0.244433 8 -2.024066 1.126685 -0.568434	3107.8281, 3110.5178, 3132.1775, 3214.0095

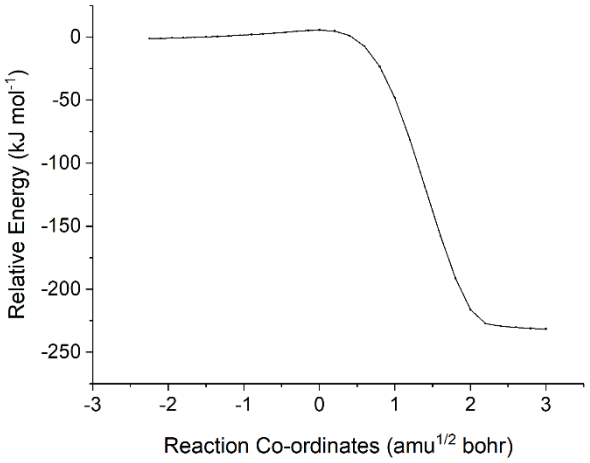
Compound: iPrCHCH$_2$ + O$_3$ TS$_{OZO}$ 1.2	**Energy (kJ mol^{-1}):** -421.477477773765
Reaction Coordinates: 6 1.383613 0.069998 -0.290670 6 0.302309 -0.434735 0.625615 6 -0.474409 -1.519811 0.352818 1 -1.110048 -1.960187 1.105829 1 -0.347954 -2.079743 -0.563065 1 0.266601 -0.009842 1.622575 6 1.773708 1.517508 0.017802 1 2.166706 1.603550 1.033809 1 0.922406 2.188965 -0.073392 1 2.551535 1.858130 -0.666436 1 0.995642 0.019690 -1.312085 6 2.617519 -0.851120 -0.208379 1 2.369722 -1.877923 -0.476169 1 3.032748 -0.857686 0.801378 1 3.394836 -0.498647 -0.888065 8 -2.288794 -0.573860 -0.625463 8 -2.366177 0.466716 0.124415 8 -1.327358 1.222477 0.055111	**Frequencies (cm^{-1}):** -155.6518, 44.7862, 70.8365, 130.7102, 187.6012, 221.8311, 241.6815, 268.1595, 320.9395, 368.9074, 407.5938, 465.3902, 492.7118, 713.3698, 745.9637, 801.2743, 922.0225, 937.5032, 960.0778, 967.5409, 996.7537, 1016.4088, 1092.3878, 1112.8757, 1116.8791, 1185.9805, 1209.1299, 1303.6601, 1317.3723, 1339.7409, 1399.0018, 1419.979, 1457.607, 1489.1537, 1491.0063, 1503.5512, 1512.3702, 1588.4372, 3015.9815, 3021.8266, 3027.5657, 3079.7276, 3086.359, 3096.3688, 3116.3783, 3146.4653, 3152.1784, 3241.2519
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ POZ1.2	**Energy (kJ mol^{-1}):** -421.579433158252
Reaction Coordinates: 6 -1.318544 0.027796 -0.327615 6 0.025972 0.016434 0.395519 6 0.995057 1.184109 0.054426 1 1.211392 1.790185 0.935932 1 0.633659 1.812138 -0.758538 8 2.174623 0.545869 -0.427571 8 2.122436 -0.740952 0.230515 8 0.769749 -1.136855 -0.017407 1 -0.124678 -0.028228 1.478942 6 -2.147353 1.238645 0.114334	**Frequencies (cm^{-1}):** 67.067, 97.6952, 183.5727, 218.8699, 237.4027, 312.5247, 328.4754, 411.2599, 421.8582, 461.2679, 690.5704, 732.4875, 745.6522, 829.7053, 896.7526, 929.6827, 937.8114, 967.3374, 986.7387, 1003.3089, 1024.1176, 1044.4486, 1144.78, 1183.8341, 1197.3571, 1238.3924, 1317.9712, 1333.5507, 1346.8571, 1354.0138, 1403.2977, 1406.3155,

1 -3.097640 1.260012 -0.419338 1 -2.370310 1.191432 1.182578 1 -1.639529 2.184155 -0.081022 1 -1.104556 0.117847 -1.396948 6 -2.085743 -1.276585 -0.092353 1 -2.300641 -1.415488 0.969830 1 -3.037795 -1.258114 -0.624162 1 -1.520704 -2.140838 -0.437439	1428.5174, 1489.8272, 1493.9072, 1507.0454, 1511.0334, 1513.5464, 3002.0141, 3017.4191, 3022.472, 3027.9418, 3038.5592, 3079.8884, 3084.2202, 3093.3431, 3101.5292, 3109.0159

Compound: $iPrCHCH_2 + O_3$ PRC1.3	**Energy (kJ mol^{-1}):** -421.487419417331
Reaction Coordinates: 6 -1.881925 0.096932 0.246370 6 -0.752279 -0.500656 1.040881 6 -0.044907 -1.592418 0.746041 1 -0.226171 -2.179427 -0.143297 1 0.729840 -1.950572 1.410060 1 -0.523639 0.023508 1.965052 6 -2.162944 -0.612629 -1.077328 1 -3.011569 -0.148906 -1.581227 1 -2.400812 -1.666584 -0.929812 1 -1.302935 -0.549977 -1.746437 1 -2.775829 -0.002316 0.876952 6 -1.656847 1.603895 0.037488 1 -0.786389 1.779329 -0.595009 1 -1.488851 2.114894 0.986662 1 -2.526141 2.058269 -0.439637 8 2.195983 -0.661616 -0.817313 8 2.581242 0.216253 -0.001302 8 1.886015 1.264243 0.098113	**Frequencies (cm^{-1}):** 18.6081, 31.3964, 40.847, 53.1454, 80.6257, 153.4446, 203.8197, 235.448, 256.719, 287.8633, 359.7377, 389.4496, 533.0584, 678.1061, 742.935, 781.3382, 923.514, 933.9275, 956.0575, 971.2865, 1027.0128, 1037.846, 1113.807, 1157.7633, 1174.0399, 1205.8223, 1209.0919, 1315.1434, 1335.3552, 1366.213, 1401.6822, 1417.3702, 1456.9933, 1491.5292, 1494.2689, 1504.7235, 1515.4136, 1668.8334, 2963.1433, 3025.4874, 3028.9973, 3086.1546, 3088.1527, 3090.3695, 3098.7163, 3116.7035, 3145.7298, 3224.0228

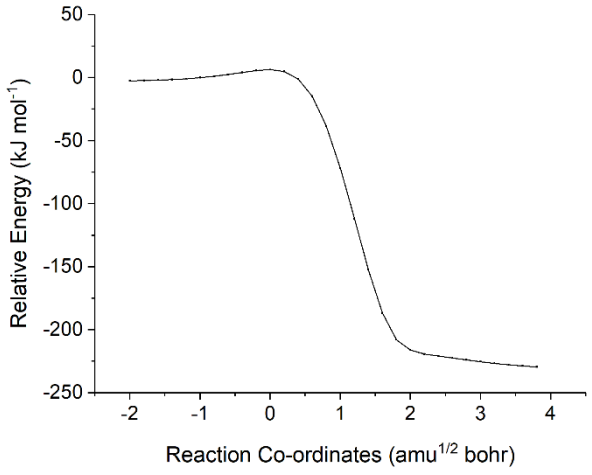
Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -421.478853556703
Reaction Coordinates: 6 1.585337 -0.274088 0.238839 6 0.275998 -0.371233 0.978534 6 -0.652685 -1.360599 0.830804 1 -1.447282 -1.482178 1.550663 1 -0.521256 -2.160607 0.118569 1 0.172495 0.293214 1.828488 6 1.555998 -0.880248 -1.167070 1 0.830297 -0.364071 -1.794541 1 1.301022 -1.939944 -1.153926 1 2.538060 -0.788715 -1.631877 1 2.289713 -0.866380 0.840654 6 2.125262 1.161709 0.226137 1 2.158713 1.580429 1.233197 1 1.500269 1.809261 -0.387096 1 3.137624 1.182670 -0.178328 8 -2.143908 -0.431698 -0.570572 8 -2.092706 0.765250 -0.101292 8 -0.925776 1.301833 -0.211795	**Frequencies (cm^{-1}):** -182.6792, 57.3358, 74.8137, 133.533, 187.7176, 215.7944, 235.1529, 286.8336, 333.5935, 366.6959, 411.9175, 478.5036, 523.4547, 709.5612, 741.668, 780.7328, 926.1582, 931.4445, 958.0195, 973.2032, 998.8914, 1043.986, 1086.1847, 1099.4574, 1117.365, 1167.5873, 1209.1177, 1306.3356, 1322.3109, 1347.7984, 1403.0918, 1417.4109, 1453.9285, 1491.5591, 1494.6521, 1506.8973, 1515.1754, 1581.7822, 2950.4076, 3031.5388, 3036.9535, 3088.2036, 3091.8749, 3107.1981, 3110.3428, 3150.3316, 3164.3506, 3250.2012
IRC:	



Compound: $iPrCHCH_2 + O_3$ POZ1.3	**Energy (kJ mol^{-1}):** -421.578348006076
Reaction Coordinates: 6 1.377131 0.280261 0.355442 6 -0.023540 -0.285670 0.611541 6 -1.156018 0.743486 0.886773 1 -1.638234 0.542207 1.845046 1 -0.823094 1.778336 0.841416 8 -2.070795 0.563434 -0.187855 8 -1.913265 -0.841576 -0.475932 8 -0.485220 -0.963894 -0.565012 1 0.014893 -0.999198 1.439498 6 2.399688 -0.852621 0.210373 1 3.408403 -0.449279 0.116584 1 2.194444 -1.451478 -0.677745 1 2.383432 -1.517797 1.075315 1 1.626968 0.840681 1.263416 6 1.437008 1.238518 -0.837675 1 1.220887 0.715686 -1.768229 1 2.434234 1.672601 -0.915565 1 0.726700 2.060694 -0.748068	**Frequencies (cm^{-1}):** 61.6595, 83.8675, 202.8082, 204.169, 249.8785, 272.2855, 341.7976, 390.5216, 432.3574, 566.7256, 679.3514, 738.2273, 743.4427, 795.1247, 895.7239, 927.7753, 935.7532, 965.329, 968.2765, 1001.2376, 1032.006, 1048.3324, 1136.7663, 1158.4649, 1206.165, 1230.0199, 1324.2179, 1332.9331, 1346.4274, 1375.9762, 1390.7964, 1408.0304, 1430.9027, 1488.4539, 1493.2623, 1503.5889, 1512.7592, 1515.2632, 2994.1971, 3013.7958, 3027.5007, 3037.5209, 3041.5696, 3087.6979, 3091.8076, 3095.0245, 3108.4168, 3112.2936

Compound: $iPrCHCH_2 + O_3$ PRC 2.1	**Energy (kJ mol^{-1}):** -421.488119294631
Reaction Coordinates: 6 1.529544 -0.202130 0.336244 6 0.579810 -0.283115 -0.828452 6 -0.059663 0.727687 -1.421317 1 -0.712682 0.553825 -2.264049 1 0.057681 1.754485 -1.102957 1 0.433419 -1.283416 -1.224899 6 1.734500 1.208371 0.887193 1 2.397229 1.183081 1.752738 1 0.794198 1.662285 1.201529 1 2.190408 1.861675 0.140581 1 1.092914 -0.815316 1.134674 6 2.871968 -0.855283 -0.037119 1 3.372962 -0.286147 -0.822319	**Frequencies (cm^{-1}):** 28.9197, 35.6144, 43.2668, 73.194, 84.5012, 159.5007, 233.9537, 240.4621, 260.4736, 292.9114, 358.7737, 389.2604, 540.9129, 677.0492, 742.6851, 782.5319, 921.6178, 933.4301, 960.3162, 969.8545, 1024.2714, 1038.3023, 1114.6272, 1154.753, 1169.789, 1199.6556, 1207.3639, 1315.8098, 1336.4725, 1367.6129, 1401.3587, 1417.5024, 1458.2759, 1490.5952, 1494.1826, 1504.6191, 1514.1995, 1665.1274, 2976.1106,

1 2.731157 -1.874432 -0.399599 1 3.534643 -0.894687 0.828424 8 -2.600096 0.780385 -0.047218 8 -2.337657 -0.175570 0.732233 8 -2.040857 -1.284132 0.207059	3022.0546, 3026.9234, 3082.824, 3087.1324, 3088.7391, 3092.1121, 3127.1823, 3149.7378, 3230.526

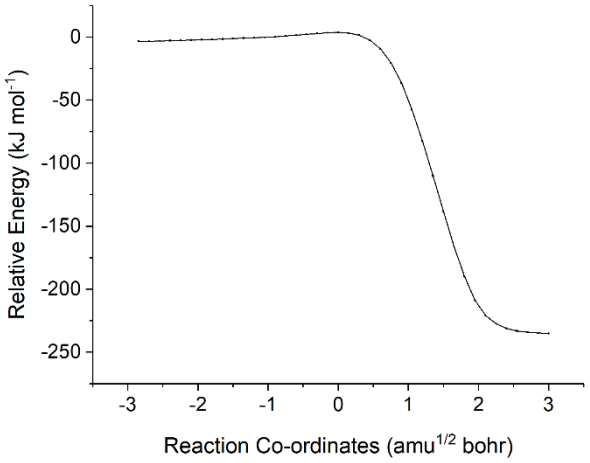
Compound: iPrCHCH$_2$ + O$_3$ TS$_{OZO}$ 2.1	**Energy (kJ mol^{-1}):** -421.478267576213
Reaction Coordinates: 6 1.368332 0.233744 0.318267 6 0.320906 -0.841820 0.177528 6 -0.380220 -1.130003 -0.962773 1 -0.943087 -2.046146 -1.039296 1 -0.233800 -0.571583 -1.874761 1 0.292732 -1.566924 0.981013 6 2.761446 -0.422983 0.362488 1 2.993625 -0.909375 -0.586586 1 2.824870 -1.174209 1.150711 1 3.527276 0.330017 0.553664 1 1.207422 0.706538 1.290203 6 1.304749 1.320760 -0.755709 1 0.320264 1.785659 -0.805759 1 1.544183 0.923371 -1.743963 1 2.030950 2.103715 -0.535894 8 -2.327603 -0.102259 -0.637759 8 -1.959555 0.703213 0.301162 8 -1.439806 0.081640 1.308081	**Frequencies (cm^{-1}):** -219.5759, 45.0444, 76.7721, 135.7788, 202.6958, 229.5637, 259.3776, 272.841, 296.8255, 372.1941, 437.0431, 515.2529, 559.4586, 727.5397, 742.7696, 784.913, 912.6843, 936.8623, 955.1531, 967.8978, 1003.1363, 1037.0108, 1075.7696, 1104.1093, 1114.7786, 1149.2049, 1205.6943, 1295.5947, 1329.6573, 1375.6841, 1402.188, 1415.6317, 1449.9339, 1489.8547, 1494.6528, 1506.3371, 1513.2298, 1573.8658, 3022.2136, 3024.3902, 3030.3188, 3083.7976, 3089.4315, 3090.3065, 3099.3316, 3161.8556, 3168.8215, 3257.3082
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ POZ 2.1	**Energy (kJ mol^{-1}):** -421.578381691063
Reaction Coordinates: 6 -1.360596 0.261009 0.342888 6 0.010564 -0.349909 0.663693 6 0.710421 -1.107264 -0.496292 1 0.226755 -0.913108 -1.454083 1 0.784937 -2.178369 -0.321442 8 2.039404 -0.602487 -0.493929 8 1.821406 0.768272 -0.130017 8 0.987678 0.634403 1.045021	**Frequencies (cm^{-1}):** 82.821, 91.1279, 208.8996, 220.8818, 245.3416, 270.0356, 335.8478, 381.5129, 476.0959, 546.1964, 663.2283, 719.5096, 758.6486, 796.0831, 890.6758, 919.0307, 936.1909, 964.8696, 982.6438, 991.8508, 1019.8782, 1034.204, 1140.9352, 1161.544, 1210.05, 1236.8865, 1303.7757,

1 -0.082212 -0.998618 1.536805 6 -2.380278 -0.849138 0.063939 1 -3.377944 -0.427563 -0.060136 1 -2.142265 -1.393767 -0.852535 1 -2.424817 -1.571070 0.881713 1 -1.667748 0.769399 1.261409 6 -1.330837 1.307867 -0.772571 1 -1.107126 0.867631 -1.745573 1 -2.305652 1.790921 -0.851910 1 -0.587478 2.077648 -0.572792	1333.3372, 1355.0743, 1365.2876, 1399.0781, 1406.6604, 1428.9707, 1489.3204, 1493.3134, 1504.7897, 1511.1692, 1512.835, 3012.7296, 3020.4437, 3032.4462, 3047.309, 3051.6637, 3075.9805, 3085.0632, 3090.7566, 3111.8654, 3118.3225

Compound: $iPrCHCH_2 + O_3$ PRC 2.2	**Energy (kJ mol^{-1}):** -421.487885829932
Reaction Coordinates: 6 1.737850 -0.025217 -0.359528 6 0.705920 0.716044 0.441616 6 -0.075361 1.694433 -0.015482 1 -0.019375 2.029415 -1.044477 1 -0.781369 2.202017 0.625389 1 0.627398 0.428836 1.487324 6 1.454081 -1.534852 -0.371863 1 2.213134 -2.063428 -0.950724 1 0.480285 -1.754737 -0.808877 1 1.463617 -1.940787 0.641881 1 1.694109 0.341721 -1.389128 6 3.145309 0.256504 0.191133 1 3.231696 -0.078656 1.227154 1 3.375256 1.321630 0.163088 1 3.899847 -0.272008 -0.393876 8 -2.776477 0.561860 -0.553041 8 -2.462420 -0.615581 -0.233418 8 -2.010027 -0.803212 0.927333	**Frequencies (cm^{-1}):** 22.2532, 28.7929, 35.8731, 61.6081, 76.1121, 136.9736, 205.2682, 220.7184, 238.6001, 319.3567, 332.0031, 349.0046, 504.0223, 701.1698, 743.0489, 801.63, 928.7501, 933.479, 960.1529, 964.4562, 1008.4367, 1026.7976, 1110.7958, 1175.5333, 1183.8735, 1208.4116, 1219.354, 1321.5608, 1336.3527, 1341.4563, 1397.6683, 1416.7472, 1462.6721, 1487.8229, 1489.8931, 1502.1771, 1510.1935, 1673.181, 3011.9313, 3019.4781, 3024.2273, 3077.2472, 3084.0094, 3093.1686, 3095.4646, 3115.4852, 3132.5411, 3223.2408

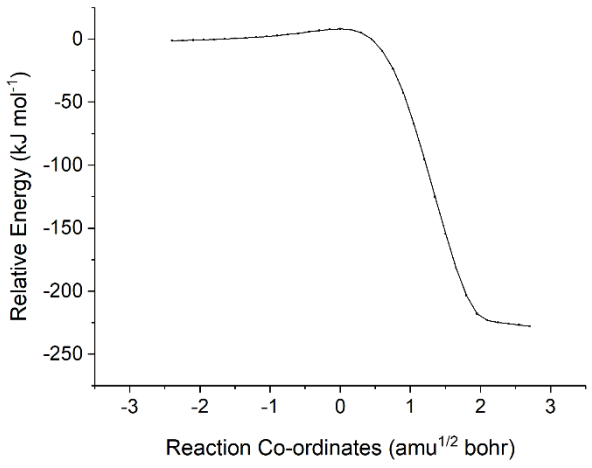
Compound: $iPrCHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -421.478621062929
Reaction Coordinates: 6 1.306992 0.076256 -0.277846 6 0.293489 -0.466937 0.693251 6 -0.515916 -1.530106 0.418630 1 -1.111591 -1.989621 1.191008 1 -0.446717 -2.056977 -0.523082 1 0.339702 -0.102422 1.712352 6 1.749261 1.497439 0.076023 1 2.221931 1.520542 1.060943 1 0.902292 2.180784 0.091864 1 2.477303 1.864835 -0.647910 1 0.840665 0.089478 -1.269090 6 2.524389 -0.868605 -0.354958 1 2.233574 -1.873870 -0.658180 1 3.021658 -0.939834 0.614230 1 3.248687 -0.489166 -1.077224 8 -2.390258 -0.569682 -0.369642 8 -1.928934 0.614274 -0.581490 8 -1.415408 1.148905 0.472943	**Frequencies (cm^{-1}):** -178.2678, 42.4411, 74.4126, 133.5783, 186.9028, 224.4401, 246.0529, 263.4133, 338.0879, 370.4337, 416.7443, 487.0257, 496.7457, 720.7394, 742.5421, 802.6306, 923.0864, 938.2613, 955.6553, 967.9145, 996.1365, 1015.8222, 1083.35, 1107.6349, 1115.7812, 1186.0039, 1208.6418, 1296.3545, 1319.6997, 1337.0796, 1398.5342, 1419.2666, 1454.8105, 1490.1718, 1490.3326, 1502.3198, 1513.86, 1583.0894, 2995.9028, 3022.4382, 3026.8751, 3080.5498, 3087.175, 3098.1911, 3113.4499, 3153.2697, 3157.4253, 3248.2157
IRC:	



Compound: $iPrCHCH_2 + O_3$ POZ 2.2	**Energy (kJ mol^{-1}):** -421.579950919226
Reaction Coordinates: 6 1.255989 0.003868 -0.324021 6 -0.020796 0.038356 0.518784 6 -1.016141 1.165007 0.124608 1 -0.718706 1.635515 -0.814736 1 -1.152237 1.916081 0.899837 8 -2.262739 0.500970 -0.024434 8 -1.842211 -0.764521 -0.559207 8 -0.818599 -1.150723 0.382948 1 0.229306 0.084872 1.581503 6 2.092863 -1.236301 -0.003788 1 2.979371 -1.273888 -0.638062 1 2.429966 -1.222178 1.035794 1 1.522645 -2.150207 -0.161178 1 0.946466 -0.045892 -1.372619 6 2.069334 1.285243 -0.109591 1 2.379250 1.379325 0.934115 1 2.972842 1.268972 -0.719369 1 1.511989 2.184549 -0.375698	**Frequencies (cm^{-1}):** 75.4874, 99.7448, 196.6689, 218.3046, 237.882, 313.3533, 350.0876, 380.7715, 445.2364, 489.7946, 686.5078, 717.3874, 764.0131, 819.2826, 894.6433, 919.4475, 937.0786, 961.2906, 983.1729, 992.7684, 1023.6189, 1033.5331, 1134.686, 1184.5308, 1194.982, 1246.2535, 1295.0786, 1317.6712, 1348.6174, 1357.4479, 1396.0621, 1404.672, 1426.4327, 1489.9379, 1494.0473, 1502.9313, 1507.0626, 1514.5139, 3010.1784, 3019.5683, 3023.9182, 3035.4585, 3042.9211, 3077.049, 3082.0234, 3091.726, 3109.6292, 3116.1887

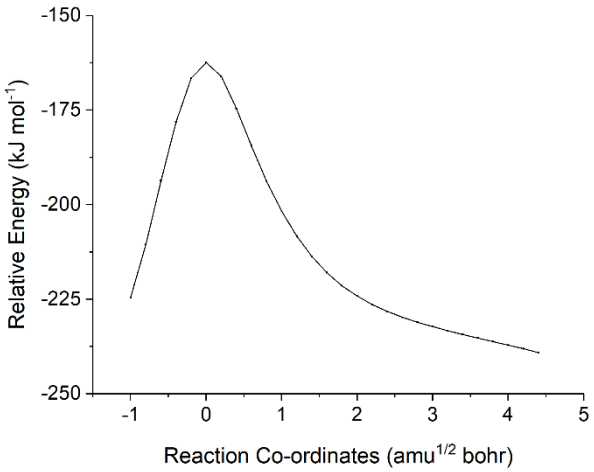
Compound: $iPrCHCH_2 + O_3$ PRC 2.3	**Energy (kJ mol^{-1}):** -421.487653574376
Reaction Coordinates: 6 -1.890354 0.094090 0.253611 6 -0.724686 -0.482650 1.011480 6 -0.016909 -1.570875 0.704537 1 -0.227708 -2.173005 -0.168889 1 0.791975 -1.904079 1.337973 1 -0.462573 0.057365 1.916800 6 -2.243363 -0.658213 -1.028542 1 -3.116383 -0.208618 -1.502675 1 -2.474055 -1.705685 -0.832580 1 -1.421743 -0.623144 -1.746854 1 -2.752363 0.024611 0.930325 6 -1.668645 1.591802 -0.018571 1 -0.835947 1.743072 -0.707256	**Frequencies (cm^{-1}):** 21.5074, 27.5017, 44.4695, 61.0739, 85.3627, 152.4376, 207.7332, 232.1118, 256.8658, 287.3985, 358.6663, 389.0178, 535.2522, 678.3333, 742.6699, 780.5801, 923.369, 932.7311, 958.85, 970.5403, 1027.4387, 1038.7355, 1113.8301, 1156.2272, 1174.783, 1205.9861, 1208.1864, 1315.3885, 1335.3112, 1366.9361, 1402.0741, 1418.148, 1458.394, 1489.9575, 1493.1345, 1504.2896, 1513.6497, 1669.2411,

1 -1.441341 2.133122 0.900525 1 -2.559975 2.037881 -0.461664 8 2.533801 -0.723897 -0.547862 8 2.233525 0.499002 -0.594617 8 1.953156 1.071590 0.492379	2967.0229, 3023.7992, 3027.5309, 3083.1816, 3089.6231, 3089.9387, 3092.1859, 3123.3605, 3148.8981, 3230.0246

Compound: iPrCHCH$_2$ + O$_3$ TS$_{OZO}$ 2.3	**Energy (kJ mol^{-1}):** -421.480159923043
Reaction Coordinates: 6 1.539942 0.347304 -0.183543 6 0.263875 0.480294 -0.976333 6 -0.725909 1.398955 -0.754514 1 -1.467718 1.590406 -1.512651 1 -0.678749 2.099073 0.065786 1 0.249297 -0.047855 -1.921629 6 1.426222 0.785552 1.279843 1 0.724676 0.155468 1.827011 1 1.100823 1.821053 1.377938 1 2.397574 0.702601 1.767781 1 2.241144 1.035346 -0.678240 6 2.146646 -1.055183 -0.306437 1 2.244349 -1.353743 -1.351434 1 1.518136 -1.791284 0.193832 1 3.139445 -1.082368 0.143717 8 -2.321400 0.244128 0.267457 8 -1.613864 -0.744142 0.698365 8 -0.986440 -1.358765 -0.249098	**Frequencies (cm^{-1}):** -213.9187, 51.3942, 77.6188, 140.3079, 189.2169, 218.3342, 243.4297, 286.0037, 349.0132, 366.6713, 422.2983, 487.6518, 538.0044, 722.9933, 739.5276, 776.2754, 926.825, 932.0731, 955.9065, 972.2425, 999.4838, 1045.1925, 1078.4575, 1096.5003, 1113.934, 1166.4033, 1210.0641, 1301.1189, 1318.1692, 1347.9535, 1404.8921, 1417.6824, 1450.2877, 1492.0982, 1493.867, 1506.7324, 1514.7236, 1574.3482, 2947.3346, 3029.5286, 3036.4307, 3088.01, 3094.3135, 3100.3378, 3105.6766, 3159.1343, 3167.4466, 3256.0347
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ POZ 2.3	**Energy (kJ mol^{-1}):** -421.578474925015
Reaction Coordinates: 6 1.324954 0.108329 0.470433 6 -0.012596 -0.637985 0.374389 6 -1.186545 0.011220 1.153167 1 -0.927810 1.012166 1.501905 1 -1.532133 -0.600130 1.984402 8 -2.252694 0.060050 0.214384 8 -1.543249 0.292716 -1.013072 8 -0.525914 -0.734274 -0.965732	**Frequencies (cm^{-1}):** 76.1168, 94.3256, 204.5056, 217.4719, 257.6352, 274.1457, 343.5553, 394.9057, 433.8583, 589.0905, 671.5651, 718.1744, 754.702, 795.7339, 894.2209, 917.3276, 933.15, 965.0168, 969.6548, 1001.5387, 1030.8053, 1046.4645, 1124.3664, 1158.6629, 1205.0961, 1233.8928,

1 0.125054 -1.674107 0.688618 6 1.298037 1.497663 -0.173521 1 2.264203 1.985839 -0.042165 1 1.100807 1.423026 -1.242656 1 0.538307 2.147947 0.258872 1 1.516343 0.227167 1.544279 6 2.453434 -0.744405 -0.118474 1 2.292097 -0.914755 -1.184063 1 3.416429 -0.246531 -0.001539 1 2.517865 -1.717495 0.371745	1297.9056, 1322.3441, 1350.2114, 1363.4691, 1389.5238, 1406.4913, 1429.4218, 1488.172, 1493.628, 1503.8142, 1511.9128, 1514.6951, 2981.1382, 3024.885, 3036.9716, 3044.9516, 3050.257, 3085.173, 3091.4369, 3095.6789, 3104.9246, 3113.762

Compound: $iPrCHCH_2 + O_3$ TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -421.547189931544
Reaction Coordinates: 6 1.434798 -0.293902 -0.346699 6 -0.047938 -0.098096 -0.561609 6 -0.874712 1.218496 0.531676 1 -0.354995 1.056524 1.486237 1 -0.505563 2.073018 -0.054236 1 -0.363701 0.332016 -1.507713 6 2.187181 1.028569 -0.535717 1 1.973334 1.727897 0.273115 1 3.261236 0.845955 -0.539452 1 1.928692 1.509878 -1.479979 1 1.749762 -0.961580 -1.158741 6 1.781644 -0.973228 0.980588 1 1.278519 -1.932357 1.087110 1 2.856451 -1.146267 1.034293 1 1.502037 -0.350155 1.830794 8 -0.821213 -1.110342 -0.166074 8 -2.091895 -0.888630 -0.467569 8 -2.113342 0.943227 0.461035	**Frequencies (cm^{-1}):** -435.9236, 67.8681, 127.5494, 180.5956, 215.2753, 218.2486, 247.7444, 328.531, 342.0147, 423.5645, 452.3003, 516.4436, 561.3426, 630.504, 831.8429, 869.3616, 937.5885, 966.0389, 979.1071, 1015.5748, 1075.5023, 1097.6756, 1155.3994, 1180.6131, 1211.5498, 1225.078, 1263.7704, 1328.11, 1356.9643, 1387.1325, 1391.2113, 1409.8749, 1434.9429, 1490.4757, 1494.6364, 1508.3109, 1513.4167, 1544.2581, 2922.8952, 2977.8745, 2986.0991, 3032.6127, 3039.9123, 3093.4661, 3096.7007, 3102.6798, 3115.4865, 3120.0678
IRC:  	

Compound: $iPrCHCH_2 + O_3$ C_{ANTI} 1	**Energy (kJ mol^{-1}):** -421.586931902890
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.618349 0.117599 -0.367647 6 -0.181988 0.331910 -0.681051 1 0.309646 -0.175311 -1.502394 8 0.484958 1.184415 -0.044691 8 1.836735 1.267128 -0.365357 6 -2.088207 0.845945 0.890533 1 -3.156379 0.683314 1.029387 1 -1.568455 0.468073 1.770830 1 -1.910504 1.918338 0.828866 1 -2.152999 0.525930 -1.238110 6 -1.912942 -1.394207 -0.328296 1 -2.984981 -1.549866 -0.213421 1 -1.592176 -1.889141 -1.244694 1 -1.392665 -1.862425 0.504852 6 2.377690 -0.790924 0.419923 1 2.696854 -0.305152 1.351508 1 3.124554 -0.822688 -0.384930 8 1.324543 -1.408169 0.347215	38.391, 81.2123, 91.8229, 125.4783, 191.5909, 211.029, 219.668, 266.0438, 303.1194, 323.4634, 365.3149, 453.553, 465.6094, 557.0607, 601.3829, 832.2031, 921.8562, 931.758, 942.7771, 976.4191, 979.7163, 1108.8914, 1145.4921, 1153.7702, 1208.1421, 1252.2418, 1293.483, 1348.1802, 1375.0067, 1410.3279, 1429.6557, 1488.6357, 1491.4389, 1503.177, 1510.3392, 1512.401, 1562.0059, 1699.3343, 2952.3503, 2957.8868, 3015.1473, 3041.7013, 3044.1515, 3105.4434, 3107.8928, 3113.0262, 3124.5827, 3178.8921

Compound: $iPrCHCH_2 + O_3$ TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -421.548092509859
Reaction Coordinates: 6 -1.379505 0.040935 -0.321837 6 0.005536 -0.140589 0.243875 6 1.216241 1.274782 -0.143081 1 0.911384 1.518562 -1.172155 1 0.812877 1.948216 0.628010 1 0.132603 -0.121598 1.323193 6 -2.265986 -1.149587 0.084347 1 -3.261497 -1.036428 -0.345838 1 -1.847446 -2.092558 -0.264635 1 -2.374233 -1.205176 1.169240 1 -1.289108 0.047914 -1.410743 6 -1.996762 1.366717 0.134648 1 -3.013625 1.451808 -0.247360 1 -2.048023 1.422712 1.223902 1 -1.434460 2.227466 -0.224709 8 0.723932 -1.090232 -0.356296 8 1.905411 -1.243297 0.219268 8 2.362456 0.769220 0.053701	**Frequencies (cm^{-1}):** -424.7614, 61.1361, 139.3668, 166.4674, 222.0182, 228.4909, 258.0556, 284.9804, 352.1543, 448.1485, 466.8311, 517.2809, 530.0917, 598.285, 846.5374, 873.0835, 938.6112, 945.848, 972.7136, 1006.8368, 1083.6508, 1123.1305, 1161.4369, 1187.3312, 1190.0226, 1225.2325, 1256.3155, 1321.4042, 1340.878, 1392.4036, 1403.2855, 1413.1291, 1434.2443, 1489.6905, 1493.2323, 1506.8123, 1513.7905, 1543.4192, 2911.7332, 2974.2782, 3027.8386, 3029.6273, 3036.7375, 3088.7906, 3095.1576, 3106.3509, 3107.9816, 3115.245
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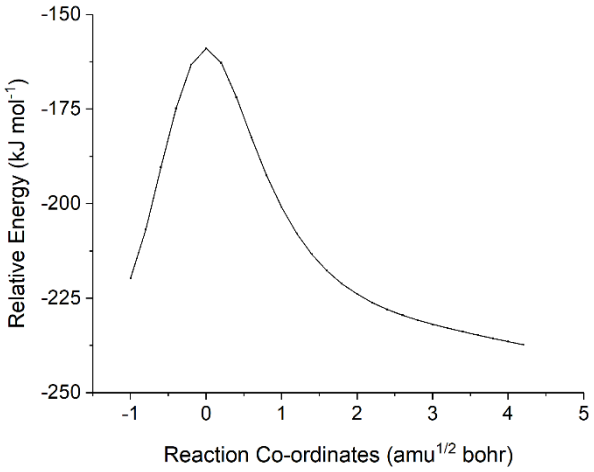
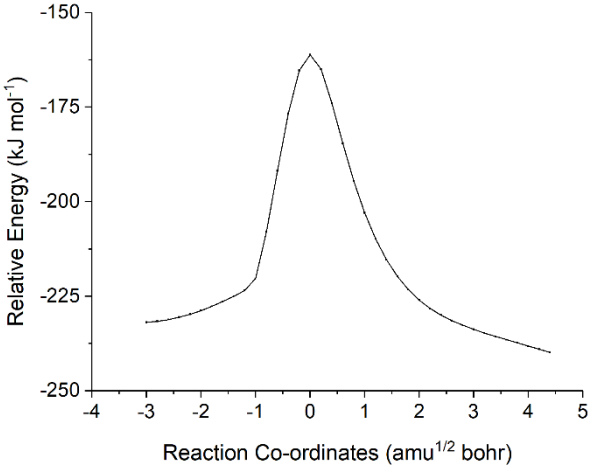


Compound: iPrCHCH$_2$ + O$_3$ C$_{ANTI}$ 2	**Energy (kJ mol^{-1}):** -421.586344391043
Reaction Coordinates: 6 -1.540785 0.023982 -0.339574 6 -0.232307 -0.408863 0.212080 1 0.068217 -0.210567 1.234490 8 0.528677 -1.116905 -0.493112 8 1.756654 -1.449180 0.067840 6 -2.667427 -0.765579 0.357071 1 -3.630376 -0.449503 -0.043972 1 -2.564912 -1.838156 0.195862 1 -2.673918 -0.577417 1.431786 1 -1.542869 -0.216384 -1.403835 6 -1.716330 1.540060 -0.153870 1 -2.673769 1.846037 -0.575410 1 -1.710736 1.807132 0.903754 1 -0.917363 2.091820 -0.643233 6 2.581687 0.669642 0.095904 1 3.082249 0.441237 -0.854452 1 3.119014 0.368948 1.005662 8 1.576599 1.363761 0.140232	**Frequencies (cm^{-1}):** 38.6458, 78.3218, 92.3284, 115.713, 184.2876, 210.0883, 213.0463, 265.8411, 297.9685, 316.0486, 358.569, 459.6574, 480.0233, 533.9852, 554.659, 855.2013, 923.6637, 942.1476, 951.8172, 953.7826, 971.8611, 1099.4272, 1151.8702, 1183.9198, 1205.8007, 1252.6154, 1327.8699, 1331.7046, 1370.9554, 1402.8871, 1424.9574, 1487.7594, 1489.8949, 1500.9809, 1510.5609, 1512.6128, 1568.6591, 1701.937, 2951.6084, 3014.3968, 3031.4826, 3037.5118, 3055.7466, 3095.0921, 3101.35, 3106.1457, 3129.2749, 3173.6931

Compound: iPrCHCH$_2$ + O$_3$ TS$_{ANTI}$ 3	**Energy (kJ mol^{-1}):** -421.547656378960
Reaction Coordinates: 6 1.384417 0.357138 -0.280146 6 -0.018480 -0.181869 -0.417208 6 -1.354485 1.144492 -0.493721 1 -0.971360 1.871503 0.236334 1 -1.162555 1.408849 -1.545088 1 -0.282585 -0.668597 -1.351450 6 1.712600 0.848950 1.132395 1 0.993119 1.586984 1.485020 1 1.720411 0.024311 1.844539 1 2.699680 1.310547 1.140884 1 1.438023 1.208058 -0.966260 6 2.399587 -0.693093 -0.764086 1 2.388024 -1.570766 -0.116593	**Frequencies (cm^{-1}):** -429.4656, 63.8621, 124.4903, 180.1246, 213.8114, 225.6088, 251.5155, 265.3578, 370.3811, 411.7229, 501.9678, 535.676, 556.2467, 628.9939, 831.3387, 875.4722, 933.5634, 965.2874, 968.2175, 1027.999, 1064.0366, 1118.9303, 1139.8519, 1181.2976, 1205.0042, 1219.7457, 1263.0199, 1329.9255, 1363.0165, 1385.4375, 1397.503, 1407.6313, 1435.0188, 1489.1033, 1494.051, 1505.1349, 1512.7008, 1543.2454,

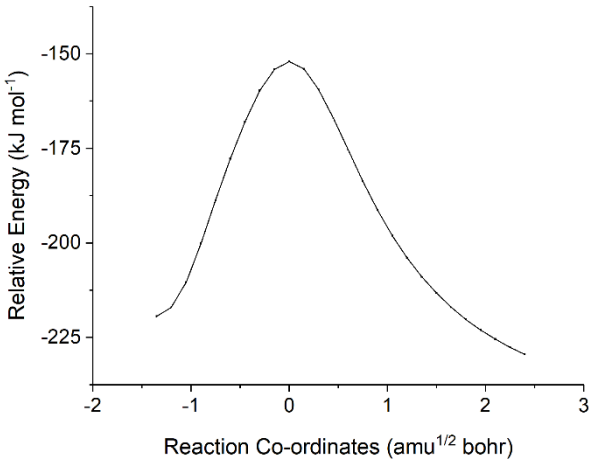
1 2.186605 -1.019502 -1.782539 1 3.406497 -0.275346 -0.749082 8 -0.501730 -0.817264 0.652772 8 -1.711739 -1.298124 0.414555 8 -2.431243 0.524169 -0.224724	2915.0002, 2978.5, 3013.8477, 3029.6345, 3041.6779, 3094.9243, 3096.8056, 3104.7435, 3107.9205, 3121.1286

IRC:

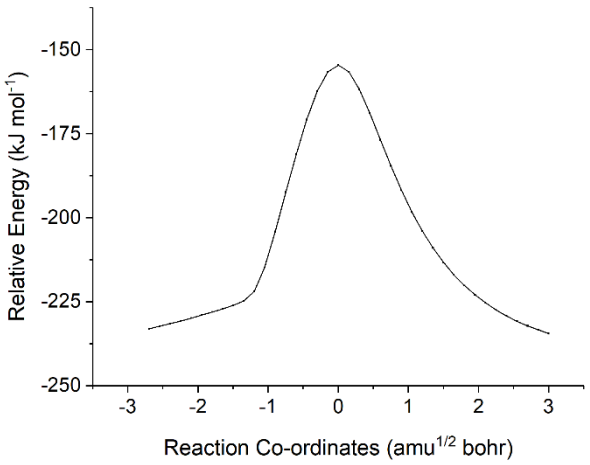


Compound: iPrCHCH$_2$ + O$_3$ C$_{ANTI}$ 3	**Energy (kJ mol^{-1}):** -421.586605259940
Reaction Coordinates: 6 -1.472596 -0.431394 0.018575 6 -0.185451 0.129104 -0.464481 1 0.241295 -0.156184 -1.418003 8 0.405578 1.021690 0.192298 8 1.654236 1.403122 -0.290557 6 -1.879454 0.061114 1.405754 1 -2.792873 -0.443001 1.719430 1 -1.104490 -0.143951 2.142228 1 -2.068375 1.134761 1.404220 1 -1.286320 -1.511431 0.060987 6 -2.564636 -0.194368 -1.044275 1 -3.474775 -0.717842 -0.753953 1 -2.796797 0.867278 -1.133989 1 -2.262080 -0.563580 -2.024435 6 2.640339 -0.602604 0.082878 1 3.036856 -0.189623 1.019667 1 3.235566 -0.404664 -0.818793 8 1.695535 -1.380171 0.074752	**Frequencies (cm^{-1}):** 40.5508, 68.2226, 90.6279, 121.8514, 183.5761, 207.153, 220.4663, 259.7288, 310.3963, 331.5203, 367.7272, 459.9734, 472.8484, 558.9194, 611.0441, 825.8833, 922.661, 931.9843, 944.2274, 975.4644, 976.3257, 1108.8443, 1141.0819, 1151.2537, 1207.7155, 1251.9502, 1296.534, 1354.8658, 1378.1782, 1408.1939, 1428.6715, 1489.3811, 1493.543, 1505.4138, 1509.8474, 1511.835, 1563.329, 1695.9717, 2953.4456, 3000.0683, 3016.6486, 3033.8952, 3042.5708, 3098.966, 3103.2322, 3107.0985, 3115.8251, 3182.5965

Compound: iPrCHCH$_2$ + O$_3$ TS$_{FO}$ 1.1	**Energy (kJ mol^{-1}):** -421.545748006541
Reaction Coordinates: 6 -1.404819 -0.300214 0.302582 6 -0.086226 0.179504 0.939912 6 0.886367 1.254290 -0.250220 1 0.230695 1.858478 -0.863866	**Frequencies (cm^{-1}):** -429.0408, 50.0879, 112.5355, 197.6485, 230.3899, 238.4293, 260.4259, 295.1199, 352.0777, 446.7248, 494.3333, 520.1074, 600.0698, 668.6648, 771.6225, 893.1327,

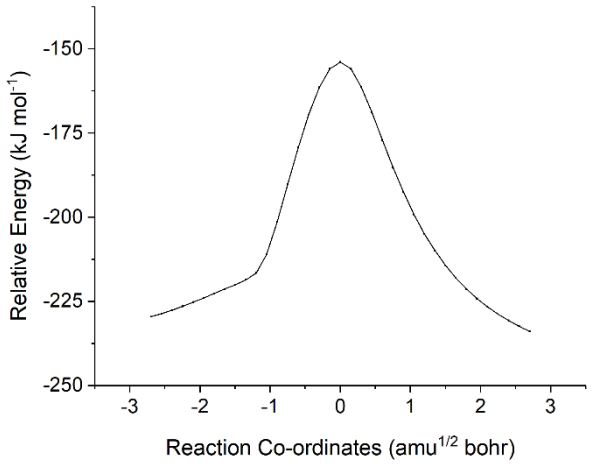
1 1.528067 1.748146 0.468511 1 -0.234104 1.023766 1.641360 6 -1.204429 -1.323812 -0.813465 1 -2.154273 -1.793850 -1.071201 1 -0.809327 -0.857611 -1.717363 1 -0.508445 -2.101719 -0.504439 1 -1.894090 -0.816416 1.137295 6 -2.316738 0.855811 -0.109300 1 -3.325507 0.493901 -0.308997 1 -2.390788 1.613143 0.674662 1 -1.967732 1.345077 -1.021163 8 1.469021 0.286967 -0.953801 8 2.269559 -0.426686 -0.184098 8 0.796490 -0.673580 1.281417	903.5004, 936.0764, 973.6742, 994.4658, 1050.1105, 1079.646, 1140.6606, 1175.5804, 1206.7204, 1221.7753, 1269.2457, 1313.609, 1336.7479, 1351.0271, 1403.1212, 1418.8442, 1454.9626, 1480.6044, 1488.8813, 1496.0494, 1509.581, 1511.2623, 2862.6227, 2987.1409, 3017.7151, 3032.9216, 3071.7465, 3085.7072, 3089.2958, 3112.9217, 3113.7352, 3229.5423
IRC:  	

Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (kJ mol^{-1}):** -421.584591848636
Reaction Coordinates: 6 -1.737228 0.145395 -0.240931 6 -0.447784 0.471603 -0.960289 1 -0.219359 -0.184589 -1.820225 8 0.265936 1.422289 -0.715075 1 -2.501414 0.565614 -0.913727 6 -1.975289 -1.366611 -0.171787 1 -1.869503 -1.831965 -1.152975 1 -2.982140 -1.575678 0.190253 1 -1.259263 -1.838348 0.499553 6 -1.851468 0.836264 1.114627 1 -1.664828 1.905694 1.031614 1 -2.847274 0.690009 1.533694 1 -1.126804 0.418605 1.814888 6 2.489259 0.535606 0.447457 1 3.361250 1.071747 0.098566 1 1.790455 0.911185 1.180878 8 2.327672 -0.599553 -0.049718 8 1.213134 -1.305963 0.315170	**Frequencies (cm^{-1}):** 32.5363, 45.8444, 76.1397, 100.4113, 133.9843, 196.1479, 208.482, 219.3935, 240.548, 272.141, 350.5085, 419.7441, 524.0043, 607.0652, 677.2844, 795.4341, 885.5102, 913.994, 925.8915, 948.6476, 974.9734, 993.4003, 1134.6038, 1153.764, 1207.5932, 1240.8374, 1307.6504, 1341.6215, 1401.6542, 1413.0093, 1416.061, 1432.2307, 1487.075, 1494.2573, 1502.2446, 1512.3964, 1566.7968, 1747.5955, 2915.7895, 2946.8097, 3032.2684, 3035.7606, 3089.579, 3093.1937, 3109.0526, 3110.5548, 3132.7528, 3277.7519

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 1.2	**Energy (kJ mol^{-1}):** -421.546199608323
Reaction Coordinates: 6 -1.233947 0.052880 -0.323585 6 -0.089776 -0.214373 0.667901 6 1.254540 1.083928 0.427709 1 0.829481 2.060966 0.238667 1 1.808382 0.919981 1.343454 1 -0.293850 0.131163 1.700491 6 -1.975443 1.354792 -0.018451 1 -2.825227 1.476926 -0.690303 1 -2.365825 1.352317 1.002537 1 -1.346056 2.238438 -0.132772 1 -0.793209 0.107146 -1.321983 6 -2.193843 -1.144669 -0.295262 1 -2.665606 -1.245062 0.685279 1 -1.662315 -2.069451 -0.511244 1 -2.985702 -1.016249 -1.034374 8 1.799135 0.561676 -0.666320 8 2.325625 -0.621077 -0.402591 8 0.591583 -1.284539 0.565208	**Frequencies (cm^{-1}):** -426.7675, 45.2426, 106.5045, 189.9068, 207.0405, 244.7019, 292.6715, 309.9316, 346.8872, 410.0374, 491.7873, 533.7123, 593.8846, 635.7118, 802.661, 891.6734, 900.1371, 935.4753, 960.5648, 970.7853, 1048.7729, 1109.1655, 1141.1874, 1169.1915, 1188.6523, 1223.3313, 1266.9753, 1303.1086, 1338.1968, 1344.5213, 1399.6804, 1419.889, 1458.3583, 1478.9255, 1488.4485, 1492.7372, 1506.8467, 1511.6104, 2864.0565, 3019.2365, 3021.9619, 3033.2449, 3075.7067, 3081.8889, 3090.3795, 3113.8663, 3114.0978, 3232.4232
IRC:  	

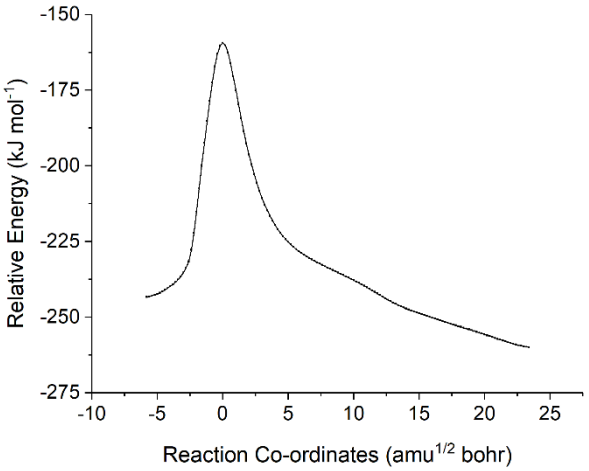
Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (kJ mol^{-1}):** -421.582016760602
Reaction Coordinates: 6 1.270095 -0.243268 -0.032876 6 1.061279 1.239056 0.107996 6 -2.452486 0.672674 -0.178545 1 -2.839793 1.475961 0.431775 1 -2.129072 0.785172 -1.203876 1 1.989445 1.823073 0.286617 6 1.834188 -0.792924 1.287518 1 2.015317 -1.863297 1.190748 1 2.781276 -0.314988 1.548848 1 1.135991 -0.645025 2.111281 1 0.303717 -0.709677 -0.235291 6 2.230125 -0.507376 -1.203035 1 3.195598 -0.020401 -1.047099 1 1.817413 -0.152443 -2.147723 1 2.408694 -1.578471 -1.297354	**Frequencies (cm^{-1}):** 31.3179, 37.8505, 63.4785, 85.6428, 96.4421, 108.3427, 194.87, 201.0697, 223.6026, 332.4769, 338.221, 357.4928, 519.6694, 549.5742, 678.1157, 852.3677, 864.9531, 912.0022, 939.3054, 960.9398, 983.6271, 991.164, 1132.2432, 1180.0211, 1193.0407, 1235.2515, 1350.9305, 1365.3009, 1398.0626, 1412.1988, 1413.47, 1428.2433, 1486.3739, 1492.1875, 1503.184, 1510.8698, 1566.5035, 1771.8818, 2863.346, 3021.7069, 3022.7783, 3044.1451,

8 -2.405981 -0.449511 0.367064 8 -1.888672 -1.499073 -0.354797 8 0.002429 1.822475 0.047199	3083.1966, 3088.2553, 3098.3332, 3101.2328, 3133.3937, 3277.3572

Compound: iPrCHCH$_2$ + O$_3$ TS$_{FO}$ 1.3	**Energy (kJ mol^{-1}):** -421.545697186692
Reaction Coordinates: 6 -1.319832 0.155799 0.422566 6 -0.162534 -0.805291 0.096118 6 1.326218 -0.363364 1.132707 1 1.021134 0.003395 2.105408 1 1.858731 -1.304385 1.073110 1 -0.273236 -1.788609 0.593306 6 -1.159348 1.529288 -0.226237 1 -2.030664 2.149786 -0.013407 1 -0.276279 2.053102 0.137629 1 -1.063247 1.431808 -1.307024 1 -1.359835 0.270232 1.510884 6 -2.626523 -0.520793 -0.021001 1 -3.486199 0.089422 0.258623 1 -2.638985 -0.652732 -1.103860 1 -2.749714 -1.502701 0.439778 8 1.818953 0.609811 0.370650 8 2.175460 0.135698 -0.808961 8 0.336888 -0.835903 -1.076610	**Frequencies (cm^{-1}):** -418.9059, 52.0246, 109.3219, 193.5729, 206.0677, 243.9031, 265.0664, 305.9954, 329.9836, 394.3882, 493.3689, 578.8569, 632.1809, 667.3136, 762.6743, 897.5366, 905.8476, 935.8951, 969.0417, 997.115, 1049.2376, 1097.0817, 1113.2446, 1175.3603, 1197.1513, 1221.9977, 1272.3986, 1311.7039, 1339.216, 1353.034, 1400.9797, 1416.1922, 1463.159, 1480.0523, 1489.14, 1492.7161, 1502.64, 1513.2438, 2863.1442, 2998.1789, 3022.6606, 3038.3629, 3082.9674, 3092.5045, 3097.7443, 3105.8822, 3110.3199, 3222.2288
IRC:  	

Compound: iPrCHCH$_2$ + O$_3$ CPr$_{FO}$ 1.3	**Energy (kJ mol^{-1}):** -421.581572894556
Reaction Coordinates: 6 -1.722636 -0.305606 -0.339316 6 -1.132967 1.081061 -0.380817 1 -1.637211 1.770975 -1.089374 8 -0.201225 1.480593 0.277090 1 -1.608884 -0.680429 -1.365898 6 -3.233419 -0.193682 -0.064800 1 -3.723034 0.493448 -0.756897 1 -3.417609 0.158993 0.951326	**Frequencies (cm^{-1}):** 22.7539, 37.1159, 49.3316, 70.0925, 83.7541, 117.5065, 139.6232, 218.2234, 242.228, 279.7377, 348.7099, 401.8489, 521.6848, 640.8711, 671.4196, 793.0007, 877.1105, 915.2473, 929.4863, 950.8389, 977.2944, 986.0585, 1131.597, 1154.9966, 1203.2643, 1239.1947, 1298.623,

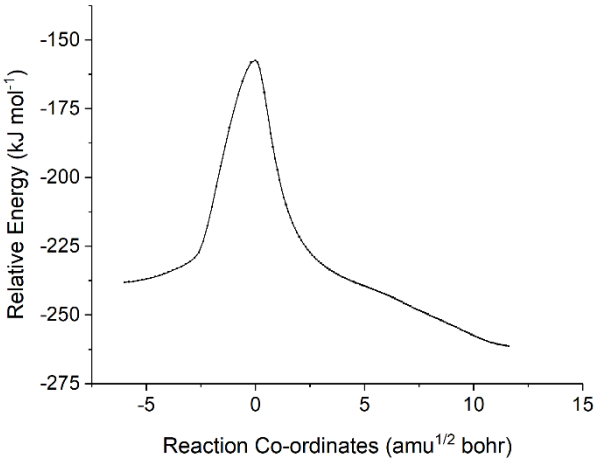
1 -3.705916 -1.169300 -0.172574 6 -1.004987 -1.243055 0.624118 1 -1.068048 -0.867991 1.646898 1 -1.467798 -2.230058 0.599509 1 0.047442 -1.356024 0.364323 6 2.481840 0.735245 0.541850 1 2.710156 1.783998 0.417945 1 2.065207 0.298812 1.439385 8 2.715881 0.010927 -0.448580 8 2.420182 -1.322294 -0.368617	1357.7339, 1404.7236, 1413.9475, 1416.2259, 1436.6102, 1491.1116, 1494.9449, 1507.3512, 1518.2229, 1564.0054, 1780.1142, 2869.8082, 2975.9613, 3025.8981, 3028.6648, 3086.142, 3090.1801, 3100.4348, 3100.9371, 3131.5684

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 2.1	**Energy (kJ mol^{-1}):** -421.544395875342
Reaction Coordinates: 6 1.502390 -0.231591 0.309800 6 0.052185 -0.056060 0.831507 6 -0.801908 1.037413 -0.453065 1 -0.577765 2.081352 -0.275821 1 -0.409801 0.558938 -1.341170 1 -0.009059 0.651744 1.678353 6 2.222963 1.100910 0.103796 1 3.294606 0.939901 -0.016312 1 1.876480 1.620911 -0.791882 1 2.086814 1.767515 0.958094 1 1.987207 -0.733894 1.154726 6 1.606012 -1.163801 -0.893694 1 2.646428 -1.441827 -1.065966 1 1.026311 -2.070410 -0.732064 1 1.246176 -0.692282 -1.811198 8 -2.062660 0.751171 -0.163721 8 -2.306529 -0.530280 -0.364131 8 -0.712967 -1.071288 0.884500	**Frequencies (cm^{-1}):** -439.8666, 78.1629, 82.1265, 199.5032, 210.1044, 244.3427, 267.333, 293.6905, 362.9446, 461.5462, 485.116, 509.9775, 593.3666, 605.2207, 783.6659, 892.0257, 914.4268, 936.922, 970.0781, 985.5263, 1063.5387, 1065.4273, 1140.0712, 1175.9006, 1201.8547, 1234.7876, 1265.9508, 1323.3098, 1338.2654, 1362.9375, 1403.1488, 1419.8783, 1459.5708, 1481.1859, 1490.2068, 1498.5271, 1508.9077, 1509.9834, 2885.7259, 2992.5428, 3019.3287, 3026.4885, 3074.4581, 3078.6545, 3087.432, 3113.1138, 3117.5042, 3232.3755
IRC:  	

Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 2.1	**Energy (kJ mol^{-1}):** -421.580054966628
Reaction Coordinates:	**Frequencies (cm^{-1}):**

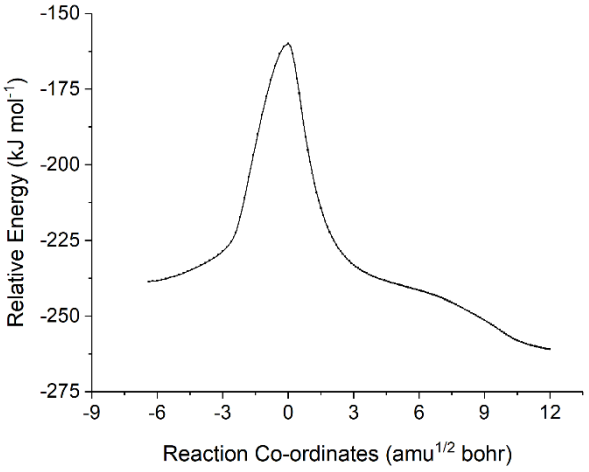
6 -2.381222 -0.219392 -0.353093 6 -1.813590 1.156944 -0.112782 1 -2.573632 1.941267 0.081837 8 -0.641389 1.447646 -0.112654 1 -3.030986 -0.098736 -1.231012 6 -3.288703 -0.601388 0.829947 1 -4.036837 0.166852 1.030926 1 -3.814077 -1.530990 0.614395 1 -2.700763 -0.749307 1.736966 6 -1.313200 -1.265773 -0.648207 1 -1.776329 -2.225636 -0.876271 1 -0.694598 -0.975376 -1.496235 1 -0.654173 -1.404707 0.209150 6 2.571165 0.824812 0.001522 1 3.353665 1.574761 -0.021868 1 1.508202 1.019122 -0.066625 8 2.898563 -0.379528 0.117504 8 4.214428 -0.704176 0.209452	10.2663, 13.699, 30.8959, 46.7721, 68.2393, 99.6978, 112.5829, 206.316, 230.6987, 271.3233, 344.3995, 399.7786, 533.256, 641.3325, 712.3574, 792.5133, 900.2259, 914.3051, 929.1468, 947.2759, 974.8744, 999.1053, 1128.3924, 1155.4511, 1201.9968, 1249.955, 1300.4892, 1358.273, 1405.4629, 1412.8991, 1414.5469, 1434.2356, 1487.4563, 1492.9102, 1505.5189, 1510.3041, 1553.5416, 1786.5053, 2879.0591, 2973.9358, 3029.4267, 3039.9024, 3090.2591, 3099.2232, 3099.8437, 3103.3811, 3108.0653, 3251.5759

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 2.2	**Energy (kJ mol^{-1}):** -421.545516836548
Reaction Coordinates: 6 1.372831 0.030970 -0.334805 6 0.091169 -0.278473 0.468021 6 -1.115802 1.098860 -0.060019 1 -0.955977 1.997570 0.521446 1 -0.862965 1.098060 -1.113290 1 0.162307 -0.005869 1.537733 6 1.954879 1.408111 -0.013839 1 2.120230 1.521123 1.060409 1 2.919410 1.537176 -0.505383 1 1.314560 2.227479 -0.343419 1 1.109516 -0.025607 -1.394085 6 2.391678 -1.077537 -0.037176 1 3.304941 -0.919903 -0.612909 1 2.662394 -1.085867 1.021304 1 1.983292 -2.054404 -0.290056 8 -2.256009 0.507254 0.255131 8 -2.418937 -0.598369 -0.447382 8 -0.565833 -1.331554 0.190396	**Frequencies (cm^{-1}):** -431.9894, 70.1263, 85.5435, 183.1117, 218.2563, 245.8348, 291.6001, 314.5512, 357.1555, 410.4524, 473.9286, 521.7679, 573.598, 599.763, 823.4206, 886.9454, 906.8937, 935.4618, 969.3827, 973.972, 1061.1257, 1090.7668, 1135.2166, 1170.2598, 1188.0958, 1236.8674, 1267.2271, 1311.4285, 1345.4199, 1355.2409, 1400.2544, 1420.4841, 1454.9737, 1483.5552, 1489.2393, 1491.5733, 1507.4891, 1511.4468, 2880.9168, 3020.4031, 3022.1115, 3028.4609, 3076.9525, 3082.1693, 3089.5753, 3106.5812, 3111.4255, 3229.7746
IRC:	



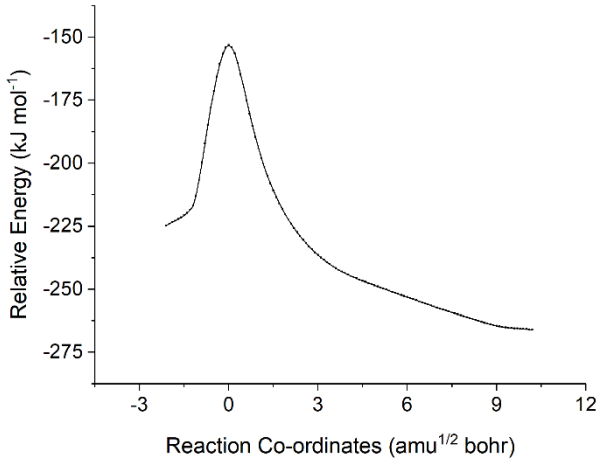
Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 2.2	**Energy (kJ mol^{-1}):** -421.580059414362
Reaction Coordinates: 6 -1.554286 -0.364474 0.000006 6 -1.543689 1.141772 -0.000016 1 -2.549843 1.612705 -0.000036 8 -0.557834 1.840481 -0.000013 6 -2.259649 -0.865076 -1.269671 1 -2.293874 -1.954545 -1.270341 1 -3.287480 -0.499551 -1.321467 1 -1.737665 -0.543515 -2.170986 6 -2.259683 -0.865039 1.269679 1 -3.287515 -0.499513 1.321436 1 -2.293908 -1.954508 1.270380 1 -1.737723 -0.543450 2.170999 1 -0.516861 -0.701445 0.000024 6 2.554197 0.892629 0.000010 1 3.558975 1.299323 0.000027 1 1.631242 1.459840 0.000002 8 2.410418 -0.352642 -0.000003 8 3.509081 -1.152116 0.000005	**Frequencies (cm^{-1}):** 15.319, 17.9783, 36.2105, 52.9113, 70.3453, 101.4084, 120.1214, 204.291, 226.2996, 332.0817, 333.2352, 354.6993, 531.7041, 545.7917, 715.0699, 847.4752, 900.5975, 912.8478, 934.7637, 961.7208, 981.7952, 1000.3116, 1132.8093, 1182.3677, 1187.4294, 1256.2312, 1329.3982, 1345.5344, 1400.0033, 1409.2685, 1413.547, 1429.1656, 1487.5636, 1492.1449, 1504.1205, 1511.5049, 1546.0075, 1785.1476, 2866.0719, 3024.8071, 3027.1485, 3057.9279, 3086.013, 3092.9092, 3094.8721, 3099.7301, 3100.4623, 3247.4671

Compound: $iPrCHCH_2 + O_3$ TS_{FO} 2.3	**Energy (kJ mol^{-1}):** -421.544980801193
Reaction Coordinates: 6 1.402278 -0.058026 0.418528 6 0.109907 -0.601790 -0.241893 6 -1.186692 -0.315182 1.081621 1 -1.151968 -1.109649 1.817085 1 -0.885364 0.682454 1.375346 1 0.066744 -1.705708 -0.254434 6 2.596299 -0.772165 -0.230881 1 3.526712 -0.475344 0.255248 1 2.508693 -1.856684 -0.149806 1 2.667275 -0.516896 -1.289034 1 1.387816 -0.337832 1.477580 6 1.525161 1.457912 0.296003 1 2.437382 1.801385 0.784972	**Frequencies (cm^{-1}):** -425.0795, 73.4791, 82.5356, 189.9308, 200.5459, 243.528, 278.3522, 305.3909, 334.2694, 411.8505, 470.5816, 572.4617, 596.7529, 632.5925, 784.8118, 895.4903, 910.2779, 940.1711, 966.4427, 999.401, 1059.0369, 1091.4508, 1110.5105, 1178.8193, 1195.1416, 1230.5333, 1265.3799, 1325.1646, 1336.0476, 1364.0623, 1402.6247, 1419.5203, 1461.0714, 1478.8689, 1486.9106, 1491.87, 1501.4695, 1508.556, 2890.9125,

1 1.558322 1.755677 -0.750866 1 0.686179 1.984867 0.752395 8 -2.278564 -0.382925 0.333498 8 -2.278847 0.577960 -0.572706 8 -0.378028 -0.005880 -1.255636	2992.4776, 3024.5372, 3035.325, 3085.9546, 3088.2018, 3093.3389, 3106.5334, 3110.5634, 3224.0383
IRC:  	

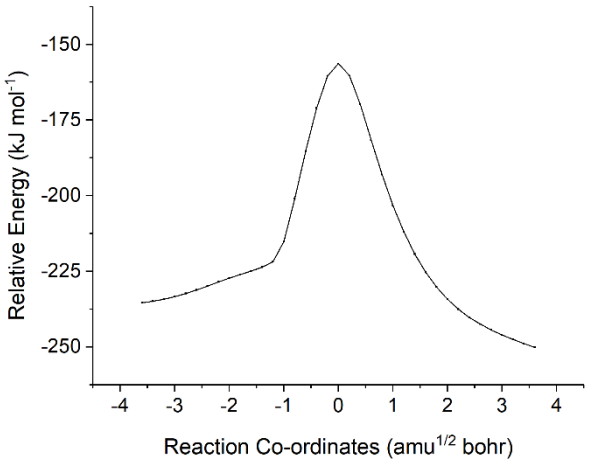
Compound: $iPrCHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (kJ mol^{-1}):** -421.580054966628
Reaction Coordinates: 6 -2.663058 -0.000063 0.262332 6 -1.185849 -0.000084 -0.030573 1 -0.926143 0.000323 -1.110573 8 -0.309246 -0.000497 0.800799 6 -3.296368 -1.269699 -0.326607 1 -4.370600 -1.270696 -0.141020 1 -3.146234 -1.321408 -1.406978 1 -2.875115 -2.170964 0.118918 6 -3.296139 1.270145 -0.325617 1 -3.146002 1.322666 -1.405948 1 -4.370370 1.271194 -0.140023 1 -2.874719 2.170987 0.120606 1 -2.776528 -0.000477 1.347363 6 2.969497 -0.000497 0.723987 1 3.639149 -0.001082 1.576662 1 1.886648 -0.000518 0.769399 8 3.465956 0.000280 -0.426985 8 4.817217 0.000362 -0.567506	**Frequencies (cm^{-1}):** 8.5524, 9.0358, 27.351, 56.1687, 64.5374, 90.8277, 93.9906, 205.5799, 226.6681, 331.437, 333.0352, 355.1537, 534.2178, 549.0834, 716.6831, 846.0596, 900.732, 913.7206, 934.0091, 962.4529, 981.823, 1000.9913, 1133.0875, 1181.9587, 1187.25, 1252.1426, 1324.0491, 1343.4769, 1400.4597, 1411.6399, 1417.1095, 1429.3722, 1488.3531, 1492.1805, 1504.3814, 1511.9163, 1554.4803, 1786.3737, 2867.9827, 3025.438, 3027.7871, 3054.3511, 3086.3454, 3089.3871, 3092.9249, 3099.0212, 3099.653, 3241.2498

Compound: $iPrCHCH_2 + O_3$ TS_{SYN} 1	**Energy (kJ mol^{-1}):** -421.543111711376
Reaction Coordinates: 6 1.191518 0.216488 -0.350071 6 0.011713 0.769454 0.446775 6 -0.958854 -0.620538 1.243752 1 -0.067181 -1.202491 1.527608	**Frequencies (cm^{-1}):** -425.6826, 42.4759, 163.0627, 201.9057, 235.2443, 247.3714, 271.8856, 287.6304, 375.5968, 378.3112, 474.657, 523.043,

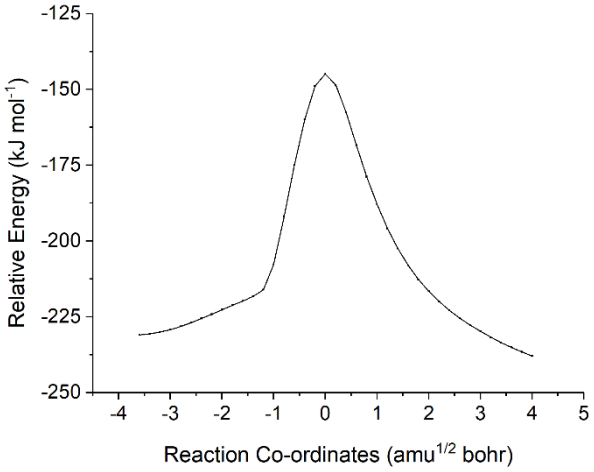
1 -1.433388 -0.086571 2.078896 1 0.284189 1.452789 1.247566 6 2.455757 0.315183 0.512516 1 2.398654 -0.354309 1.373692 1 3.328813 0.022174 -0.069622 1 2.623540 1.328193 0.880728 1 1.280100 0.931702 -1.178084 6 1.062261 -1.177155 -0.971576 1 1.943081 -1.368262 -1.585971 1 1.023840 -1.953858 -0.206804 1 0.174593 -1.262066 -1.587868 8 -1.049021 1.291965 -0.183650 8 -1.522686 0.470900 -1.102107 8 -1.694619 -1.078851 0.314693	576.7051, 701.7327, 842.6803, 880.0824, 925.4797, 932.8609, 965.3255, 975.1141, 1077.7901, 1087.0651, 1149.7792, 1180.8192, 1203.4167, 1224.7214, 1228.8614, 1309.2695, 1338.9401, 1382.9508, 1407.2224, 1418.8307, 1437.2069, 1488.3174, 1491.6007, 1504.8096, 1509.8563, 1543.1175, 2911.6633, 2975.575, 2982.2825, 3024.1978, 3038.792, 3081.4737, 3088.1309, 3100.2355, 3117.5079, 3161.3862
IRC  	

Compound: $iPrCHCH_2 + O_3$ CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -421.581568558205
Reaction Coordinates: 6 -1.637752 -0.075464 0.236235 6 -0.757728 0.606676 -0.734714 1 -0.888131 0.535149 -1.810645 8 0.223614 1.328898 -0.421023 8 0.521543 1.489429 0.915408 6 -3.008563 -0.368417 -0.378281 1 -2.925435 -1.045594 -1.230775 1 -3.651824 -0.845804 0.360304 1 -3.505086 0.542804 -0.713657 1 -1.725314 0.609842 1.084101 6 -0.943363 -1.356204 0.756142 1 -1.567609 -1.806581 1.527917 1 -0.810033 -2.082191 -0.045897 1 0.028387 -1.122486 1.182233 6 3.205163 -0.276724 0.070742 1 2.669689 0.522564 0.608865 1 4.307907 -0.303427 0.166219 8 2.619956 -1.091262 -0.598061	**Frequencies (cm^{-1}):** 16.4307, 31.6879, 50.5018, 56.3772, 94.834, 124.7594, 147.6384, 194.5855, 208.0262, 224.1906, 270.9433, 335.2989, 413.2968, 543.5479, 669.4131, 843.9531, 856.9582, 878.8069, 939.6224, 949.2709, 976.1609, 1109.1502, 1175.761, 1191.5474, 1224.4204, 1282.0887, 1310.7447, 1321.8813, 1376.8559, 1396.9894, 1423.729, 1485.777, 1492.5953, 1502.5179, 1510.4661, 1535.8649, 1569.5776, 1788.7012, 2875.5333, 2979.4695, 3026.0924, 3030.7939, 3040.3919, 3087.5305, 3100.1869, 3102.4617, 3137.7985, 3147.7344

Compound: $iPrCHCH_2 + O_3$ TS_{SYN} 2	**Energy (kJ mol^{-1}):** -421.547239590041

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.083471 0.104408 -0.288535 6 0.022308 0.055170 0.750483 6 1.359156 1.254732 0.191279 1 0.651000 2.052943 -0.073064 1 1.908997 1.426899 1.127071 1 -0.254905 0.312017 1.770928 6 -2.003180 1.300613 -0.034042 1 -1.473658 2.252668 -0.076493 1 -2.487741 1.226578 0.942270 1 -2.787911 1.331446 -0.789431 1 -0.621366 0.198762 -1.269787 6 -1.875804 -1.213888 -0.251879 1 -1.236831 -2.069708 -0.457578 1 -2.355034 -1.360025 0.718161 1 -2.658244 -1.186507 -1.010612 8 0.855294 -0.995501 0.790980 8 1.943347 0.649210 -0.762050 8 1.301563 -1.302620 -0.414592	-438.0669, 75.1877, 137.3063, 197.3475, 210.5116, 235.2839, 270.9712, 312.34, 365.4871, 379.2968, 440.4712, 534.6052, 588.6387, 692.7415, 847.9495, 878.2453, 913.3437, 942.0642, 951.6442, 970.1266, 1068.8619, 1109.3333, 1149.4259, 1186.37, 1190.8205, 1214.1843, 1223.1497, 1326.2098, 1349.3214, 1383.8076, 1401.2727, 1416.3731, 1436.087, 1487.5095, 1494.9006, 1505.4112, 1514.0674, 1539.6042, 2930.5106, 2991.1026, 3024.5625, 3030.6495, 3072.5147, 3085.1524, 3095.4342, 3100.0758, 3114.1698, 3121.7063
IRC  	

Compound: $iPrCHCH_2 + O_3$ CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -421.586425541548
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.147352 0.247239 -0.218730 6 -0.405696 -0.306595 0.933722 6 2.499406 0.492058 -0.507544 1 3.217947 -0.140991 0.035070 1 2.438255 0.324402 -1.594330 1 -0.655972 -0.060126 1.962126 6 -1.754342 1.607748 0.126956 1 -0.978857 2.326604 0.388050 1 -2.456744 1.533007 0.960191 1 -2.301287 1.997110 -0.731331 1 -0.429856 0.343163 -1.032068 6 -2.213025 -0.787740 -0.653013 1 -1.749045 -1.739706 -0.902974 1 -2.955076 -0.945773 0.130858 1 -2.729599 -0.411450 -1.535876 8 0.519305 -1.156032 0.866802 8 1.859045 1.356566 0.046379 8 0.962436 -1.543347 -0.384188	42.9884, 70.9648, 76.9079, 98.1581, 131.5534, 202.8051, 214.9906, 226.7022, 246.7321, 275.3181, 333.9789, 367.5326, 415.5029, 537.0638, 667.3596, 846.9731, 868.391, 884.7019, 939.9079, 947.5612, 976.0918, 1109.3031, 1168.8733, 1181.766, 1191.8521, 1258.692, 1310.7745, 1323.0421, 1379.8692, 1394.8593, 1421.7396, 1487.6545, 1496.1031, 1501.451, 1513.9828, 1526.6834, 1574.6767, 1763.4748, 2930.2457, 2991.6529, 3027.0187, 3033.3404, 3079.2176, 3090.9542, 3102.4676, 3110.5939, 3120.8249, 3143.9122

Compound: iPrCHCH$_2$ + O$_3$ TS$_{SYN}$ 3	**Energy (kJ mol^{-1}):** -421.542915962916
Reaction Coordinates: 6 -1.171447 0.404197 0.420856 6 -0.002221 -0.504293 0.778348 6 1.574450 0.539575 0.918625 1 1.058977 1.412862 1.349133 1 2.139969 -0.060094 1.645705 1 -0.122695 -1.014712 1.731411 6 -2.386336 -0.497045 0.122405 1 -2.582748 -1.200546 0.932424 1 -3.274283 0.121300 -0.009762 1 -2.230248 -1.064309 -0.794935 1 -1.375222 0.933553 1.356951 6 -0.979400 1.450389 -0.679341 1 -0.872300 0.982462 -1.654106 1 -1.855118 2.101168 -0.698730 1 -0.099177 2.067053 -0.514161 8 0.520333 -1.382599 -0.082677 8 0.842559 -0.827281 -1.237525 8 2.012430 0.630421 -0.268458	**Frequencies (cm^{-1}):** -424.0332, 54.1921, 164.6446, 197.4006, 217.3173, 248.4357, 257.2572, 282.7579, 367.2125, 413.2314, 423.4476, 535.5042, 586.4836, 726.4006, 810.2204, 873.0259, 916.2233, 943.0544, 960.0004, 974.2364, 1062.304, 1112.1514, 1126.3256, 1173.6415, 1206.3856, 1224.8545, 1243.9622, 1328.8789, 1372.3091, 1387.4639, 1404.9105, 1423.9809, 1446.1428, 1484.739, 1491.4015, 1501.9742, 1510.407, 1547.5422, 2912.0253, 2975.7323, 3008.9695, 3031.6489, 3043.12, 3094.3905, 3104.4193, 3111.7935, 3114.4054, 3138.1181
IRC  	

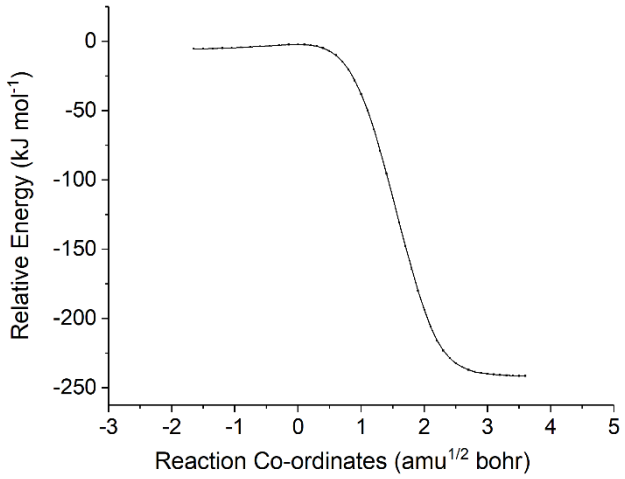
Compound: iPrCHCH$_2$ + O$_3$ CPr$_{SYN}$ 3	**Energy (kJ mol^{-1}):** -421.580710676361
Reaction Coordinates: 6 1.520893 -0.494771 0.434653 6 0.632919 0.533198 1.038950 6 -2.677840 -0.094173 -0.447107 1 -3.054048 0.939278 -0.384252 1 -2.510007 -0.481893 -1.465478 1 0.652659 0.746200 2.103686 6 2.568970 0.176148 -0.481282 1 3.163645 0.912462 0.059771 1 3.244516 -0.591736 -0.858341 1 2.081957 0.664538 -1.321305 1 2.047527 -0.940660 1.281674 6 0.758547 -1.617616 -0.295244	**Frequencies (cm^{-1}):** 38.1986, 61.1304, 72.3379, 83.2116, 123.8316, 181.9359, 201.4732, 218.3971, 234.9382, 239.8214, 301.3795, 341.5884, 420.4379, 531.4752, 742.5517, 796.7005, 864.0164, 876.8295, 945.3088, 962.7793, 974.8579, 1100.9033, 1127.4171, 1177.2125, 1197.9032, 1259.3898, 1332.5329, 1374.3637, 1391.6872, 1399.2576, 1422.9729, 1482.0066, 1494.9367, 1501.3647, 1521.5603, 1528.6612, 1573.8011, 1782.731,

1 0.309503 -1.241983 -1.209453 1 1.467993 -2.408103 -0.542104 1 -0.030059 -2.039044 0.325524 8 -0.174913 1.290629 0.444551 8 -0.357978 1.157600 -0.915332 8 -2.491435 -0.770200 0.534588	2920.2097, 2980.2964, 3031.5362, 3038.4957, 3044.4801, 3097.1427, 3110.1583, 3134.2327, 3146.1413, 3148.9663

6.6 Ozonolysis of 3,3-dimethyl-1-butene (Alkene 4)

Compound: $tBuCHCH_2 + O_3$ PRC1	**Energy (kJ mol^{-1}):** -460.747918632232
Reaction Coordinates: 6 -1.556018 0.113564 0.050119 6 -0.501900 -0.475325 -0.858447 6 0.229484 -1.571762 -0.658509 1 0.933169 -1.914470 -1.404965 1 0.140387 -2.177469 0.232239 1 -0.367284 0.065792 -1.791902 6 -1.666092 -0.630005 1.385704 1 -2.431535 -0.166096 2.009419 1 -0.724579 -0.601572 1.935257 1 -1.945848 -1.674711 1.242427 6 -1.208285 1.593016 0.311663 1 -1.126842 2.148823 -0.624120 1 -0.259717 1.684714 0.839394 1 -1.986945 2.063635 0.914729 6 -2.908423 0.043277 -0.691849 1 -3.197299 -0.990701 -0.884005 1 -2.860724 0.563782 -1.649922 1 -3.692660 0.512151 -0.094436 8 2.629291 -0.656208 0.703386 8 2.969371 0.173683 -0.179812 8 2.299749 1.238717 -0.268100	**Frequencies (cm^{-1}):** 20.9752, 27.8085, 39.6346, 50.3155, 73.444, 141.2924, 198.0121, 226.7068, 266.0898, 285.0322, 294.4728, 322.6663, 351.7982, 389.5477, 403.2121, 526.4817, 703.8628, 714.621, 743.0282, 881.4047, 928.2036, 939.5606, 956.6683, 965.7845, 1017.0365, 1029.8113, 1047.9629, 1092.1299, 1174.8823, 1207.951, 1219.7564, 1230.4804, 1291.0803, 1339.909, 1396.373, 1400.8877, 1423.0517, 1457.7487, 1481.7299, 1488.8813, 1492.7353, 1504.6754, 1505.6074, 1523.5818, 1668.6011, 3018.4823, 3022.2676, 3028.9033, 3078.6139, 3082, 3086.1262, 3089.7601, 3092.1707, 3103.6297, 3110.9391, 3144.7203, 3222.9043

Compound: $tBuCHCH_2 + O_3$ TS_{OZO} 1	**Energy (kJ mol^{-1}):** -460.740227572465
Reaction Coordinates: 6 -1.320621 -0.060305 0.038067 6 -0.128798 0.417549 -0.764193 6 0.650210 1.498675 -0.468364 1 0.487708 2.089416 0.420142 1 1.321619 1.912694 -1.204706 1 -0.037132 -0.013605 -1.754615 6 -1.563594 -1.556746 -0.223158 1 -2.481449 -1.879181 0.270574 1 -0.742824 -2.163747 0.153255 1 -1.671411 -1.756263 -1.291010 6 -1.147131 0.182542 1.543873 1 -1.067774 1.244163 1.780290 1 -0.256939 -0.318691 1.920326 1 -2.013882 -0.204432 2.081610 6 -2.548449 0.731656 -0.474503 1 -2.697168 0.585824 -1.545667	**Frequencies (cm^{-1}):** -173.2116, 53.4758, 74.0635, 130.8142, 188.982, 217.698, 244.989, 267.9473, 277.7023, 294.9671, 356.5905, 366.1715, 405.9267, 417.1546, 485.37, 523.1124, 714.8721, 726.8844, 750.2925, 874.9262, 928.6709, 939.9683, 957.8883, 967.1893, 1003.7728, 1021.1489, 1044.0821, 1086.1013, 1089.1421, 1114.0191, 1213.0876, 1234.2879, 1280.6594, 1315.8212, 1396.066, 1402.4889, 1420.6554, 1454.6801, 1482.1928, 1488.2208, 1491.684, 1503.5983, 1508.1665, 1522.5692, 1579.1913, 3019.6457, 3027.5951, 3034.0885, 3080.5521, 3083.6631, 3087.5153,

1 -2.433335 1.800209 -0.291243 1 -3.449215 0.390465 0.039254 8 2.429120 0.574547 0.539637 8 2.517897 -0.469015 -0.208189 8 1.476996 -1.226415 -0.142517	3092.8533, 3111.5893, 3117.4544, 3147.2671, 3163.2733, 3248.8463
IRC:  	

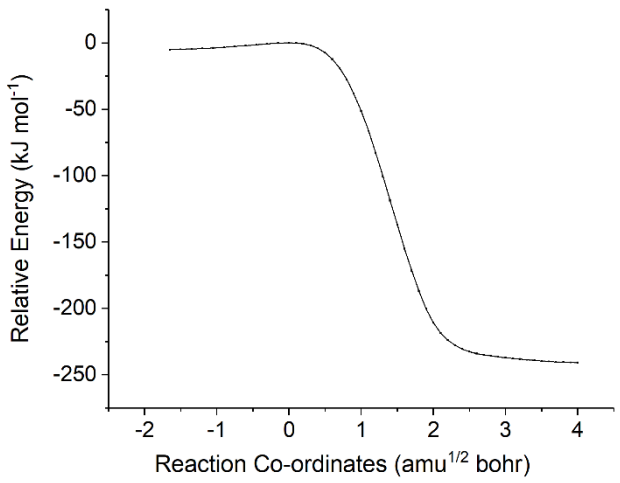
Compound: $tBuCHCH_2 + O_3$ POZ1	**Energy (kJ mol^{-1}):** -460.838705022718
Reaction Coordinates: 6 1.213628 0.005510 0.026760 6 -0.200625 -0.036284 -0.585733 6 -1.153672 1.159420 -0.294663 1 -1.489873 1.622156 -1.224120 1 -0.727867 1.910043 0.366647 8 -2.247924 0.581625 0.407574 8 -2.291035 -0.747106 -0.152567 8 -0.918934 -1.153258 -0.044096 1 -0.116040 -0.163878 -1.669072 6 1.169812 0.174585 1.552218 1 2.185017 0.173935 1.951597 1 0.704530 1.115009 1.850108 1 0.618116 -0.636795 2.023564 6 1.930948 -1.310124 -0.322648 1 2.956443 -1.290487 0.049118 1 1.426098 -2.167057 0.121942 1 1.969221 -1.463830 -1.402892 6 1.973919 1.177962 -0.614300 1 1.520158 2.141126 -0.374652 1 3.000992 1.200547 -0.248043 1 2.012287 1.082740 -1.701285	**Frequencies (cm^{-1}):** 63.0022, 90.2637, 195.919, 204.6776, 248.0985, 257.9683, 283.7115, 316.6226, 344.562, 373.7176, 402.9304, 450.8961, 515.0404, 679.2781, 727.8234, 739.4805, 779.3151, 855.7517, 928.387, 936.6766, 940.5285, 967.5225, 979.334, 1002.6263, 1013.9617, 1027.9546, 1077.1193, 1085.0174, 1219.6125, 1236.7113, 1244.0733, 1282.9195, 1332.0103, 1353.4994, 1382.2459, 1403.8872, 1405.4683, 1438.0277, 1482.1043, 1489.3438, 1491.1048, 1500.5784, 1509.3446, 1515.9998, 1521.8631, 3008.5396, 3020.7625, 3025.7262, 3035.0635, 3042.741, 3079.9965, 3083.095, 3085.4142, 3090.1413, 3102.3099, 3112.5156, 3119.0168

Compound: $tBuCHCH_2 + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -460.748808987932
Reaction Coordinates: 6 -1.580837 -0.099835 0.061272 6 -0.476522 0.428974 -0.825274 6 0.259609 1.526268 -0.650386 1 0.133012 2.182676 0.199753 1 1.010695 1.810622 -1.372802	**Frequencies (cm^{-1}):** 19.8797, 24.4339, 34.6225, 58.879, 73.3649, 137.9603, 198.6455, 225.6877, 263.6759, 284.5335, 293.2917, 324.5644, 350.3662, 389.846, 402.5291, 526.8701, 703.1615, 714.3252, 743.0764, 881.3986,

1 -0.298790 -0.166473 -1.717040 6 -1.229392 -1.544327 0.473327 1 -2.043880 -1.982889 1.052822 1 -0.326401 -1.571760 1.083953 1 -1.061075 -2.174181 -0.401481 6 -1.791684 0.753105 1.316965 1 -2.070846 1.776777 1.063953 1 -0.891519 0.789722 1.932142 1 -2.593076 0.331903 1.925651 6 -2.882288 -0.123204 -0.768454 1 -2.763693 -0.725425 -1.670778 1 -3.171576 0.883750 -1.071339 1 -3.698432 -0.551926 -0.183771 8 2.946779 0.739053 0.424096 8 2.696567 -0.495441 0.427848 8 2.354437 -1.024697 -0.662666	927.134, 938.6203, 959.5706, 964.1097, 1016.9046, 1031.535, 1047.9162, 1091.9431, 1176.316, 1209.7032, 1219.159, 1230.5441, 1290.3448, 1340.0585, 1396.4477, 1400.4938, 1423.2024, 1459.005, 1481.9508, 1487.1665, 1491.2365, 1504.6562, 1505.5852, 1521.7693, 1669.9023, 3018.7848, 3021.3882, 3028.3661, 3080.0748, 3083.0896, 3087.0553, 3088.2139, 3090.9622, 3092.1076, 3116.0388, 3148.8821, 3229.0675

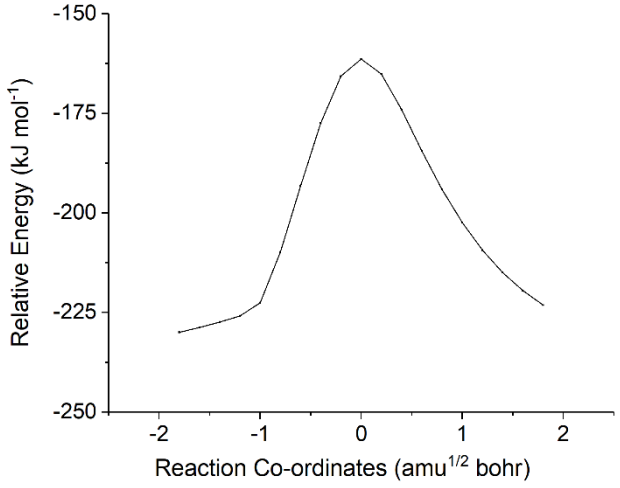
Compound: $tBuCHCH_2 + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -460.737652627627
Reaction Coordinates: 6 1.285637 0.055460 0.046996 6 0.136293 -0.502482 -0.768149 6 -0.678974 -1.538343 -0.400520 1 -0.589166 -2.019802 0.561671 1 -1.283996 -2.040466 -1.137707 1 0.129005 -0.210278 -1.811216 6 1.577454 1.505102 -0.374332 1 2.467835 1.874755 0.136348 1 0.741379 2.158749 -0.132820 1 1.757306 1.572258 -1.449075 6 1.023021 -0.002139 1.559048 1 0.880007 -1.023685 1.912298 1 0.145163 0.580959 1.835256 1 1.878827 0.409117 2.096030 6 2.524048 -0.812412 -0.288970 1 2.735945 -0.804062 -1.359270 1 2.375904 -1.847675 0.018735 1 3.401289 -0.421873 0.230371 8 -2.572348 -0.563436 0.221600 8 -2.125891 0.627827 0.433775 8 -1.532308 1.128220 -0.598508	**Frequencies (cm^{-1}):** -202.764, 49.6219, 77.2099, 137.875, 188.8331, 218.2524, 252.4732, 270.1137, 274.6331, 295.8577, 358.3615, 373.0666, 406.5721, 428.1607, 502.4985, 530.3318, 712.853, 736.7001, 747.7878, 873.5424, 928.3474, 939.8311, 956.0588, 967.2812, 1004.035, 1021.6765, 1044.2414, 1078.371, 1091.9471, 1107.0619, 1212.1957, 1233.4846, 1278.6349, 1311.0007, 1396.1306, 1404.006, 1419.7254, 1452.1761, 1481.6375, 1488.4197, 1492.4708, 1503.3567, 1507.462, 1522.3168, 1572.2168, 3019.9344, 3026.7451, 3034.5833, 3080.6697, 3084.7692, 3089.3558, 3094.1474, 3104.545, 3113.6269, 3155.5359, 3166.1779, 3254.8358

IRC:



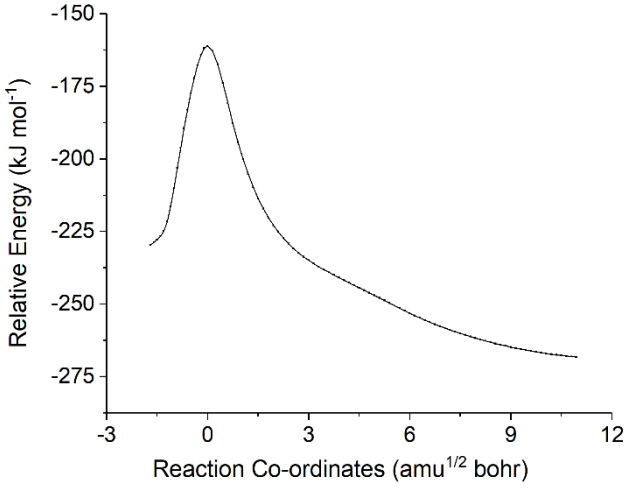
Compound: $tBuCHCH_2 + O_3$ POZ 2	**Energy (kJ mol^{-1}):** -460.838967030957
Reaction Coordinates: 6 -1.189225 0.018606 0.042206 6 0.186079 0.093560 -0.657133 6 1.166633 1.181269 -0.143814 1 0.850758 1.591874 0.815105 1 1.325979 1.981874 -0.862865 8 2.407416 0.501189 -0.011428 8 1.972152 -0.788134 0.441419 8 0.954839 -1.117064 -0.534157 1 0.026415 0.209977 -1.731335 6 -2.003818 -1.095306 -0.636219 1 -2.995770 -1.168089 -0.187948 1 -2.133020 -0.898031 -1.702513 1 -1.511675 -2.061603 -0.528672 6 -1.058802 -0.295533 1.539374 1 -2.051394 -0.400153 1.980144 1 -0.518605 -1.227675 1.698907 1 -0.540691 0.491376 2.087763 6 -1.905818 1.363702 -0.161391 1 -2.000979 1.608595 -1.221581 1 -2.912021 1.319581 0.257409 1 -1.384539 2.186561 0.330775	**Frequencies (cm^{-1}):** 80.9414, 96.4614, 200.2032, 212.8671, 256.9378, 259.0956, 285.0313, 313.8699, 338.6867, 383.4462, 398.0554, 467.1194, 525.9153, 662.9698, 719.4099, 753.0161, 767.4469, 857.8242, 921.1223, 935.8654, 939.3792, 965.7049, 982.5149, 990.666, 1019.1262, 1022.2703, 1057.7392, 1096.5216, 1224.2869, 1237.3991, 1243.1293, 1277.1558, 1315.738, 1346.8597, 1380.6907, 1402.4183, 1404.8018, 1436.5986, 1482.7128, 1488.6269, 1491.328, 1500.52, 1509.9568, 1514.1966, 1521.3757, 3018.5691, 3023.4876, 3033.3006, 3040.9736, 3055.3828, 3077.4865, 3081.8167, 3084.7365, 3089.6497, 3100.2864, 3108.6759, 3119.808

Compound: $tBuCHCH_2 + O_3$ TS_{ANTI}	**Energy (kJ mol^{-1}):** -460.807913787771
Reaction Coordinates: 6 1.253997 0.031559 -0.008810 6 -0.204651 -0.140817 -0.395275 6 -1.384421 1.279574 0.056988 1 -0.996555 1.569809 1.043229 1 -1.070531 1.931455 -0.771088 1 -0.436465 -0.138641 -1.457013 6 1.757867 1.377363 -0.555548 1 2.832148 1.459731 -0.389759 1 1.580681 1.465801 -1.628852 1 1.279969 2.221311 -0.058837 6 2.039212 -1.113083 -0.688769 1 1.918274 -1.090629 -1.772842 1 1.705670 -2.086091 -0.328699 1 3.102587 -1.012645 -0.467501 6 1.457541 -0.036583 1.511750 1 0.911823 0.753204 2.027524 1 1.130055 -0.992196 1.917949 1 2.516366 0.083873 1.742786 8 -0.864880 -1.084895 0.277728 8 -2.093877 -1.239154 -0.190941 8 -2.540154 0.754917 -0.009152	**Frequencies (cm^{-1}):** -427.9662, 66.9154, 124.4447, 175.8749, 213.3112, 221.0846, 253.6687, 264.0743, 281.5983, 333.5843, 348.8622, 385.5841, 431.0333, 500.0593, 523.79, 556.6287, 595.2725, 786.8686, 861.2057, 920.7543, 939.9291, 951.295, 971.0386, 1016.8353, 1036.0295, 1056.1023, 1112.769, 1161.4557, 1218.2013, 1225.7495, 1232.7398, 1264.3559, 1286.1197, 1382.8615, 1385.9267, 1402.8658, 1408.6055, 1442.1557, 1482.9166, 1489.3431, 1490.6338, 1504.9593, 1508.8828, 1522.8035, 1543.6492, 2924.5942, 2988.4185, 3026.3829, 3030.4646, 3039.8335, 3088.6793, 3092.8236, 3097.3189, 3100.8688, 3103.2336, 3112.1022, 3113.5968
IRC:	

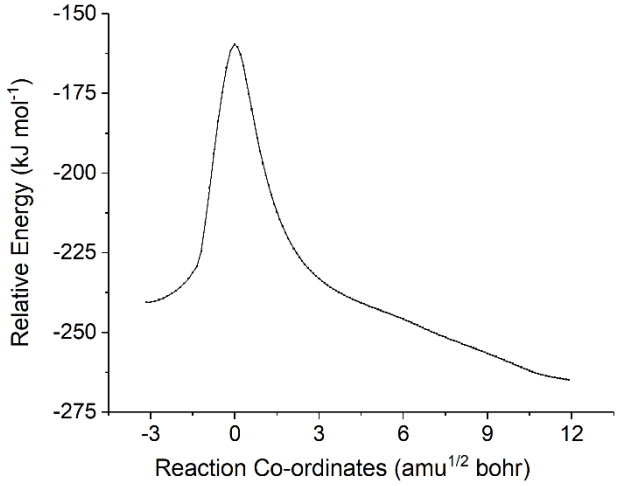


Compound: $tBuCHCH_2 + O_3$ C_{ANTI}	**Energy (kJ mol^{-1}):** -460.847128143048
Reaction Coordinates: 6 1.376085 -0.088090 -0.003468 6 0.016669 0.337877 0.441104 1 -0.386018 0.045284 1.403969 8 -0.660550 1.137025 -0.249674 8 -1.931465 1.442326 0.232323 6 1.468528 -1.617188 0.184869 1 2.475304 -1.946699 -0.073527 1 1.271647 -1.903719 1.218333 1 0.750235 -2.132789 -0.448688 6 2.384829 0.608838 0.943385 1 2.351173 1.692408 0.830799 1 3.392145 0.269670 0.699853 1 2.191382 0.363675 1.988313 6 1.651196 0.298184 -1.460381 1 0.933745 -0.171362 -2.132207 1 1.598094 1.376004 -1.608455 1 2.650541 -0.035315 -1.740026 6 -2.794631 -0.636466 -0.060129 1 -3.406317 -0.427315 0.828095 1 -3.203408 -0.285290 -1.016964 8 -1.812307 -1.362286 -0.010371	**Frequencies (cm^{-1}):** 33.0919, 80.1483, 91.6569, 115.8148, 180.2764, 198.1683, 211.5521, 264.1308, 264.4729, 299.1032, 313.7726, 339.0733, 349.2545, 382.1285, 470.2727, 486.7746, 552.5522, 563.5184, 777.4799, 915.9002, 923.4633, 929.0515, 959.6401, 961.2806, 976.0332, 1045.146, 1068.0272, 1151.7019, 1211.557, 1229.7521, 1252.526, 1299.9684, 1366.0551, 1400.1321, 1409.1103, 1434.8701, 1478.9601, 1488.4947, 1490.0079, 1501.6571, 1503.35, 1511.7506, 1519.6371, 1560.7447, 1701.5902, 2951.1797, 3013.4332, 3029.0496, 3035.5221, 3041.5008, 3094.5849, 3098.5467, 3101.2529, 3105.8247, 3111.5433, 3125.6409, 3172.6784

Compound: $tBuCHCH_2 + O_3$ TS_{FO} 1	**Energy (kJ mol^{-1}):** -460.806199784381
Reaction Coordinates: 6 1.201369 0.045991 0.079732 6 -0.046206 -0.295242 -0.776657 6 -1.380335 1.016967 -0.643277 1 -1.930250 0.771341 -1.543015 1 -0.955838 2.007542 -0.547608 1 0.112311 -0.076139 -1.851531 6 0.899908 -0.037922 1.579254 1 1.825305 0.043928 2.151725 1 0.235332 0.762135 1.905411 1 0.427642 -0.987992 1.824760	**Frequencies (cm^{-1}):** -415.1607, 47.0558, 111.4634, 192.4328, 221.2597, 246.8507, 256.4116, 279.7969, 290.5369, 320.2342, 361.6341, 382.5604, 427.3794, 500.7077, 550.8053, 602.5383, 658.581, 735.4148, 846.7866, 896.359, 932.0378, 944.9353, 966.8849, 988.5781, 1037.7826, 1051.0339, 1054.0568, 1156.0679, 1219.5508, 1223.3527,

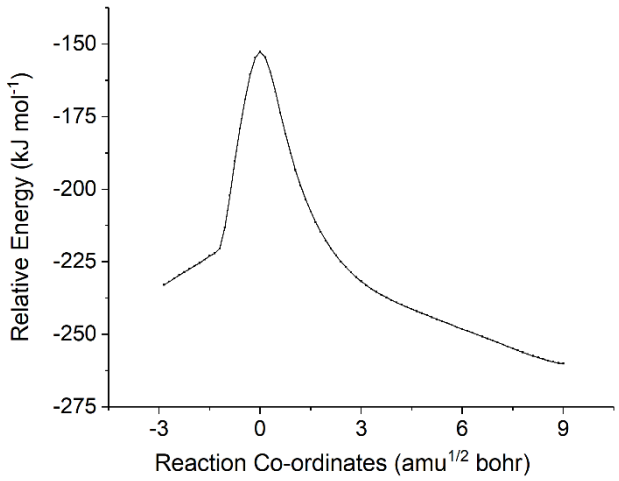
6 1.764730 1.422710 -0.292090 1 1.140028 2.238900 0.073735 1 2.753659 1.556650 0.147982 1 1.873136 1.533382 -1.374122 6 2.239030 -1.034392 -0.293794 1 3.168691 -0.867621 0.252639 1 1.864364 -2.027242 -0.047508 1 2.469632 -1.014184 -1.361152 8 -1.946422 0.610029 0.489598 8 -2.468335 -0.593155 0.339173 8 -0.717117 -1.348045 -0.522561	1240.9579, 1259.8389, 1273.9136, 1328.3108, 1396.8159, 1402.3367, 1419.9622, 1452.7957, 1479.8323, 1483.743, 1487.2575, 1492.1477, 1504.6588, 1512.2248, 1520.732, 2853.5784, 3015.7191, 3021.6464, 3033.7038, 3073.935, 3079.3968, 3084.1055, 3090.4353, 3103.575, 3111.3411, 3114.6542, 3232.1718
IRC:  	

Compound: $tBuCHCH_2 + O_3$ CPr_{FO} 1	**Energy (kJ mol^{-1}):** -460.844648712719
Reaction Coordinates: 6 1.466008 -0.073528 -0.048353 6 0.276263 0.495922 0.705736 1 0.081865 0.015772 1.683446 8 -0.379433 1.454849 0.358900 6 1.446832 0.355815 -1.515891 1 0.581423 -0.063741 -2.029259 1 2.345717 0.001273 -2.022455 1 1.403805 1.440137 -1.609536 6 1.467590 -1.603525 0.084340 1 0.602536 -2.041086 -0.410645 1 1.445042 -1.910357 1.131655 1 2.373523 -2.014528 -0.364013 6 2.708227 0.506518 0.668196 1 2.712389 0.256167 1.730826 1 3.612878 0.087693 0.224892 1 2.748832 1.591870 0.572042 6 -2.844089 0.670853 -0.349858 1 -3.591717 1.369487 -0.000054 1 -2.215221 0.825930 -1.214791 8 -2.742582 -0.380363 0.318179 8 -1.781243 -1.283355 -0.046720	**Frequencies (cm^{-1}):** 23.6945, 42.1485, 64.5446, 85.2077, 123.4399, 175.5768, 202.7348, 210.7067, 246.5091, 252.9231, 277.4417, 329.0533, 352.9024, 387.4666, 408.2708, 523.3427, 592.3784, 676.3936, 762.754, 878.7673, 885.5079, 926.9349, 950.8518, 962.2543, 969.7092, 991.9368, 1057.1577, 1066.5102, 1221.2595, 1240.1147, 1240.6531, 1290.0316, 1394.4655, 1401.0826, 1412.4319, 1415.6833, 1436.1343, 1478.7043, 1488.8281, 1490.3426, 1499.859, 1505.1063, 1521.6685, 1566.3558, 1752.8124, 2908.2859, 3021.1246, 3027.0042, 3033.9386, 3081.0367, 3084.9192, 3092.1511, 3094.6096, 3105.9819, 3113.9051, 3132.0401, 3276.994

Compound: $tBuCHCH_2 + O_3$ TS_{FO} 2	**Energy (kJ mol^{-1}):** -460.804325711020
Reaction Coordinates: 6 -1.281058 0.040659 0.046612 6 0.096344 -0.236835 -0.634762 6 1.274441 1.103341 -0.003805 1 0.976684 1.085070 1.036260 1 1.151053 2.016732 -0.570950 1 0.102393 0.070453 -1.697524 6 -2.260595 -0.909933 -0.673528 1 -3.272978 -0.764894 -0.292593 1 -2.277468 -0.722742 -1.748965 1 -1.974269 -1.949105 -0.515507 6 -1.731664 1.487092 -0.188276 1 -1.664243 1.758208 -1.244585 1 -2.772893 1.610805 0.112451 1 -1.145971 2.205736 0.387262 6 -1.252942 -0.300436 1.538141 1 -2.264721 -0.272710 1.945449 1 -0.842027 -1.295580 1.698167 1 -0.656529 0.406713 2.117513 8 2.428087 0.511911 -0.274101 8 2.547471 -0.610513 0.409942 8 0.721169 -1.307900 -0.352499	**Frequencies (cm^{-1}):** -428.0647, 75.3955, 79.608, 193.1875, 205.3238, 251.616, 257.8282, 287.8297, 291.2593, 316.8282, 364.852, 380.5214, 448.9984, 474.8079, 548.2433, 589.1872, 599.8295, 747.6811, 848.583, 897.2119, 932.4715, 944.4808, 967.5839, 983.9385, 1033.7093, 1045.8249, 1064.5262, 1153.4286, 1219.2475, 1234.0057, 1240.9096, 1252.7717, 1269.8245, 1356.1125, 1398.0518, 1402.781, 1421.6824, 1453.4631, 1478.1369, 1484.706, 1489.3613, 1491.3458, 1505.7067, 1512.2151, 1518.9386, 2875.7615, 3017.7196, 3022.5193, 3030.7187, 3075.9134, 3078.3586, 3080.7929, 3085.3566, 3103.6193, 3114.6758, 3115.3432, 3276.994
IRC  	

Compound: $tBuCHCH_2 + O_3$ CPr_{FO} 2	**Energy (kJ mol^{-1}):** -460.840586382727
Reaction Coordinates: 6 2.005352 0.212990 0.012082 6 1.430106 -1.176427 -0.177979 1 2.185193 -1.948984 -0.434167 8 0.268313 -1.487847 -0.076311 6 2.701963 0.593459 -1.310145 1 3.205542 1.554099 -1.196390 1 3.453408 -0.144941 -1.595734 1 1.983597 0.682912 -2.125793 6 3.056302 0.112757 1.136165 1 3.815000 -0.639198 0.911696 1 3.562457 1.071708 1.252621 1 2.593602 -0.143204 2.090031	**Frequencies (cm^{-1}):** 11.396, 15.5758, 30.163, 48.5833, 67.9821, 98.3662, 102.6532, 200.7514, 245.4581, 249.6845, 275.5111, 322.7194, 347.8046, 387.2013, 400.3139, 533.3561, 595.4158, 713.2967, 763.0783, 880.0023, 901.0339, 925.1852, 949.9415, 963.6473, 967.9614, 999.6208, 1056.6407, 1072.8871, 1225.0375, 1234.1683, 1250.6413, 1294.5485, 1396.9002, 1402.8015, 1411.0335, 1414.6575, 1437.8096, 1480.4426, 1487.8731,

6 0.915532 1.223205 0.368666 1 1.351854 2.213479 0.503560 1 0.162642 1.288925 -0.416086 1 0.407981 0.947513 1.292635 6 -2.935821 -0.836935 0.076434 1 -3.733822 -1.563266 0.180982 1 -1.876275 -1.059617 0.060770 8 -3.238879 0.373842 -0.038906 8 -4.548406 0.734790 -0.029216	1488.9687, 1500.7793, 1506.9716, 1520.3942, 1553.0467, 1785.6276, 2871.0095, 3023.2964, 3026.3714, 3038.2247, 3086.1542, 3089.2872, 3094.0904, 3094.9936, 3099.1029, 3101.0861, 3106.6603, 3251.5731

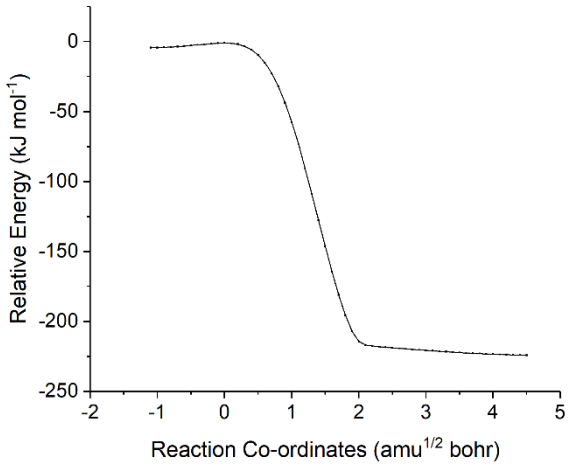
Compound: $tBuCHCH_2 + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -460.803227474852
Reaction Coordinates: 6 -1.077889 -0.070118 0.057406 6 0.145941 0.080572 -0.859902 6 1.463167 -1.214706 -0.439821 1 0.735763 -2.010831 -0.219555 1 1.958812 -1.309768 -1.416219 1 -0.085491 -0.047677 -1.915238 6 -1.970511 -1.157147 -0.566009 1 -1.484363 -2.133849 -0.562467 1 -2.890984 -1.248827 0.010172 1 -2.244491 -0.916546 -1.594863 6 -1.816074 1.287791 -0.003445 1 -2.747169 1.214236 0.559323 1 -2.063448 1.565984 -1.029040 1 -1.215236 2.082065 0.435859 6 -0.792636 -0.424778 1.524041 1 -0.278966 -1.379696 1.620562 1 -0.182397 0.331306 2.006747 1 -1.743965 -0.503917 2.052954 8 2.113478 -0.719334 0.530386 8 1.459820 1.275960 0.458328 8 0.992945 1.111853 -0.766446	**Frequencies (cm^{-1}):** -425.4144, 64.6248, 159.5897, 196.802, 217.8585, 246.8033, 262.3699, 263.6354, 290.013, 327.4105, 362.1603, 401.2858, 412.0539, 448.2173, 530.1381, 575.555, 666.662, 802.7782, 858.9804, 885.9071, 935.2734, 936.3068, 964.9808, 973.0021, 1038.6298, 1063.5455, 1080.85, 1155.7967, 1215.7806, 1224.1488, 1225.3731, 1241.812, 1266.0181, 1385.7089, 1399.9014, 1408.858, 1418.4304, 1446.0029, 1480.6968, 1487.578, 1489.5069, 1502.4986, 1507.8014, 1519.9426, 1545.8924, 2920.2693, 2979.9551, 3024.785, 3030.8529, 3041.511, 3084.3356, 3090.8071, 3096.538, 3102.3258, 3111.1659, 3114.6553, 3150.7715
IRC  	

Compound: $tBuCHCH_2 + O_3$ CPr_{SYN}	**Energy (kJ mol^{-1}):** -460.840483767952
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 1.351542 0.204034 0.043843 6 0.418919 -0.304587 -1.007634 1 0.569428 -0.056402 -2.054980 8 -0.568410 -1.070800 -0.872154 8 -0.954270 -1.494987 0.381025 6 2.373664 1.117694 -0.653897 1 1.888934 1.984614 -1.105621 1 3.097778 1.481800 0.073989 1 2.922859 0.586008 -1.433190 6 2.074160 -1.007135 0.682417 1 2.752675 -0.638246 1.452626 1 2.665748 -1.549810 -0.055994 1 1.359968 -1.689332 1.135669 6 0.593026 1.003221 1.126650 1 0.013982 1.815533 0.689540 1 -0.082302 0.360413 1.681476 1 1.327794 1.429691 1.811217 6 -3.009798 0.237824 0.281116 1 -3.482952 -0.590481 -0.269965 1 -2.972504 0.124529 1.377271 8 -2.586131 1.220210 -0.275996	32.7984, 61.5297, 69.6683, 82.648, 128.3829, 179.6098, 197.3123, 215.4722, 236.5807, 245.008, 268.44, 294.5096, 313.784, 371.082, 393.3987, 397.7969, 539.7448, 662.4144, 787.8568, 862.2408, 874.5096, 922.6193, 939.7233, 949.0031, 975.612, 1048.0368, 1063.4722, 1177.9835, 1213.0975, 1232.5551, 1259.4505, 1272.4446, 1390.3855, 1396.4722, 1402.308, 1430.8369, 1474.9881, 1491.7168, 1493.6594, 1498.4805, 1508.2745, 1525.5754, 1528.888, 1564.637, 1783.9352, 2919.4713, 2979.5986, 3025.4131, 3032.5372, 3039.0573, 3085.6635, 3091.283, 3101.7293, 3105.8382, 3133.8889, 3139.0096, 3151.1234

6.7 Ozonolysis of Methyl Vinyl Ketone (Alkene 5)

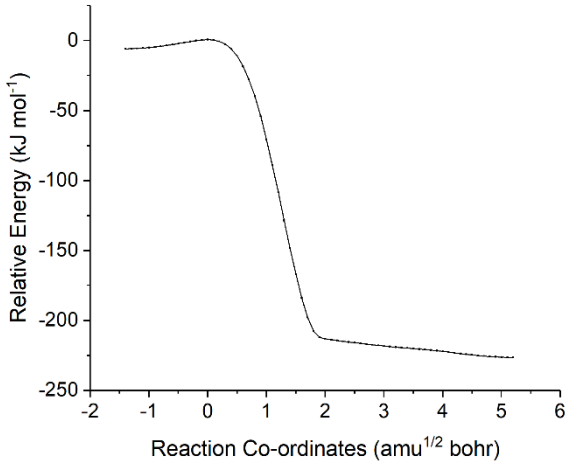
Compound: MVK + O_3 PRC1.1	**Energy (kJ mol^{-1}):** -456.186204464071
Reaction Coordinates: 6 -2.273787 -1.242740 0.247655 6 -1.606138 0.056432 -0.132229 6 -0.652748 0.626881 0.870014 6 0.041622 1.738571 0.622672 1 0.718606 2.162211 1.351241 1 -0.076771 2.253296 -0.321510 1 -0.553592 0.108487 1.816209 8 -1.827993 0.612675 -1.187072 1 -2.827528 -1.121718 1.181878 1 -1.518433 -2.011960 0.423356 1 -2.948578 -1.562280 -0.541270 8 2.319742 0.458297 -0.638151 8 2.367762 -0.558589 0.100102 8 1.409563 -1.375245 0.030299	**Frequencies (cm^{-1}):** 25.1652, 36.7223, 47.9539, 64.4328, 85.0549, 121.6927, 147.0794, 215.8379, 268.6036, 415.6833, 469.5476, 601.0617, 688.15, 743.2286, 775.8423, 959.8374, 1017.9065, 1021.0631, 1046.9848, 1084.0799, 1173.4141, 1194.4722, 1218.4815, 1325.2825, 1385.51, 1438.9693, 1464.814, 1474.0953, 1650.2706, 1764.2321, 3026.8467, 3078.3873, 3142.2081, 3143.8808, 3158.8657, 3236.7308

Compound: MVK + O_3 TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -456.176463083769
Reaction Coordinates: 6 -2.387645 -0.934084 0.233370 6 -1.455063 0.208841 -0.074384 6 -0.297634 0.391824 0.856578 6 0.598738 1.403158 0.664869 1 1.324943 1.660246 1.420186 1 0.445514 2.092756 -0.152282 1 -0.266929 -0.211445 1.753227 8 -1.615027 0.946886 -1.022435 1 -2.792920 -0.829673 1.242583 1 -1.837258 -1.876817 0.205661 1 -3.198787 -0.958906 -0.488492 8 2.143118 0.389185 -0.503316 8 2.037601 -0.799215 -0.018277 8 0.881191 -1.323681 -0.213908	**Frequencies (cm^{-1}):** -213.8916, 61.1693, 79.3428, 109.1123, 120.8863, 217.2586, 275.777, 336.6449, 426.9135, 445.1228, 559.8212, 602.238, 728.0088, 751.1871, 779.7145, 960.3026, 989.447, 1012.0367, 1047.4411, 1078.1309, 1083.7317, 1125.7044, 1196.8924, 1294.8229, 1387.4039, 1434.7779, 1465.6856, 1474.2813, 1565.1569, 1760.2754, 3029.5558, 3082.5417, 3144.1747, 3161.2936, 3183.7802, 3259.794
IRC:  	

Compound: MVK + O_3 POZ1.1	**Energy (kJ mol^{-1}):** -456.263917668777
Reaction Coordinates: 6 -0.035951 0.105209 0.554340 6 -1.390499 -0.239308 -0.078842 8 -1.527315 -1.161856 -0.838353 6 -2.523306 0.677331 0.320785 1 -2.216017 1.725159 0.311114 1 -3.369917 0.529193 -0.343738 1 -2.826409 0.444475 1.344747 6 0.752804 1.185595 -0.263745 1 1.028745 2.025201 0.375819 1 0.229191 1.532983 -1.152714 8 1.896499 0.482653 -0.716978 8 2.127428 -0.434473 0.363108 8 0.817870 -1.022275 0.528469 1 -0.179736 0.457638 1.579588	**Frequencies (cm^{-1}):** 39.8319, 64.6811, 121.8034, 189.8977, 270.7646, 351.0622, 392.0579, 565.2609, 590.1198, 691.094, 726.7123, 743.5035, 802.4903, 921.9484, 944.6164, 965.3995, 989.9505, 1011.3885, 1077.248, 1090.1017, 1181.7339, 1233.4949, 1297.5734, 1351.4365, 1371.1221, 1389.3099, 1463.1151, 1475.8535, 1504.5401, 1807.0867, 3019.1587, 3028.4968, 3044.3941, 3079.2975, 3111.176, 3142.0824

Compound: MVK + O_3 PRC1.2	**Energy (kJ mol^{-1}):** -456.185692055393
Reaction Coordinates: 6 -1.768361 0.036796 -1.411546 6 -1.681642 -0.171711 0.083263 6 -0.804362 0.714471 0.894428 6 -0.114090 1.755807 0.427646 1 0.483356 2.373488 1.084577 1 -0.129655 2.036837 -0.616063 1 -0.784401 0.460127 1.947507 8 -2.315808 -1.046687 0.639997 1 -0.783363 -0.060808 -1.870142 1 -2.140734 1.036440 -1.642461 1 -2.441777 -0.703923 -1.833106 8 2.416744 0.469248 -0.606318 8 2.421691 -0.495439 0.202843 8 1.478286 -1.321415 0.134345	**Frequencies (cm^{-1}):** 13.8291, 37.3665, 39.2477, 54.8898, 69.1285, 122.3891, 147.4387, 182.7936, 277.7078, 439.5153, 492.2799, 536.6631, 699.9927, 746.0101, 760.1504, 946.7037, 999.3233, 1036.6146, 1051.9076, 1075.5961, 1180.009, 1229.3615, 1268.5212, 1309.8637, 1390.1629, 1447.6621, 1473.5714, 1479.3107, 1666.3367, 1742.7163, 3037.2747, 3092.84, 3142.0878, 3146.1354, 3164.5181, 3228.9736

Compound: MVK + O_3 TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -456.175776837179
Reaction Coordinates: 6 -1.683259 0.752385 -1.148698 6 -1.524203 -0.078889 0.100801 6 -0.312699 0.120778 0.948818 6 0.489210 1.230402 0.901369 1 1.193767 1.433839 1.693466 1 0.286139 2.039912 0.217758 1 -0.223990 -0.584943 1.763210 8 -2.348474 -0.901566 0.440423 1 -0.779529 0.713055 -1.757325 1 -1.862604 1.797958 -0.888416 1 -2.532403 0.381308 -1.715324 8 2.090443 0.578254 -0.421748 8 2.075054 -0.681791 -0.136095 8 0.946018 -1.236045 -0.398468	**Frequencies (cm^{-1}):** -239.7593, 68.4941, 75.2044, 116.3488, 130.2459, 224.2828, 274.6178, 340.3414, 443.9796, 499.1452, 535.892, 556.2633, 732.935, 755.1696, 763.2777, 945.8152, 981.5062, 1013.1847, 1047.4781, 1072.5014, 1077.995, 1122.6638, 1260.3178, 1282.465, 1390.5992, 1430.1312, 1470.6713, 1478.9834, 1566.142, 1750.676, 3035.2025, 3093.5565, 3144.24, 3166.099, 3189.4041, 3255.4817
IRC:	

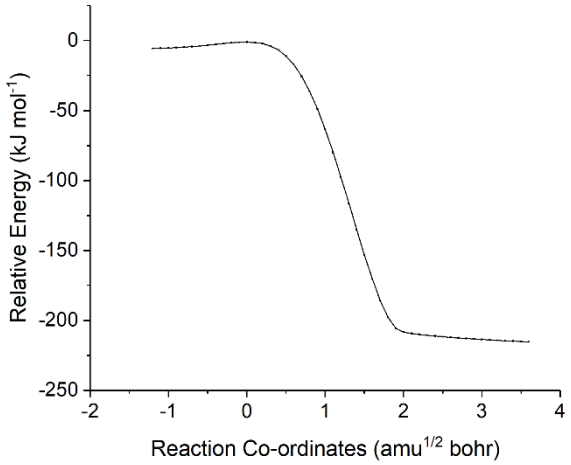


Compound: MVK + O_3 POZ1.2	**Energy (kJ mol^{-1}):** -456.270363446280
Reaction Coordinates: 6 -0.031285 0.358251 0.629461 6 -1.439074 0.079243 0.091395 8 -2.286821 0.923778 0.261559 6 -1.676303 -1.203757 -0.652864 1 -1.553361 -2.050217 0.025314 1 -2.678520 -1.201431 -1.071960 1 -0.928591 -1.335010 -1.437115 6 0.833086 1.162575 -0.392286 1 1.355483 1.976828 0.109527 1 0.270625 1.534856 -1.245619 8 1.744399 0.192246 -0.879231 8 2.035349 -0.541726 0.310211 8 0.698954 -0.850860 0.807377 1 -0.119236 0.909595 1.566286	**Frequencies (cm^{-1}):** 39.6444, 62.7843, 157.772, 203.0661, 259.2476, 395.745, 434.2236, 503.8204, 576.6346, 691.8455, 721.1429, 752.237, 770.8312, 917.0796, 939.2981, 973.6672, 988.9329, 1019.4325, 1051.0396, 1086.3571, 1221.5249, 1249.9633, 1277.1828, 1335.4559, 1353.1419, 1393.3151, 1457.525, 1465.6717, 1503.6053, 1783.9411, 3037.9601, 3053.8701, 3067.2296, 3090.0128, 3127.7285, 3145.6386

Compound: MVK + O_3 PRC 2.1	**Energy (kJ mol^{-1}):** -456.184296396009
Reaction Coordinates: 6 -2.510543 -0.844354 0.361809 6 -1.444574 0.043806 -0.231075 6 -0.671913 0.886659 0.729186 6 0.144838 1.855228 0.308677 1 0.696623 2.473113 1.002305 1 0.254157 2.055876 -0.748848 1 -0.813838 0.702348 1.786848 8 -1.214411 0.070406 -1.423669 1 -3.224682 -0.248693 0.934962 1 -2.055280 -1.551810 1.058946 1 -3.027598 -1.386605 -0.424643 8 2.442947 0.288365 -0.268933 8 1.838443 -0.812408 -0.346211 8 1.315993 -1.257896 0.711170	**Frequencies (cm^{-1}):** 28.5327, 47.0216, 54.3142, 62.5386, 94.0142, 120.6781, 162.2295, 244.4381, 270.1362, 411.7715, 477.3651, 602.5921, 690.6836, 747.1234, 780.215, 960.6413, 1015.0252, 1022.7784, 1046.3593, 1087.121, 1170.2996, 1197.2171, 1216.979, 1324.0682, 1386.2987, 1440.2796, 1464.4503, 1474.0336, 1646.1735, 1755.8299, 3027.2917, 3078.6339, 3142.2433, 3147.3774, 3164.6844, 3240.3602

Compound: MVK + O_3 TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -456.179368879638

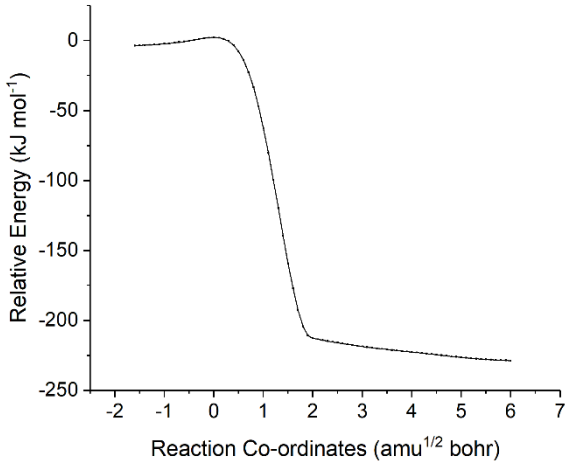
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.527927 -0.565261 -0.351627 6 1.339788 0.186823 0.190265 6 0.331211 0.659887 -0.800352 6 -0.639299 1.541955 -0.428553 1 -1.293580 1.989541 -1.159882 1 -0.635116 1.948518 0.572338 1 0.452132 0.381444 -1.837530 8 1.181462 0.396852 1.376498 1 3.064351 0.047907 -1.079365 1 2.189479 -1.462207 -0.874455 1 3.195318 -0.842919 0.459125 8 -2.264033 0.167262 0.195920 8 -1.560736 -0.869788 0.480517 8 -0.897986 -1.319665 -0.520264	-192.9949, 65.8813, 84.2054, 109.0036, 120.1139, 203.9969, 280.0962, 324.2855, 432.5692, 454.4184, 561.5867, 605.2774, 735.4113, 748.2964, 786.3104, 961.3039, 990.8427, 1011.2114, 1047.5052, 1081.9072, 1088.7532, 1131.49, 1202.0299, 1293.8501, 1387.2427, 1432.7407, 1465.2213, 1475.0606, 1568.3899, 1746.8556, 3030.0093, 3083.0507, 3143.437, 3162.745, 3188.5901, 3261.8399
IRC:	



Compound: MVK + O_3 POZ 2.1	**Energy (kJ mol^{-1}):** -456.265703924772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.035242 0.173014 0.623559 6 -1.355177 -0.250626 -0.039235 8 -1.477161 -1.314060 -0.587657 6 -2.473979 0.761864 0.060758 1 -2.132344 1.765046 -0.203161 1 -3.296286 0.468816 -0.585971 1 -2.828279 0.807665 1.093683 6 0.751479 1.197577 -0.257803 1 0.822766 2.186513 0.189161 1 0.330793 1.256701 -1.263909 8 2.060857 0.659753 -0.289564 8 1.786438 -0.748815 -0.319917 8 0.881561 -0.890936 0.800614 1 -0.232699 0.576760 1.618703	52.8009, 80.8099, 103.7238, 196.4219, 274.3911, 345.5381, 416.1223, 569.7839, 598.237, 667.9194, 713.6482, 760.1832, 809.3153, 915.5681, 944.5131, 949.5872, 984.8064, 1009.3554, 1064.4978, 1102.975, 1183.7054, 1235.1508, 1264.5745, 1350.1193, 1368.1806, 1387.8929, 1462.8419, 1476.727, 1502.2969, 1810.0178, 3026.8142, 3034.1231, 3053.519, 3078.8035, 3120.8821, 3141.2057

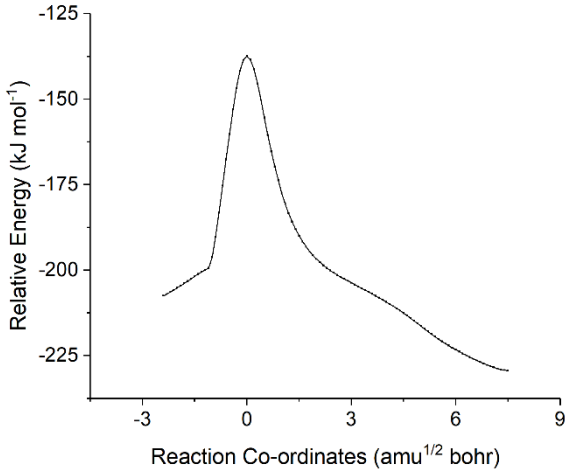
Compound: MVK + O_3 PRC 2.2	**Energy (kJ mol^{-1}):** -456.187382728015
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 2.425476 1.005867 0.680379 6 1.932136 -0.295615 0.085829 6 0.840730 -0.272955 -0.921717 6 0.213240 0.819267 -1.355136 1 -0.577141 0.757639 -2.089935 1 0.462587 1.808675 -0.996085 1 0.575191 -1.253132 -1.299348 8 2.414006 -1.362098 0.417422 1 1.615582 1.535755 1.184439 1 2.810794 1.665641 -0.098788 1 3.215332 0.790513 1.394237 8 -2.414953 0.999763 0.495639 8 -2.512945 -0.232768 0.720966 8 -2.557588 -1.010456 -0.262858	9.797, 16.8509, 25.4758, 44.4003, 54.9495, 115.0277, 126.6031, 134.7706, 278.9148, 438.2648, 492.3555, 537.7589, 701.4315, 746.4181, 760.2428, 946.3918, 1002.6917, 1041.5976, 1051.5711, 1074.9138, 1186.1202, 1240.3115, 1269.8393, 1310.5861, 1390.6799, 1448.7888, 1473.2662, 1479.277, 1673.9462, 1738.7122, 3036.8061, 3090.947, 3141.8085, 3147.7784, 3165.2429, 3230.0541

Compound: MVK + O_3 TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -456.175406279816
Reaction Coordinates: 6 1.519955 0.061624 1.424156 6 1.496447 0.001629 -0.086230 6 0.345567 0.604978 -0.816453 6 -0.505193 1.537388 -0.290670 1 -1.151260 2.112205 -0.935650 1 -0.413137 1.877649 0.729823 1 0.349622 0.415394 -1.880480 8 2.397442 -0.504411 -0.722426 1 0.579539 -0.285034 1.854822 1 1.674020 1.089708 1.759013 1 2.338716 -0.552274 1.788273 8 -2.273724 0.310659 0.238019 8 -1.668686 -0.806032 0.458157 8 -1.019801 -1.236637 -0.561327	**Frequencies (cm^{-1}):** -218.8368, 77.9261, 80.3525, 112.5567, 123.3632, 207.2237, 279.5787, 331.2025, 438.7483, 502.2717, 533.7703, 558.2824, 739.3775, 744.4426, 759.1417, 945.1165, 984.0621, 1013.1188, 1046.2286, 1075.6671, 1084.0607, 1123.9207, 1259.9483, 1284.8398, 1393.1264, 1428.8224, 1469.4788, 1479.8746, 1570.963, 1746.9756, 3034.3912, 3088.9007, 3142.9581, 3165.9298, 3193.8383, 3255.4499
IRC:  	

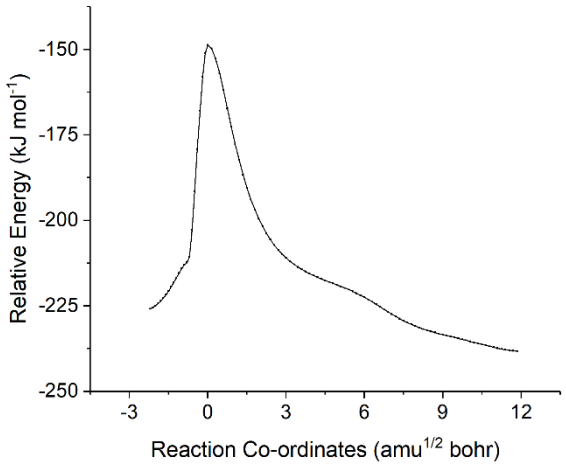
Compound: MVK + O_3 POZ 2.2	**Energy (kJ mol^{-1}):** -456.271438670647
Reaction Coordinates: 6 0.004679 0.255744 0.682591 6 -1.386097 0.202221 0.037909 8 -1.973784 1.247021 -0.122354	**Frequencies (cm^{-1}):** 34.5265, 79.0622, 153.5949, 209.6666, 275.4099, 375.1588, 452.7262, 517.9064, 587.9968, 676.0139, 717.0244, 761.6569,

6 -1.948706 -1.138616 -0.336073 1 -1.988150 -1.788880 0.539857 1 -2.941407 -1.011921 -0.758501 1 -1.289894 -1.632256 -1.052805 6 0.977789 1.183280 -0.106377 1 1.332609 2.029213 0.476566 1 0.521645 1.524366 -1.035317 8 2.105492 0.349740 -0.348915 8 1.503661 -0.947277 -0.460654 8 0.689115 -0.989517 0.737658 1 -0.116669 0.583968 1.716020	787.437, 915.128, 935.5392, 978.1459, 994.8769, 1008.856, 1040.2699, 1103.1051, 1213.7379, 1225.4835, 1262.8074, 1326.3301, 1350.5372, 1390.8592, 1457.7724, 1467.1364, 1513.2989, 1781.1544, 3037.6102, 3062.8456, 3069.4897, 3090.0735, 3132.4128, 3146.0905

Compound: MVK + O_3 TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -456.232838272659
Reaction Coordinates: 6 -2.458428 0.667027 -0.670521 6 -1.455944 -0.164573 0.088034 6 -0.040128 -0.092384 -0.424514 6 0.950213 1.220919 0.520934 1 0.499447 2.082061 0.004250 1 0.592293 1.051275 1.544311 1 0.145060 0.272464 -1.429105 8 -1.732988 -0.836843 1.050963 1 -3.404250 0.676437 -0.136674 1 -2.097605 1.687993 -0.809695 1 -2.607463 0.242763 -1.666559 8 2.153822 0.930557 0.228631 8 1.954555 -0.949425 -0.536329 8 0.736890 -1.119154 -0.067029	**Frequencies (cm^{-1}):** -449.43, 48.0396, 108.4031, 135.0767, 156.1429, 211.2839, 301.2834, 381.1411, 439.5015, 516.3249, 570.4161, 593.8925, 621.5032, 852.6618, 928.2131, 963.8644, 1015.0169, 1035.4144, 1122.2323, 1144.733, 1193.2912, 1219.5422, 1247.5718, 1373.9191, 1386.2511, 1403.7405, 1463.5923, 1472.9588, 1538.14, 1781.3333, 2925.3479, 3004.7894, 3029.8908, 3082.2954, 3140.8823, 3146.3752
IRC:  	

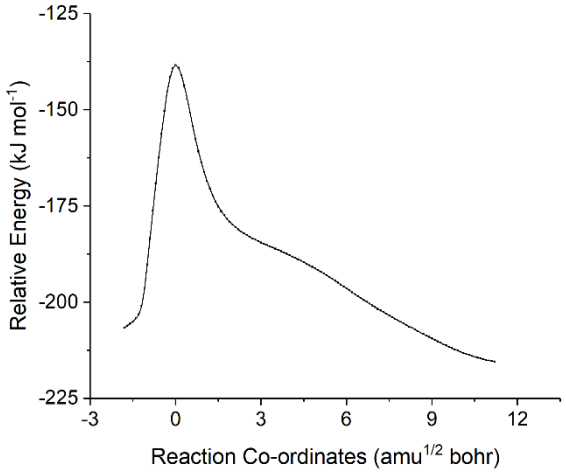
Compound: MVK + O_3 C_{ANTI} 1	**Energy (kJ mol^{-1}):** -456.267801791220
Reaction Coordinates: 6 -2.313645 1.148745 -0.444768 6 -1.629663 -0.092598 0.056606 6 -0.264681 -0.323729 -0.523253 1 0.131893 0.226325 -1.366285	**Frequencies (cm^{-1}):** 45.7147, 61.8857, 76.731, 117.3614, 125.4511, 195.9322, 238.7194, 257.1303, 289.2984, 375.6091, 410.0717, 466.1412, 566.7143, 617.4489, 894.6049, 905.2813,

8 0.455298 -1.211056 0.004113 8 1.721768 -1.342938 -0.461588 8 -2.099222 -0.859251 0.862592 1 -3.283615 1.250495 0.032610 1 -1.695079 2.023352 -0.231145 1 -2.437857 1.101040 -1.529471 6 2.453150 0.869761 0.348764 1 2.788378 0.357529 1.262191 1 3.149346 0.852082 -0.502392 8 1.406652 1.485257 0.308683	936.3848, 1028.7522, 1049.4599, 1170.7255, 1196.8241, 1257.836, 1364.7633, 1393.0743, 1463.0653, 1469.3671, 1509.0535, 1524.0342, 1737.9055, 1772.8094, 2943.3546, 3011.6883, 3028.1983, 3081.0098, 3149.6295, 3193.5725

Compound: MVK + O_3 TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -456.236589638640
Reaction Coordinates: 6 -2.057532 -0.868478 0.786278 6 -1.476243 0.134125 -0.172302 6 -0.021452 0.024332 -0.530276 6 1.010622 1.196305 0.539354 1 0.752409 2.094704 -0.037022 1 0.505212 1.110168 1.511416 1 0.280837 0.409170 -1.497265 8 -2.105202 1.047011 -0.657506 1 -3.092236 -0.609192 0.990469 1 -2.002589 -1.871275 0.358266 1 -1.484191 -0.893049 1.714253 8 2.190147 0.727559 0.425238 8 1.866597 -1.066757 -0.467415 8 0.586982 -1.102592 -0.147623	**Frequencies (cm^{-1}):** -454.4496, 66.3455, 113.74, 126.7112, 155.9432, 206.879, 315.6977, 408.9368, 459.1389, 526.205, 545.709, 590.9745, 608.6009, 830.2059, 882.2389, 1011.3585, 1015.3091, 1040.9621, 1119.7995, 1155.8763, 1214.9454, 1232.7255, 1260.9556, 1359.6662, 1369.2914, 1397.2725, 1461.5483, 1470.043, 1542.254, 1769.1678, 2935.0892, 3003.5502, 3039.3273, 3092.9248, 3148.778, 3157.962
IRC:  	

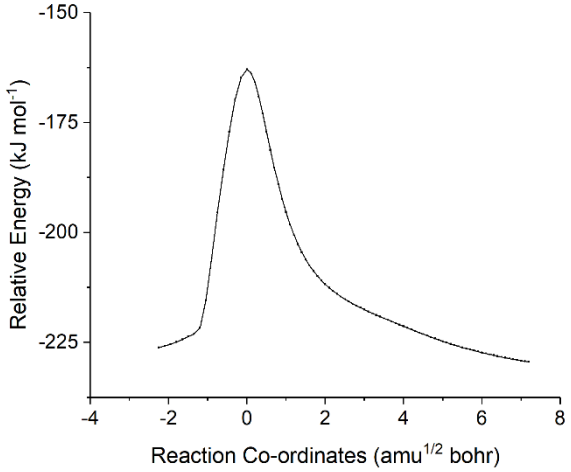
Compound: MVK + O_3 C_{ANTI} 2	**Energy (kJ mol^{-1}):** -456.269159459781
Reaction Coordinates: 6 -0.095987 1.744241 1.034569 6 0.046603 1.027027 -0.277427 6 -0.891099 -0.070254 -0.593223 1 -0.807241 -0.654813 -1.501844 8 -1.829189 -0.321468 0.213992	**Frequencies (cm^{-1}):** 31.8563, 54.4678, 65.0592, 92.0449, 99.277, 152.6856, 165.1055, 168.7825, 191.0045, 227.4592, 399.4823, 501.0133, 559.9164, 572.1996, 834.7722, 916.1473, 1008.3183, 1028.9119, 1049.1463,

8 -2.696457 -1.307620 -0.068713 8 0.887748 1.298684 -1.114904 1 0.639166 2.542132 1.085788 1 -1.100829 2.154887 1.142120 1 0.054760 1.043937 1.857150 6 2.688557 -1.094402 -0.023073 1 2.759318 -0.302587 -0.788526 1 3.577636 -1.732129 0.124772 8 1.686490 -1.255983 0.624058	1212.0972, 1248.4071, 1267.9762, 1344.9359, 1399.4626, 1463.5812, 1472.3116, 1493.5808, 1523.9992, 1729.5467, 1797.6411, 2905.0197, 2977.0259, 3043.8875, 3100.6183, 3147.7651, 3182.2422

Compound: MVK + O_3 TS_{FO} 1.1	**Energy (kJ mol^{-1}):** -456.233801783071
Reaction Coordinates: 6 -2.629214 0.312303 0.428051 6 -1.343745 -0.109337 -0.245885 6 -0.179214 -0.431588 0.718856 6 0.914085 1.169718 0.479058 1 0.326442 2.033673 0.195555 1 1.366901 1.124219 1.460933 1 -0.405375 -0.265321 1.786257 8 -1.217153 -0.214423 -1.436327 1 -3.358436 0.612078 -0.319201 1 -3.026330 -0.521053 1.012488 1 -2.452449 1.131210 1.129093 8 0.616726 -1.362508 0.415935 8 2.328084 -0.356360 -0.154706 8 1.644563 0.713119 -0.518102	**Frequencies (cm^{-1}):** -392.7443, 51.2519, 88.9853, 122.2145, 160.5978, 260.383, 294.056, 362.806, 478.4695, 512.9117, 585.4505, 619.9948, 655.6298, 777.028, 888.3772, 944.2673, 968.7236, 1025.7637, 1051.8813, 1127.388, 1169.3956, 1230.2424, 1274.0007, 1353.6089, 1383.0153, 1457.3047, 1462.4967, 1471.3267, 1485.0196, 1801.985, 2907.1447, 3027.6863, 3078.4389, 3112.8737, 3142.3558, 3234.7384
IRC:  	

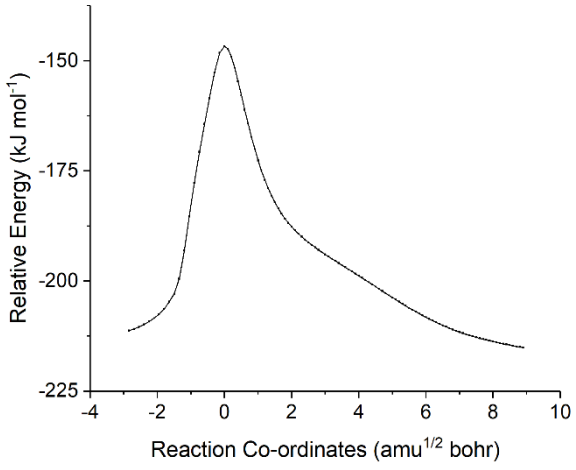
Compound: MVK + O_3 CPr_{FO} 1.1	**Energy (kJ mol^{-1}):** -456.261237431394
Reaction Coordinates: 6 -3.471710 -0.927226 0.000001 6 -2.075395 -0.376525 0.000000 6 -1.952762 1.172903 0.000005 1 -2.903106 1.740678 0.000017 8 -0.889620 1.726544 -0.000003 8 -1.073417 -1.044661 -0.000005	**Frequencies (cm^{-1}):** 12.9334, 24.298, 47.6598, 55.5461, 60.2228, 68.9387, 93.8572, 131.3223, 269.9692, 403.9261, 464.447, 527.9565, 638.8827, 704.2435, 801.0064, 880.213, 894.1198, 974.9287, 1002.235, 1076.7572,

1 -3.451577 -2.012871 -0.000003 1 -4.016866 -0.565446 0.876013 1 -4.016870 -0.565438 -0.876004 6 2.040938 -0.155399 -0.000001 1 1.230484 0.560462 -0.000009 1 1.910578 -1.230673 0.000009 8 3.199967 0.319872 -0.000004 8 4.263186 -0.527908 0.000006	1181.5843, 1231.1907, 1390.1438, 1399.8388, 1406.2772, 1458.9949, 1466.4791, 1549.7646, 1788.28, 1820.4789, 2907.3685, 3023.1795, 3070.8322, 3115.6541, 3148.6348, 3266.5354

Compound: MVK + O_3 TS_{FO} 1.2	**Energy (kJ mol^{-1}):** -456.243731375558
Reaction Coordinates: 6 1.584190 1.248293 -0.664278 6 1.422135 -0.068875 0.036400 6 0.153060 -0.260498 0.881494 6 -0.987986 -1.213735 -0.309987 1 -0.409060 -1.842610 -0.974512 1 -1.606640 -1.669346 0.452403 1 0.254268 -1.100657 1.589124 8 2.230454 -0.967500 0.002510 1 2.487109 1.238048 -1.267901 1 0.709396 1.463191 -1.279862 1 1.631960 2.046425 0.078654 8 -0.545370 0.745167 1.210764 8 -2.180950 0.593623 -0.070399 8 -1.516062 -0.167061 -0.925336	**Frequencies (cm^{-1}):** -399.1707, 58.541, 96.225, 115.3489, 165.4963, 248.2229, 300.9156, 431.8369, 475.537, 516.3623, 577.3178, 602.245, 638.934, 757.5777, 898.9444, 954.5515, 1007.2087, 1024.4438, 1050.7534, 1149.9669, 1214.1893, 1225.073, 1273.2002, 1301.795, 1390.4748, 1445.8418, 1460.4305, 1463.7953, 1486.2758, 1776.3068, 2926.6784, 3041.8535, 3094.4734, 3114.4965, 3148.2134, 3236.7337
IRC:  	

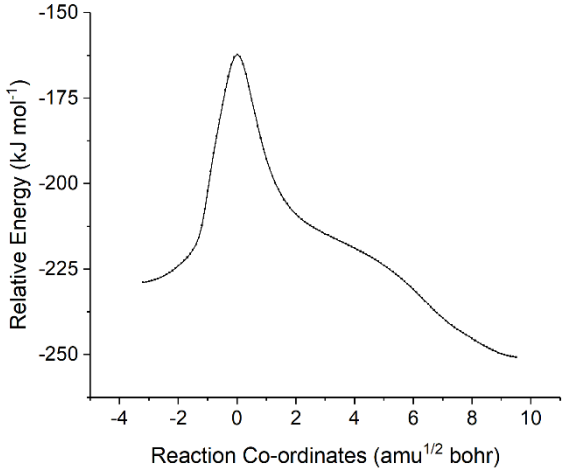
Compound: MVK + O_3 CPr_{FO} 1.2	**Energy (kJ mol^{-1}):** -456.275225635743
Reaction Coordinates: 6 1.190383 1.310987 1.000471 6 0.725366 0.640164 -0.255196 6 1.380465 -0.690316 -0.630040 1 0.908518 -1.182935 -1.498786 8 2.351372 -1.128176 -0.073536 8 -0.069630 1.127068 -1.041284 1 0.600458 2.204108 1.187318	**Frequencies (cm^{-1}):** 53.9394, 60.686, 76.1751, 104.1622, 126.9361, 177.1163, 195.0446, 226.753, 256.5464, 474.1684, 489.1827, 525.4362, 585.7249, 678.047, 785.7371, 883.2559, 922.3838, 1002.9041, 1014.9957, 1066.272, 1240.8945, 1251.3296,

1 1.126959 0.620667 1.839930 1 2.243317 1.580446 0.890716 6 -2.404595 0.015632 -0.516346 1 -3.230413 0.713732 -0.544386 1 -1.955023 -0.438451 -1.387586 8 -1.993079 -0.273829 0.628030 8 -0.919103 -1.119610 0.726724	1367.3749, 1392.1778, 1416.4431, 1455.3903, 1467.1276, 1566.9828, 1727.7281, 1795.1644, 2937.3654, 3041.4918, 3104.7907, 3132.6877, 3147.2852, 3278.1482

Compound: MVK + O_3 TS_{FO} 2.1	**Energy (kJ mol^{-1}):** -456.235933348061
Reaction Coordinates: 6 2.674078 -0.053627 0.678362 6 1.457783 0.056468 -0.207402 6 0.151656 -0.497014 0.446727 6 -0.917679 1.092169 0.238209 1 -0.648792 1.840918 0.973852 1 -0.671998 1.230406 -0.809083 1 0.201937 -0.583732 1.546082 8 1.480277 0.482159 -1.330164 1 2.500351 0.452882 1.630100 1 2.863169 -1.103960 0.910439 1 3.536950 0.375404 0.176888 8 -2.074599 0.524168 0.509964 8 -2.400842 -0.375867 -0.402107 8 -0.501916 -1.355447 -0.198148	**Frequencies (cm^{-1}):** -373.8862, 47.9332, 104.9092, 128.5647, 192.7982, 262.3019, 292.3149, 329.2256, 469.2277, 508.4486, 578.1971, 590.179, 635.4187, 781.1971, 893.6734, 942.9455, 994.9344, 1033.9196, 1051.5928, 1128.5684, 1164.1758, 1235.6424, 1265.8626, 1374.3464, 1381.9386, 1461.7703, 1462.263, 1468.5781, 1484.837, 1799.9629, 2909.0047, 3031.5805, 3084.6314, 3090.8587, 3144.0005, 3223.9552
IRC:  	

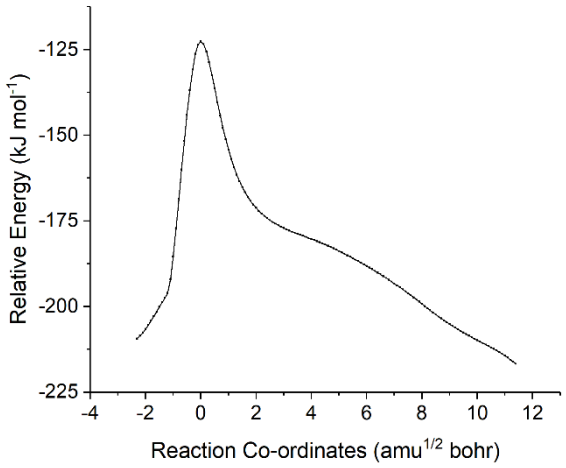
Compound: MVK + O_3 CPr_{FO} 2.1	**Energy (kJ mol^{-1}):** -456.271731817866
Reaction Coordinates: 6 -1.721235 -1.482475 0.092313 6 -0.929117 -0.287327 -0.357640 6 -1.075631 0.996973 0.475093 1 -1.536612 0.867110 1.470286 8 -0.736911 2.076456 0.065379 8 -0.277558 -0.266802 -1.388274	**Frequencies (cm^{-1}):** 59.3232, 94.9443, 107.7437, 127.4285, 139.6416, 188.7177, 216.2572, 286.1673, 297.1954, 407.7125, 507.3407, 529.2019, 647.9601, 704.8725, 838.4876, 871.6352, 907.7392, 991.3869, 1041.0014, 1060.635, 1192.0423, 1246.3283, 1391.2578,

1 -1.704627 -1.587203 1.175181 1 -2.762377 -1.345382 -0.216645 1 -1.336323 -2.383464 -0.377532 6 1.954812 0.275095 -0.574796 1 2.646569 0.050486 -1.376199 1 1.437029 1.218110 -0.468830 8 1.845731 -0.623968 0.289823 8 0.904160 -0.414842 1.281061	1400.2652, 1423.2827, 1459.141, 1476.8179, 1569.3358, 1713.6052, 1789.1469, 2931.6461, 3023.6138, 3100.183, 3127.243, 3146.0529, 3271.4158

Compound: MVK + O_3 TS_{FO} 2.2	**Energy (kJ mol^{-1}):** -456.242451639511
Reaction Coordinates: 6 1.912254 1.044420 0.745859 6 1.498110 -0.141046 -0.078343 6 0.115006 -0.058808 -0.771984 6 -0.870364 -0.972833 0.591237 1 -0.681174 -2.035210 0.506292 1 -0.521360 -0.431210 1.461742 1 0.018954 -0.798494 -1.581889 8 2.186568 -1.109132 -0.282359 1 2.206537 1.845327 0.063664 1 1.081734 1.436881 1.330714 1 2.755955 0.779525 1.377164 8 -2.067067 -0.628918 0.148927 8 -2.255744 0.676508 0.236152 8 -0.462592 1.058140 -0.862508	**Frequencies (cm^{-1}):** -382.7959, 83.3289, 93.8653, 112.8644, 168.3644, 265.3785, 275.6913, 411.6495, 474.4676, 522.5809, 573.4957, 584.1742, 591.8783, 764.769, 887.8157, 983.7593, 1001.0583, 1019.419, 1057.1311, 1138.0785, 1191.0141, 1224.6572, 1270.1325, 1335.5451, 1389.7996, 1456.5515, 1460.1777, 1466.8585, 1479.9492, 1783.6133, 2953.0055, 3042.316, 3100.474, 3109.3534, 3148.5338, 3235.1353
IRC:  	

Compound: MVK + O_3 CPr_{FO} 2.2	**Energy (kJ mol^{-1}):** -456.275122940607
Reaction Coordinates: 6 -1.247554 1.382559 0.870913 6 -0.682153 0.606821 -0.279470 6 -1.296199 -0.761873 -0.575032 1 -0.732533 -1.343716 -1.325648 8 -2.330732 -1.136621 -0.090723 8 0.142119 1.045960 -1.068018 1 -2.275115 1.666053 0.630845	**Frequencies (cm^{-1}):** 58.8116, 71.3915, 86.0205, 118.2147, 135.5804, 194.4754, 212.675, 255.0958, 269.9623, 472.6693, 487.2115, 527.8133, 591.9795, 685.0056, 785.8178, 889.4603, 931.3019, 1004.9923, 1015.2932, 1062.4168, 1237.3704, 1249.4216,

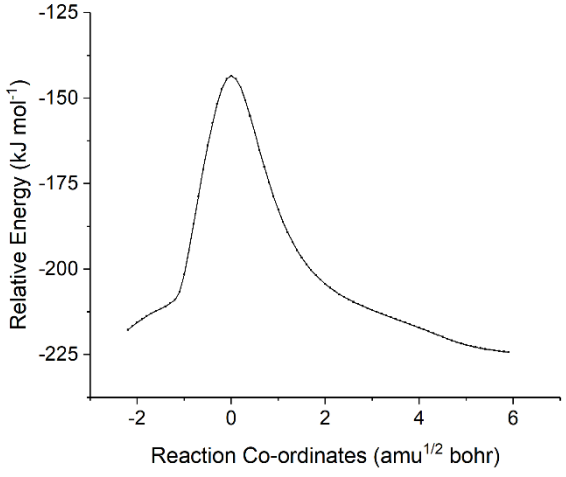
1 -1.288999 0.765117 1.766004 1 -0.658282 2.279076 1.045297 6 2.403063 0.315613 -0.142601 1 3.157830 0.343420 -0.916879 1 2.118274 1.163478 0.462928 8 1.889084 -0.806215 0.060931 8 0.876515 -0.869643 0.984635	1367.5519, 1394.5357, 1414.4214, 1456.963, 1465.5547, 1566.407, 1711.392, 1792.1496, 2941.2295, 3040.1755, 3104.7426, 3135.8213, 3144.6956, 3280.2475

Compound: MVK + O_3 TS_{SYN} 1	**Energy (kJ mol^{-1}):** -456.227716334814
Reaction Coordinates: 6 2.426203 0.672562 0.099725 6 1.236581 -0.240875 -0.097325 6 0.072437 0.049665 0.831626 6 -0.936919 1.440575 -0.120451 1 -0.104140 1.863063 -0.701729 1 -1.213333 2.012960 0.776513 1 0.352374 0.421767 1.813176 8 1.235358 -1.166289 -0.863419 1 3.035772 0.669197 -0.799809 1 2.131689 1.690750 0.352528 1 3.028338 0.286787 0.926186 8 -1.838214 0.802117 -0.737073 8 -1.460716 -1.141768 -0.193520 8 -0.938993 -0.803571 0.962973	**Frequencies (cm^{-1}):** -412.3666, 68.8092, 77.0806, 102.8744, 166.2176, 214.635, 303.8893, 348.8722, 443.0383, 517.5128, 534.1209, 607.3324, 691.7491, 826.0602, 905.1487, 946.9895, 987.6442, 1033.3464, 1079.1374, 1132.2614, 1172.1207, 1218.7098, 1232.7591, 1382.7142, 1390.2723, 1432.6396, 1467.5, 1478.2829, 1549.8312, 1795.0323, 2922.0895, 2981.0897, 3034.3827, 3094.5817, 3134.144, 3143.3892
IRC  	

Compound: MVK + O_3 CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -456.254760711605
Reaction Coordinates: 6 -1.425189 1.440524 0.003720 6 -1.411455 -0.061487 -0.045699 6 -0.047306 -0.778545 -0.117003 1 -0.218768 -1.851133 -0.227530 8 0.706005 -0.618752 1.092319 8 1.561684 0.522397 0.791353 8 -2.407208 -0.744557 -0.015773	**Frequencies (cm^{-1}):** 40.8735, 94.5141, 133.6361, 197.8858, 248.6756, 366.4592, 420.9936, 534.36, 595.9659, 728.2163, 770.948, 788.7789, 866.3244, 918.818, 962.3184, 1022.4898, 1042.8244, 1050.1093, 1098.7346, 1154.3248, 1231.5943, 1251.7324,

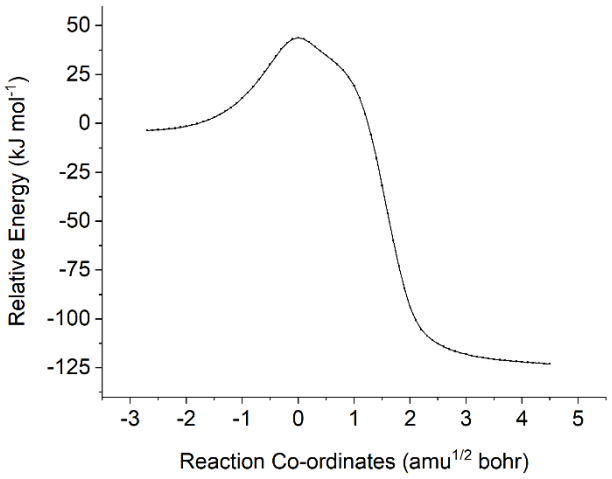
1 -2.437369 1.788714 0.189564 1 -0.746691 1.803049 0.776453 1 -1.067055 1.838842 -0.947135 6 1.956056 0.184044 -0.515482 1 2.322196 1.089429 -0.996199 1 2.702501 -0.615165 -0.505658 8 0.766087 -0.254207 -1.148238	1294.2001, 1342.3101, 1390.1755, 1390.7328, 1466.3643, 1468.781, 1519.158, 1789.2763, 3020.1158, 3042.417, 3064.6143, 3099.495, 3116.7905, 3144.441

Compound: MVK + O_3 TS_{SYN} 2	**Energy (kJ mol^{-1}):** -456.235446436955
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.405586 1.160045 -0.783167 6 -1.309263 -0.076261 0.057198 6 -0.038809 -0.406207 0.830238 6 1.057850 -1.298079 -0.439971 1 0.233184 -1.795317 -0.969724 1 1.620397 -1.947312 0.244549 1 -0.225806 -1.084522 1.656213 8 -2.211027 -0.873039 0.183576 1 -1.119898 2.043605 -0.212163 1 -0.700275 1.096177 -1.612281 1 -2.425033 1.250852 -1.148361 8 1.675215 -0.360806 -1.039178 8 1.262039 1.250734 0.174166 8 0.872808 0.503052 1.188434	-430.9151, 34.0089, 116.1417, 188.1295, 210.7973, 248.366, 308.054, 355.0012, 467.6908, 520.673, 532.1735, 606.878, 682.2697, 818.9488, 888.0324, 953.8825, 1023.8396, 1044.7669, 1069.8456, 1155.004, 1211.2032, 1217.5216, 1241.0192, 1365.5391, 1397.2773, 1400.6883, 1453.1952, 1463.6239, 1546.387, 1760.1253, 2935.1069, 3001.7206, 3046.3406, 3103.6425, 3145.2972, 3156.4383
IRC	



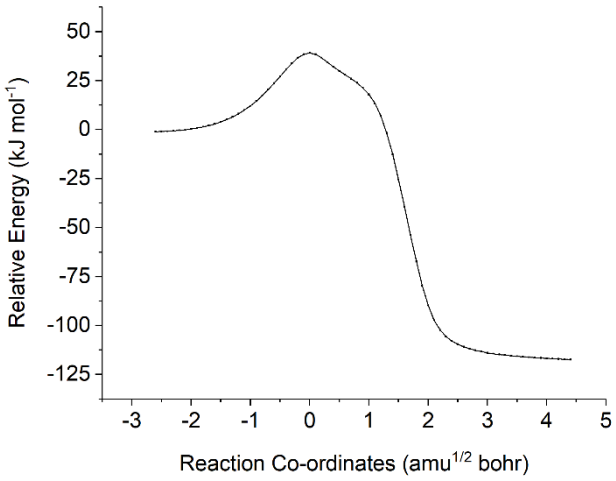
Compound: MVK + O_3 CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -456.266282922429
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.234499 -0.424668 1.440329 6 1.462391 -0.358324 -0.034013 6 0.700090 0.581001 -0.913190 1 0.903906 0.528467 -1.975872 8 -0.145538 1.469853 -0.616023 8 -0.537283 1.683428 0.660400 8 2.275421 -1.040122 -0.627906 1 1.894262 -1.177924 1.863317	27.5161, 53.8334, 60.2462, 77.6675, 79.4991, 94.2378, 117.2288, 190.828, 241.7392, 324.3854, 348.1024, 498.3069, 586.7428, 667.394, 818.0278, 861.8707, 912.8046, 1041.7754, 1051.2307, 1214.8147, 1258.3245, 1269.8904, 1361.0742, 1398.4759, 1442.5145,

1 1.408909 0.552141 1.892422 1 0.189221 -0.660725 1.637915 6 -2.786998 -0.693538 0.061734 1 -2.754285 0.281330 0.574482 1 -3.781454 -1.150814 -0.091184 8 -1.782657 -1.238071 -0.320251	1455.2084, 1503.0485, 1526.4095, 1732.9327, 1793.6549, 2899.5505, 2984.8016, 3046.6356, 3105.4746, 3145.0683, 3186.8609

Compound: MVK + O_3 TS_{EPOX} 1.1	**Energy (kJ mol^{-1}):** -456.157741160206
Reaction Coordinates: 6 2.372363 1.219189 0.145472 6 1.970434 -0.228531 -0.034048 6 0.596743 -0.558118 -0.421492 6 -0.420982 0.361131 -0.689668 1 -0.177387 1.413846 -0.727808 1 -1.228915 0.088851 -1.371390 1 0.371587 -1.616720 -0.440846 8 2.771677 -1.137223 0.129112 1 2.253593 1.775819 -0.786236 1 1.752594 1.707392 0.899753 1 3.412976 1.258793 0.453735 8 -1.314430 0.284856 0.756217 8 -2.490470 -0.371010 0.562760 8 -3.153751 0.049626 -0.451689	**Frequencies (cm^{-1}):** -363.7337, 70.6413, 76.1798, 84.4809, 124.0222, 207.0942, 284.7645, 300.9347, 423.627, 490.6217, 531.8628, 560.5861, 702.0273, 768.2866, 818.2928, 852.9195, 936.3861, 1037.872, 1048.3906, 1111.3101, 1138.6885, 1200.9445, 1261.2767, 1273.2853, 1393.6342, 1417.5546, 1469.592, 1479.968, 1530.8559, 1684.8269, 3033.0059, 3036.7886, 3086.3731, 3143.8248, 3178.9395, 3195.9407
IRC  	

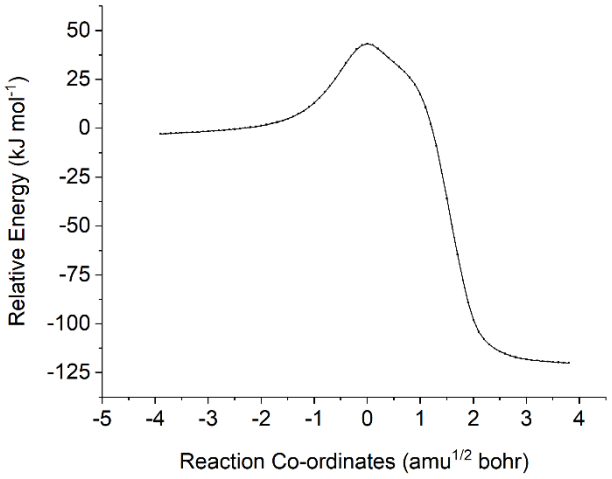
Compound: MVK + O_3 C_{EPOX} 1.1	**Energy (kJ mol^{-1}):** -456.237983457170
Reaction Coordinates: 6 -2.466710 -0.972373 -0.347683 6 -1.800689 0.351252 -0.078622 6 -0.307932 0.371180 0.112919 6 0.347410 -0.456722 1.139433 1 1.267840 -0.088363 1.585213 1 -0.233879 -1.132757 1.756100 1 0.162801 1.308445 -0.160892 8 -2.404177 1.398571 -0.019369 1 -2.165255 -1.729251 0.377202 1 -2.151484 -1.340928 -1.326042	**Frequencies (cm^{-1}):** 25.1203, 50.8199, 64.6142, 79.9012, 102.2431, 116.7645, 168.8343, 241.2261, 289.4099, 478.6073, 505.1174, 594.4314, 739.1458, 848.2764, 899.2998, 926.9053, 1010.4641, 1065.0937, 1100.3737, 1155.5005, 1163.8258, 1248.5124, 1270.2424, 1388.2352, 1393.7366, 1457.9456, 1469.3082, 1516.7315, 1554.5188, 1776.2175, 3039.7218,

1 -3.545162 -0.843779 -0.331474 8 3.219396 0.408674 0.221193 8 2.754970 0.010874 -0.826116 8 0.433894 -0.809792 -0.232756	3074.572, 3092.5363, 3145.6767, 3147.8589, 3168.1347

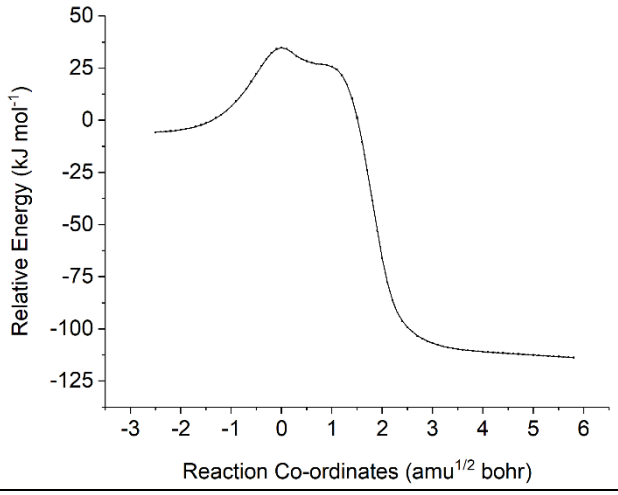
Compound: MVK + O_3 TS_{EPOX} 1.2	**Energy (kJ mol^{-1}):** -456.157706885861
Reaction Coordinates: 6 3.014242 -0.928622 0.054496 6 1.918270 0.106674 -0.031066 6 0.607854 -0.349513 -0.516208 6 -0.466132 0.528120 -0.650178 1 -0.263312 1.578892 -0.493819 1 -1.266120 0.319286 -1.359043 1 0.460984 -1.404367 -0.709081 8 2.099927 1.272407 0.285261 1 2.735758 -1.709644 0.765841 1 3.159284 -1.414683 -0.912638 1 3.941363 -0.461088 0.373183 8 -1.343355 0.147453 0.785998 8 -2.471177 -0.539072 0.501250 8 -3.187064 -0.011830 -0.423346	**Frequencies (cm^{-1}):** -357.4571, 70.5253, 74.51, 83.0025, 94.6134, 212.0457, 280.3727, 288.4289, 418.7204, 430.0018, 567.1329, 600.699, 703.0029, 778.5998, 806.8366, 865.016, 960.8074, 1036.3252, 1047.0311, 1110.9736, 1137.764, 1191.1131, 1216.2221, 1266.7283, 1388.3592, 1427.8315, 1465.1762, 1474.4465, 1518.0095, 1701.9516, 3028.5546, 3065.2749, 3079.8954, 3143.4076, 3174.3138, 3203.067
IRC  	

Compound: MVK + O_3 C_{EPOX} 1.2	**Energy (kJ mol^{-1}):** -456.234735203125
Reaction Coordinates: 6 -2.561677 1.317820 0.127750 6 -1.780184 0.042353 -0.058778 6 -0.288075 0.150714 0.162389 6 0.424578 -0.952380 0.830713 1 1.323848 -0.723407 1.399011 1 -0.135004 -1.830635 1.130949 1 0.129506 1.149012 0.236082 8 -2.290305 -1.012335 -0.349626 1 -2.270517 2.041739 -0.637536 1 -2.330747 1.770845 1.094753 1 -3.626788 1.117628 0.055544 8 3.078768 0.510274 0.431040 8 2.699711 0.412998 -0.719481	**Frequencies (cm^{-1}):** 34.6389, 46.4953, 72.4901, 91.0171, 105.0959, 135.9993, 194.9677, 245.2737, 307.073, 374.7759, 592.0944, 610.8883, 761.7105, 853.6271, 894.101, 955.6863, 994.5565, 1057.3085, 1107.2086, 1160.1364, 1164.5938, 1198.2811, 1276.333, 1385.7006, 1414.6763, 1463.3374, 1473.2375, 1496.8147, 1539.317, 1790.8004, 3026.0246, 3063.0831, 3076.7372, 3133.7968, 3144.0415, 3174.4668

8 0.529558 -0.770465 -0.568338	

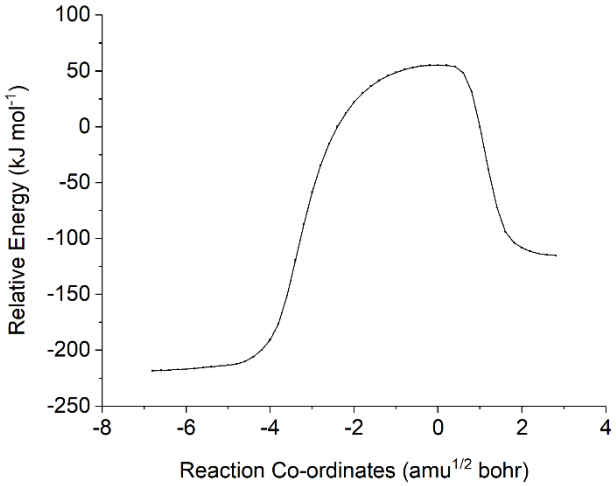
Compound: MVK + O_3 TS_{EPOX} 1.3	**Energy (kJ mol^{-1}):** -456.159268181460
Reaction Coordinates: 6 -1.100004 -1.472390 0.247930 6 -1.716304 -0.116765 0.008501 6 -0.911324 1.093518 0.203876 6 0.409197 1.134834 0.667464 1 0.828115 2.104743 0.896577 1 0.797971 0.344659 1.310857 1 -1.416309 2.012450 -0.064903 8 -2.883146 0.009446 -0.334982 1 -0.296647 -1.655242 -0.469522 1 -0.658196 -1.543019 1.243338 1 -1.863794 -2.236040 0.133481 8 1.288781 0.744845 -0.739246 8 1.880990 -0.475764 -0.624488 8 2.528309 -0.636368 0.471659	**Frequencies (cm^{-1}):** -367.6924, 62.9416, 83.0145, 129.5713, 164.9946, 229.5626, 263.4659, 304.0192, 410.1843, 491.8636, 530.175, 558.7169, 700.8537, 769.7833, 817.9027, 839.9033, 947.1561, 1038.4806, 1052.7228, 1118.1603, 1122.8942, 1194.1948, 1253.3892, 1279.4904, 1396.6796, 1424.4495, 1465.1276, 1477.7338, 1525.679, 1686.1108, 3031.8076, 3050.8528, 3084.8806, 3143.4686, 3177.4848, 3196.6632
IRC  	

Compound: MVK + O_3 C_{EPOX} 1.3	**Energy (kJ mol^{-1}):** -456.239363946836
Reaction Coordinates: 6 -0.947337 -1.544387 0.430551 6 -1.740907 -0.388633 -0.119293 6 -1.035570 0.922878 -0.336345 6 -0.304729 1.588122 0.756627 1 -0.251005 2.670719 0.760772 1 -0.228975 1.107597 1.725539 1 -1.490304 1.541761 -1.101888 8 -2.914915 -0.467467 -0.405331 1 -0.206120 -1.857279 -0.307391 1 -0.389130 -1.260583 1.323270 1 -1.618949 -2.368636 0.653078 8 0.396868 0.943959 -0.300298 8 2.580900 -0.719127 0.179568 8 3.481615 -0.170047 -0.404267	**Frequencies (cm^{-1}):** 9.1118, 27.9221, 34.1713, 53.0674, 80.1511, 97.5841, 113.6791, 235.0531, 264.1927, 477.9423, 505.4664, 595.5412, 738.6975, 855.4518, 895.1486, 930.5145, 1012.6362, 1065.7933, 1097.5099, 1154.6552, 1166.67, 1249.5061, 1272.2579, 1386.4063, 1394.6362, 1457.7288, 1469.7615, 1523.3998, 1603.3764, 1772.8361, 3040.9856, 3092.9062, 3095.3302, 3140.6298, 3145.2591, 3182.5121

Compound: MVK + O_3 TS_{EPOX} 1.4	**Energy (kJ mol^{-1}):** -456.161450630123
Reaction Coordinates: 6 2.866111 -0.343622 0.309847 6 1.435323 -0.201171 -0.152587 6 0.852398 1.131606 -0.192321 6 -0.485444 1.281591 -0.570254 1 -0.903374 2.277224 -0.616460 1 -0.904004 0.580987 -1.291808 1 1.412262 1.973692 0.192915 8 0.748401 -1.174022 -0.451960 1 2.938344 -0.107642 1.374158 1 3.204960 -1.363295 0.149176 1 3.518567 0.352434 -0.220368 8 -2.420032 -0.739798 -0.450706 8 -1.702127 -0.610001 0.589450 8 -1.285877 0.658344 0.818751	**Frequencies (cm^{-1}):** -352.1461, 66.5184, 86.5413, 91.8222, 158.4674, 224.8126, 293.1177, 308.8633, 400.0719, 445.4994, 565.2864, 604.9671, 706.1094, 784.3287, 816.3389, 846.3034, 966.4721, 1039.5382, 1049.2005, 1126.7536, 1152.712, 1204.979, 1217.6897, 1251.6471, 1389.2156, 1434.2369, 1467.2904, 1476.7039, 1512.018, 1664.9899, 3029.8556, 3065.2683, 3082.5204, 3140.0903, 3174.7555, 3205.9886
IRC  	

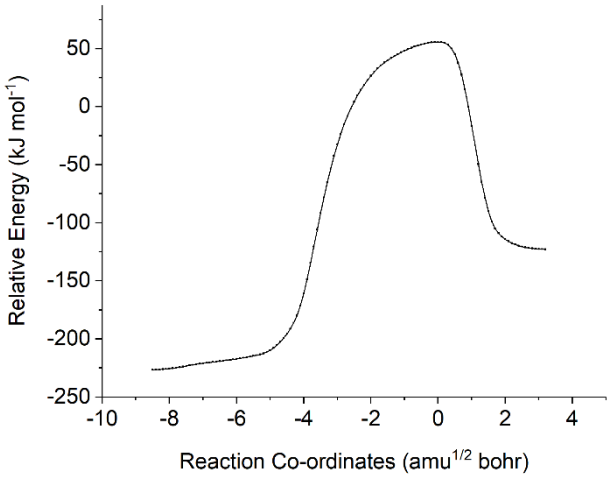
Compound: MVK + O_3 C_{EPOX} 1.4	**Energy (kJ mol^{-1}):** -456.236649707373
Reaction Coordinates: 6 -2.730401 -0.946037 0.057627 6 -1.292892 -0.503632 -0.064152 6 -1.070793 0.987399 -0.109234 6 0.001966 1.580083 0.715178 1 -0.117174 2.595753 1.076412 1 0.622634 0.916370 1.306136 1 -1.939181 1.596700 -0.340448 8 -0.369481 -1.282166 -0.110642 1 -2.778393 -2.020012 0.212785 1 -3.224668 -0.425827 0.881202 1 -3.272671 -0.683641 -0.854261 8 0.147725 1.440681 -0.688563 8 3.007038 -0.265729 -0.336832 8 2.372489 -0.978564 0.401244	**Frequencies (cm^{-1}):** 23.2229, 33.4266, 54.6209, 57.5847, 74.8451, 89.7019, 126.406, 240.0514, 264.8547, 378.2566, 594.8601, 612.5373, 765.0808, 868.8639, 890.9458, 959.1078, 992.8719, 1059.6805, 1101.4825, 1163.7047, 1168.5098, 1198.8924, 1275.2943, 1384.4136, 1413.7046, 1463.3056, 1474.0393, 1510.6709, 1595.8845, 1782.2923, 3026.5258, 3077.7903, 3089.6637, 3117.0276, 3143.4864, 3186.1079

Compound: MVK + O_3 TS_{EPOX} 2.1	**Energy (kJ mol^{-1}):** -456.207090721319
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -2.525269 1.274093 0.090767 6 -1.723976 -0.001329 -0.011252 6 -0.470436 -0.067549 0.732453 6 0.424324 -1.196506 0.581243 1 1.071414 -1.445372 1.415599 1 -0.038486 -2.073687 0.140394 1 -0.133673 0.795312 1.291221 8 -2.096697 -0.953373 -0.687533 1 -3.502370 1.131891 -0.362117 1 -2.639524 1.585563 1.130517 1 -2.000676 2.078243 -0.430637 8 1.270898 -0.610280 -0.515622 8 2.421510 0.050819 0.080373 8 2.531221 1.247308 -0.320248	-86.0721, 61.5282, 80.5549, 92.1182, 131.3281, 210.6785, 267.1186, 374.2067, 415.951, 470.0315, 547.7153, 555.5953, 600.6825, 751.2049, 799.6452, 832.2505, 961.7915, 1036.1848, 1061.7961, 1148.5126, 1191.7029, 1204.667, 1241.011, 1306.8374, 1389.6297, 1433.6452, 1466.357, 1474.9238, 1481.2252, 1669.8823, 3030.55, 3083.3839, 3104.6617, 3141.9797, 3169.7833, 3191.4557
IRC  	

Compound: MVK + O_3 C_{EPOX} 2.1	**Energy (kJ mol^{-1}):** -456.235187855083
Reaction Coordinates: 6 -2.597595 1.338121 0.296928 6 -1.817456 0.129646 -0.157397 6 -0.409673 0.021142 0.382525 6 0.094467 -1.296948 0.811670 1 0.843878 -1.343941 1.593661 1 -0.556118 -2.156043 0.696309 1 0.004901 0.907809 0.850400 8 -2.273317 -0.714642 -0.890198 1 -3.626137 1.269000 -0.045419 1 -2.570660 1.425740 1.385573 1 -2.137148 2.244382 -0.104539 8 0.523792 -0.713926 -0.409588 8 2.778965 0.318236 0.317884 8 3.523414 0.672994 -0.565391	**Frequencies (cm^{-1}):** 12.8046, 35.3243, 38.3182, 63.3625, 75.8602, 130.2572, 149.0878, 241.6124, 280.1794, 374.7716, 593.1864, 610.7994, 762.6553, 860.2161, 889.0018, 957.0572, 996.8388, 1058.9601, 1103.4358, 1160.5276, 1167.6973, 1197.5962, 1275.1535, 1384.7566, 1411.5156, 1463.4876, 1473.5678, 1504.0555, 1579.1126, 1790.0219, 3025.8806, 3076.6983, 3094.1536, 3128.5998, 3143.0947, 3190.5796

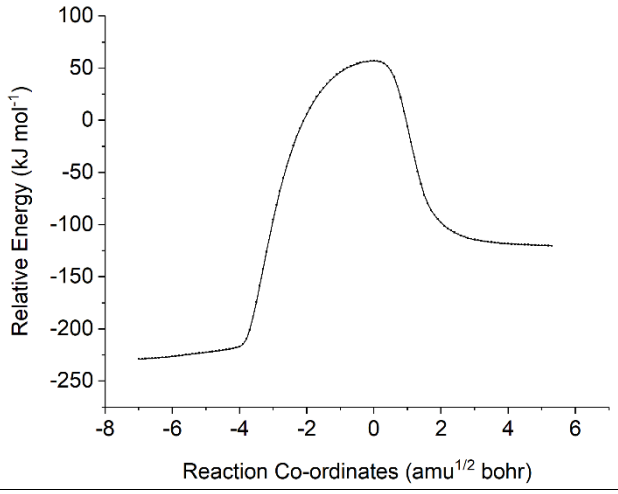
Compound: MVK + O_3 TS_{EPOX} 2.2	**Energy (kJ mol^{-1}):** -456.239749900564
Reaction Coordinates: 6 -2.198022 -0.842130 -0.798111 6 -1.725015 0.316839 0.050115 6 -0.481115 0.208743 0.798232	**Frequencies (cm^{-1}):** -140.927, 61.3467, 82.0327, 117.8929, 120.8358, 174.3052, 253.4492, 368.6125, 395.881,

6 0.353846 -0.977538 0.860630 1 1.021033 -1.052006 1.713918 1 -0.142865 -1.925697 0.678723 1 -0.129795 1.124873 1.253954 8 -2.380652 1.347681 0.152102 1 -3.081076 -0.534799 -1.350828 1 -1.422438 -1.162099 -1.495610 1 -2.454867 -1.700108 -0.172742 8 1.178417 -0.724763 -0.364927 8 2.430063 -0.041563 0.034590 8 2.586152 1.045440 -0.583342	489.7979, 514.8858, 521.7892, 565.3176, 762.7579, 811.414, 816.1383, 943.6449, 1035.4237, 1055.4192, 1144.522, 1204.4331, 1231.448, 1269.5706, 1308.9908, 1393.375, 1409.7861, 1467.8536, 1480.6684, 1496.7281, 1660.1279, 3031.7993, 3086.7827, 3097.6008, 3143.0359, 3154.2245, 3195.6897
IRC  	

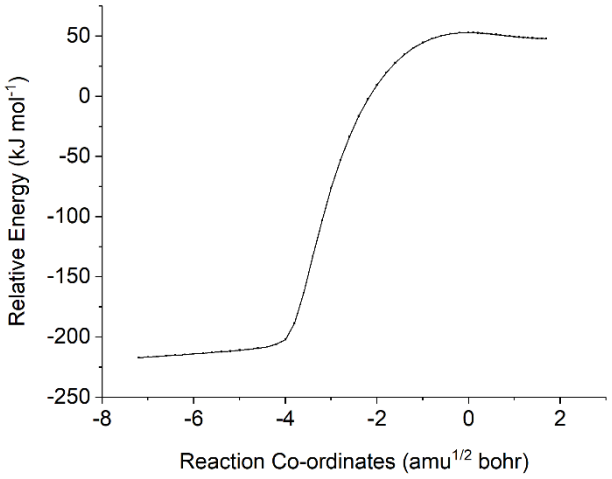
Compound: MVK + O_3 C_{EPOX} 2.2	**Energy (kJ mol^{-1}):** -456.238757609375
Reaction Coordinates: 6 -2.367449 0.991278 0.698101 6 -1.867264 -0.318038 0.146462 6 -0.438703 -0.393401 -0.320776 6 0.080158 0.530613 -1.343786 1 0.871466 0.184492 -1.998096 1 -0.558691 1.311556 -1.740680 1 -0.007462 -1.386366 -0.261381 8 -2.554253 -1.312038 0.073125 1 -3.441600 0.933126 0.849120 1 -1.870480 1.191447 1.649677 1 -2.121045 1.826180 0.041583 8 0.443986 0.681654 0.025067 8 2.756959 -0.561137 0.135563 8 3.689228 0.076129 0.563717	**Frequencies (cm^{-1}):** 13.5566, 27.7392, 38.7466, 66.8704, 89.832, 110.5237, 140.7518, 240.2713, 267.3185, 478.6085, 505.4428, 594.8274, 739.5614, 854.3641, 893.2068, 931.5211, 1011.0585, 1066.0952, 1097.0819, 1154.877, 1166.3532, 1248.4917, 1271.0409, 1386.7338, 1393.335, 1457.8282, 1469.3377, 1519.1993, 1585.0243, 1774.8071, 3039.7628, 3092.6438, 3096.3196, 3143.6444, 3145.5243, 3185.9899

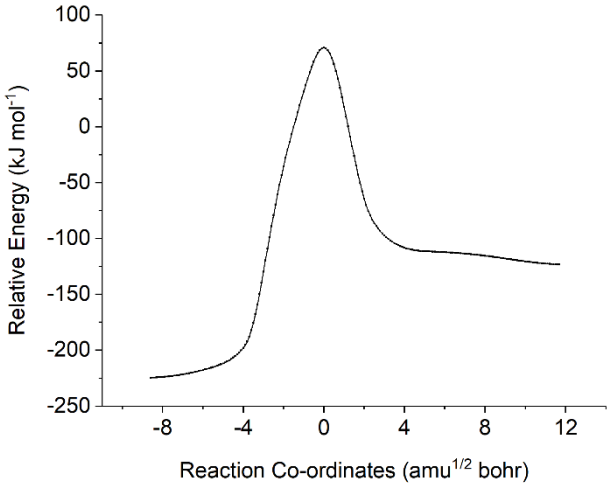
Compound: MVK + O_3 TS_{EPOX} 2.3	**Energy (kJ mol^{-1}):** -456.239534637013
Reaction Coordinates: 6 1.382671 -1.073501 0.998718 6 1.582362 -0.066321 -0.109978 6 0.674141 1.063942 -0.245949 6 -0.448286 1.380006 0.623101 1 -0.483209 0.866937 1.579755 1 -0.657625 2.438824 0.751545	**Frequencies (cm^{-1}):** -143.8671, 66.0133, 88.3301, 125.9508, 144.7397, 214.3804, 266.7079, 358.8235, 369.6951, 483.4673, 517.0622, 528.9597, 578.6371, 763.1323, 800.161, 833.3356, 938.1357, 1036.81,

1 0.834580 1.686808 -1.115275 8 2.541813 -0.129904 -0.871658 1 1.652910 -0.630438 1.960515 1 0.347328 -1.406391 1.066171 1 2.029797 -1.926761 0.816491 8 -1.541068 0.861038 -0.245332 8 -1.946615 -0.495044 0.232647 8 -1.912768 -1.342807 -0.697477	1051.1124, 1163.9752, 1191.7029, 1231.4974, 1272.4487, 1306.667, 1396.7201, 1404.2236, 1466.3143, 1479.996, 1491.6341, 1654.6656, 3032.7011, 3087.6458, 3095.4503, 3143.661, 3145.9739, 3198.7947
IRC	



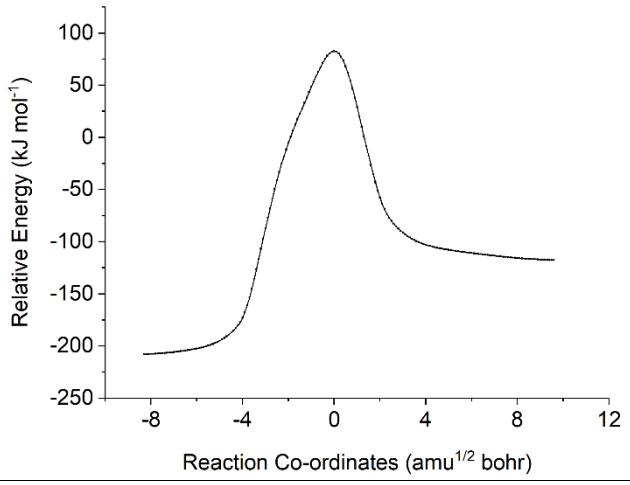
Compound: MVK + O_3 TS_{EPOX} 2.4	**Energy (kJ mol^{-1}):** -456.170075488032
Reaction Coordinates: 6 -2.527515 -0.516057 -0.494703 6 -1.310040 0.079714 0.168222 6 -0.561201 1.124309 -0.474544 6 0.662505 1.562053 0.173797 1 1.068386 2.504332 -0.182465 1 0.650043 1.505711 1.257245 1 -0.772239 1.426473 -1.490242 8 -0.908239 -0.334102 1.264440 1 -3.387173 -0.398271 0.165851 1 -2.748769 -0.054463 -1.455370 1 -2.370423 -1.584974 -0.637814 8 1.673328 0.571186 -0.343110 8 1.561657 -0.714260 0.340070 8 1.420465 -1.635189 -0.498130	**Frequencies (cm^{-1}):** -114.9096, 35.2276, 62.0296, 98.3181, 190.8973, 303.1027, 330.8209, 380.3819, 438.5761, 466.5193, 537.0944, 572.1773, 602.3298, 763.3434, 787.4825, 839.994, 995.7693, 1044.4555, 1048.6377, 1142.9794, 1187.0258, 1231.0255, 1255.3566, 1315.5502, 1395.6089, 1418.2141, 1466.6435, 1474.373, 1486.9352, 1596.0938, 3041.7783, 3099.4685, 3104.3762, 3120.5399, 3164.0651, 3201.0748
IRC	



Compound: MVK + O_3 TS_{EPOX} 2.5	**Energy (kJ mol^{-1}):** -456.140995312962
Reaction Coordinates: 6 2.244027 1.241931 0.075347 6 1.664927 -0.132289 -0.098745 6 0.135124 -0.176100 -0.327525 6 -0.593388 -1.339473 0.165593 1 -1.290241 -1.908305 -0.426688 1 -0.445722 -1.619850 1.196857 1 -0.045996 0.033562 -1.389680 8 2.307067 -1.152116 -0.084070 1 1.923658 1.897917 -0.736133 1 3.328151 1.179572 0.109006 1 1.860640 1.682043 0.997080 8 -2.801311 -0.185309 0.127790 8 -2.195945 0.774277 -0.377679 8 -0.564139 0.709478 0.504152	**Frequencies (cm^{-1}):** -582.8387, 36.408, 88.6967, 98.073, 128.0061, 238.3455, 275.1063, 300.5924, 358.7715, 436.4891, 457.6764, 523.0491, 575.4716, 654.2201, 715.7341, 916.568, 955.4286, 965.945, 1021.9861, 1071.9431, 1172.866, 1206.0052, 1250.1492, 1306.4664, 1319.9653, 1388.4954, 1457.6884, 1463.9446, 1489.7269, 1785.0036, 2985.9202, 3039.8861, 3094.6417, 3145.3742, 3182.252, 3298.1299
IRC  	

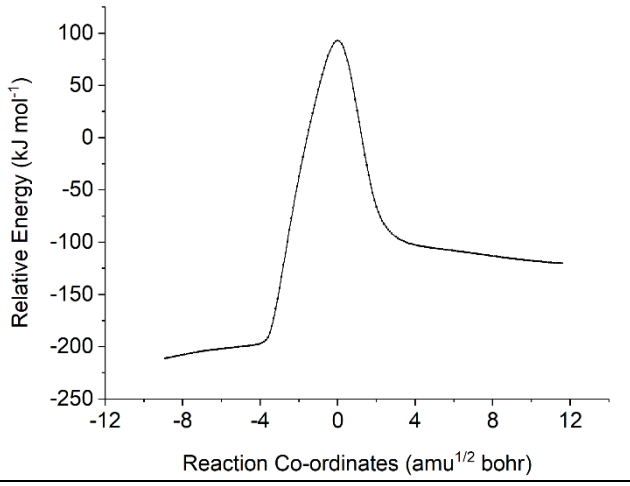
Compound: MVK + O_3 TS_{EPOX} 2.6	**Energy (kJ mol^{-1}):**
Reaction Coordinates: IP	**Frequencies (cm^{-1}):**

IRC



Compound: MVK + O_3 TS_{EPOX} 2.7	**Energy (kJ mol^{-1}):** -456.131026262361
Reaction Coordinates: 6 1.559630 1.335613 0.446486 6 1.324371 -0.064243 -0.051866 6 0.165934 -0.885134 0.568704 6 -0.772768 -0.277559 1.505843 1 -1.465600 -0.931894 2.011692 1 -0.871480 0.783319 1.662291 1 0.589083 -1.836485 0.903597 8 2.012122 -0.599072 -0.881974 1 1.681000 1.343000 1.532930 1 0.699576 1.965105 0.211142 1 2.451388 1.740940 -0.023129 8 -2.038945 0.922954 -0.337820 8 -1.171608 0.380109 -1.071316 8 -0.894940 -1.168496 -0.348081	**Frequencies (cm^{-1}):** -612.1042, 48.9171, 79.9614, 171.1517, 179.1742, 201.3574, 283.7233, 329.6669, 385.9884, 449.8581, 480.121, 512.5975, 595.6981, 622.9532, 733.6496, 869.1024, 930.1304, 948.0312, 1032.2486, 1071.5627, 1154.2291, 1206.9229, 1216.3691, 1242.1888, 1334.183, 1387.1018, 1464.0067, 1474.0593, 1499.3154, 1797.2576, 3026.0223, 3027.791, 3083.2109, 3143.0931, 3182.6501, 3295.4538

IRC



Compound: MVK + O_3 C_{EPOX} 2.7	**Energy (kJ mol^{-1}):** -456.239011910976
Reaction Coordinates: 6 -0.721038 -1.369346 0.901061 6 -1.542402 -0.593314 -0.094557 6 -1.081022 0.787273 -0.475011 6 -0.847589 1.822895 0.546905 1 -1.013508 2.860364 0.279868 1 -0.967274 1.580926 1.597156 1 -1.407842 1.102608 -1.459761 8 -2.545364 -1.032453 -0.612145 1 -0.500346 -0.776903 1.789599 1 0.242267 -1.620696 0.452434 1 -1.250324 -2.277288 1.175834 8 3.397034 -0.220028 0.241116 8 2.660443 -0.529221 -0.660439 8 0.244054 1.187445 -0.106721	**Frequencies (cm^{-1}):** 14.4582, 18.8435, 34.5707, 40.6433, 43.7643, 93.0459, 124.065, 235.1491, 262.7402, 477.9341, 505.8821, 596.6135, 739.489, 856.8866, 896.4518, 931.2599, 1013.5987, 1066.161, 1097.5602, 1155.0101, 1166.1634, 1249.5477, 1272.3087, 1387.3625, 1394.8734, 1459.2456, 1469.572, 1524.0603, 1615.3489, 1772.8742, 3039.3582, 3091.2514, 3093.62, 3139.6631, 3144.7228, 3179.8683

Compound: MVK + O_3 TS_{EPOX} 2.8	**Energy (kJ mol^{-1}):** -456.145645098218
Reaction Coordinates: 6 1.949533 -1.110688 0.213964 6 1.268653 0.172000 -0.156985 6 0.152354 0.676282 0.787241 6 -0.854189 1.503362 0.133579 1 -1.583622 1.997480 0.756505 1 -0.938010 1.577966 -0.938275 1 0.678614 1.180987 1.613499 8 1.577922 0.872556 -1.088212 1 1.222403 -1.921946 0.223970 1 2.351365 -1.032155 1.227014 1 2.750605 -1.323921 -0.488288 8 -2.095908 -0.461871 -0.834762 8 -1.169550 -1.144952 -0.371325 8 -0.759897 -0.256252 1.261646	**Frequencies (cm^{-1}):** -574.156, 58.1182, 92.0327, 110.7515, 180.2315, 225.1498, 275.1356, 297.7817, 354.8015, 426.1749, 430.8497, 522.81, 597.5208, 611.6522, 747.5041, 908.9684, 953.2755, 977.7138, 1062.4634, 1092.9248, 1146.6984, 1198.0341, 1215.1123, 1307.5732, 1333.0691, 1390.9814, 1459.3196, 1469.081, 1479.5574, 1789.5379, 2935.2123, 3037.5242, 3101.2038, 3147.7217, 3178.7451, 3297.6719

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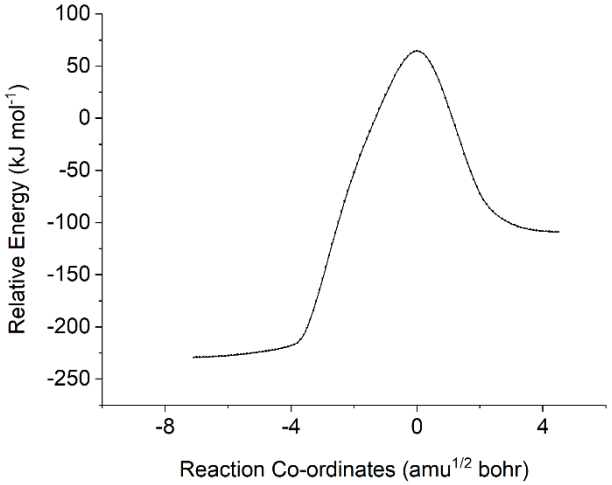
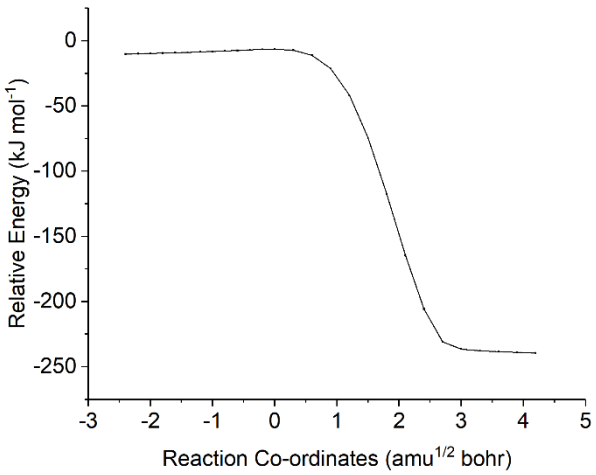


6.8 Ozonolysis of 2-methyl-2-butene (Alkene 6)

Compound: $MeCHCMe_2 + O_3$ PRC1	**Energy (kJ mol^{-1}):** -421.490704382920
Reaction Coordinates: 6 0.617958 -1.738134 -0.847548 6 1.160318 -0.482303 -0.232014 6 0.817788 0.722130 -0.730886 6 1.228567 2.075100 -0.254696 1 0.345186 2.656941 0.020752 1 1.728190 2.627048 -1.055503 1 1.895261 2.049366 0.603867 1 0.161888 0.725122 -1.595772 6 2.072541 -0.693526 0.940121 1 1.566970 -1.279829 1.711620 1 2.416178 0.232472 1.392362 1 2.951302 -1.269950 0.637003 1 1.424669 -2.429968 -1.104406 1 -0.026102 -2.267153 -0.136714 1 0.036317 -1.536620 -1.745393 8 -2.692863 0.200343 -0.511708 8 -2.104248 -0.355829 0.471919 8 -1.188250 0.304608 1.042579	**Frequencies (cm^{-1}):** 27.1784, 50.1606, 53.6577, 75.2081, 102.8604, 118.194, 127.0791, 178.0945, 255.2214, 276.1835, 298.1965, 388.2708, 456.2367, 528.1489, 731.5779, 771.3455, 838.3277, 958.8451, 970.2319, 1002.4463, 1058.0042, 1075.0445, 1096.3981, 1135.3897, 1143.4019, 1166.3998, 1244.4755, 1380.4423, 1410.1982, 1415.0271, 1420.5919, 1469.6599, 1475.4336, 1480.3338, 1489.7206, 1492.6476, 1495.7423, 1679.7275, 3001.8539, 3016.2956, 3018.3243, 3043.7022, 3054.3052, 3054.4137, 3104.8866, 3110.9907, 3128.0823, 3135.6233

Compound: $MeCHCMe_2 + O_3$ TS_{OZO} 1	**Energy (kJ mol^{-1}):** -421.488197362492
Reaction Coordinates: 6 1.141143 -1.399325 -1.095080 6 0.972841 -0.198514 -0.208950 6 0.322740 0.912992 -0.685697 6 0.249553 2.232717 0.008353 1 1.197219 2.774223 -0.079378 1 0.033345 2.116685 1.069826 1 -0.528600 2.856009 -0.427453 1 -0.021866 0.883196 -1.711558 6 1.785812 -0.175686 1.052941 1 1.820552 -1.162035 1.513466 1 1.396451 0.529878 1.782586 1 2.816863 0.114235 0.825336 1 2.149954 -1.412818 -1.520953 1 1.018188 -2.325984 -0.535149 1 0.432562 -1.394583 -1.922359 8 -1.937684 0.406110 -0.269118 8 -1.790979 -0.824332 0.080348 8 -0.914738 -0.983267 1.010801	**Frequencies (cm^{-1}):** -136.2357, 69.9513, 97.1473, 113.1259, 132.8794, 157.0309, 162.2988, 181.2724, 260.3192, 289.9223, 388.6736, 430.8786, 493.8605, 527.7861, 739.5736, 774.8147, 843.5158, 955.376, 975.3407, 1007.9985, 1040.2137, 1074.0844, 1086.2863, 1090.372, 1110.1244, 1137.0213, 1241.886, 1368.0393, 1407.6949, 1410.9587, 1419.3948, 1472.2655, 1473.4018, 1479.7303, 1482.5358, 1492.2253, 1502.9971, 1593.0708, 3007.963, 3009.7503, 3013.8158, 3071.6638, 3077.9598, 3081.9531, 3109.0578, 3114.1663, 3126.0383, 3160.7213
IRC:	



Compound: $MeCHCMe_2 + O_3$ POZ1	**Energy (kJ mol^{-1}):** -421.589334220594
Reaction Coordinates: 6 1.101822 1.196014 -1.047195 6 0.684040 0.173905 0.000722 6 -0.806760 0.278334 0.501228 6 -1.600548 1.517231 0.143171 1 -1.663038 1.656540 -0.934013 1 -2.611955 1.435145 0.539513 1 -1.139167 2.399873 0.586425 1 -0.806591 0.134098 1.585354 8 -1.445405 -0.846198 -0.105810 8 -0.397122 -1.824940 -0.078572 8 0.687478 -1.100568 -0.688230 6 1.646165 0.136944 1.183570 1 1.572065 1.055397 1.769638 1 2.674210 0.034719 0.837387 1 1.411965 -0.704448 1.834562 1 0.410532 1.206593 -1.887081 1 2.092545 0.946409 -1.426485 1 1.151512 2.194759 -0.613386	**Frequencies (cm^{-1}):** 53.6351, 213.4189, 235.2693, 251.6887, 275.9539, 292.1465, 306.9803, 346.0847, 411.0663, 480.6846, 520.2624, 600.6938, 701.9449, 724.326, 767.0573, 861.1894, 892.3931, 933.2719, 939.0378, 954.3417, 1014.6864, 1054.8716, 1098.5972, 1159.5296, 1184.6188, 1216.3731, 1264.8323, 1352.7203, 1389.2551, 1404.2704, 1416.6102, 1424.2986, 1475.6044, 1486.0936, 1489.1246, 1500.635, 1500.9913, 1515.6267, 3014.3141, 3030.0947, 3042.4794, 3046.8643, 3092.5638, 3103.2686, 3106.4043, 3112.3538, 3119.5643, 3126.7663

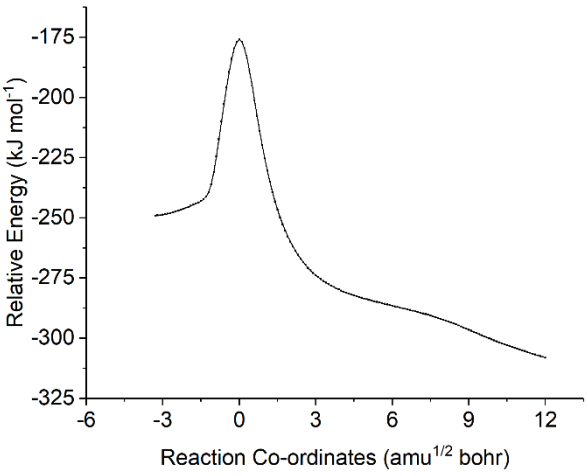
Compound: $MeCHCMe_2 + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -421.495697865614
Reaction Coordinates: 6 1.338362 -1.481189 -0.970225 6 1.224914 -0.200943 -0.196144 6 0.600374 0.866522 -0.731027 6 0.359114 2.200580 -0.105301 1 -0.714310 2.372083 0.029823 1 0.714633 3.002707 -0.756992 1 0.835919 2.315764 0.865119 1 0.219252 0.757717 -1.740579 6 1.895925 -0.219283 1.147715 1 1.547624 -1.071276 1.735089 1 1.727869 0.682519 1.729755 1 2.975271 -0.346684 1.022583 1 2.385515 -1.776619 -1.083131 1 0.837262 -2.292110 -0.434698 1 0.890144 -1.401474 -1.958703	**Frequencies (cm^{-1}):** 36.9586, 48.5349, 58.774, 75.81, 87.4943, 122.1003, 148.8737, 177.9751, 267.2774, 290.6169, 299.6627, 388.7022, 463.2547, 526.5619, 738.9726, 770.9035, 833.5889, 959.1562, 970.2212, 1006.5445, 1054.7353, 1073.1955, 1099.0366, 1132.8514, 1154.1765, 1171.5029, 1241.1897, 1377.034, 1410.2, 1415.1913, 1421.1811, 1469.0695, 1476.3614, 1477.595, 1488.3415, 1493.8922, 1496.422, 1675.6447, 3004.0927, 3009.8783, 3018.3636, 3044.5664,

8 -2.099525 -0.285338 -0.824124 8 -2.114687 -0.102944 0.430069 8 -1.277202 -0.766311 1.109258	3051.4083, 3060.9297, 3108.5119, 3110.3783, 3128.2449, 3141.4631

Compound: $MeCHCMe_2 + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -421.486931933269
Reaction Coordinates: 6 -1.559672 -1.077952 1.054445 6 -1.006578 0.001822 0.176915 6 -0.152071 0.945013 0.701523 6 0.321347 2.155449 -0.037576 1 -0.508244 2.827327 -0.277361 1 0.790687 1.883615 -0.986412 1 1.049135 2.712187 0.547865 1 0.049427 0.899998 1.762214 6 -1.669464 0.181671 -1.161013 1 -1.923591 -0.778804 -1.605857 1 -1.050939 0.732390 -1.865653 1 -2.603568 0.739424 -1.032614 1 -2.611584 -0.876738 1.281865 1 -1.518312 -2.044152 0.550601 1 -1.012411 -1.155926 1.991667 8 1.822796 -0.244108 0.679771 8 1.711213 -0.634259 -0.544601 8 0.683244 -1.393550 -0.731680	**Frequencies (cm^{-1}):** -166.479, 66.823, 128.0688, 140.1025, 151.3913, 167.7468, 175.382, 190.4718, 268.1285, 283.3042, 386.8183, 453.6647, 505.9947, 531.6042, 738.9611, 775.9025, 848.6449, 958.6579, 978.941, 1006.8509, 1037.4865, 1072.6977, 1078.3327, 1089.7411, 1105.7005, 1132.3285, 1242.2939, 1359.4497, 1409.4788, 1413.2695, 1419.6259, 1469.7945, 1474.898, 1480.0535, 1481.6523, 1490.1522, 1502.9366, 1581.474, 3006.1939, 3010.4183, 3012.2715, 3051.4727, 3071.5928, 3083.8299, 3115.8701, 3116.0134, 3124.7305, 3180.0494
IRC: Reassess	

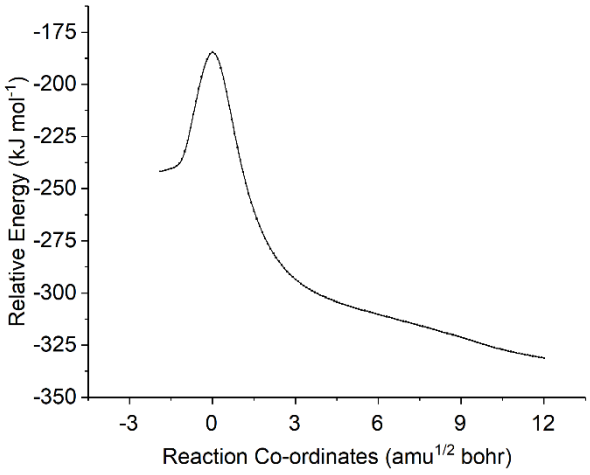
Compound: $MeCHCMe_2 + O_3$ POZ 2	**Energy (kJ mol^{-1}):** -421.588054479771
Reaction Coordinates: 6 1.822185 0.322617 -1.041390 6 0.715074 0.085934 -0.023353 6 -0.707787 0.448168 -0.593236 6 -1.445900 1.600267 0.065664 1 -2.414158 1.730562 -0.415927 1 -0.889834 2.532821 -0.043876 1 -1.613113 1.415411 1.124908 1 -0.623761 0.626479 -1.666520 6 1.038334 0.716356 1.327811 1 2.015344 0.366308 1.659275 1 0.301606 0.433953 2.076806 1 1.071231 1.803793 1.265062 1 1.932718 1.390362 -1.233219 1 2.773678 -0.051722 -0.664619 1 1.596356 -0.181472 -1.979955 8 -1.451036 -0.779588 -0.487624 8 -0.744709 -1.511813 0.542224 8 0.610557 -1.346917 0.128536	**Frequencies (cm^{-1}):** 38.6134, 214.0229, 246.9177, 269.816, 279.0017, 279.7958, 308.925, 340.7614, 434.1964, 489.808, 504.9436, 611.6695, 692.605, 740.8897, 772.0819, 862.7097, 888.8831, 932.4031, 937.883, 957.7792, 1019.0646, 1051.0518, 1074.9168, 1124.2582, 1189.5732, 1230.7942, 1246.6571, 1330.3106, 1384.6717, 1404.4642, 1412.6955, 1423.3656, 1477.6914, 1485.0787, 1489.6134, 1500.7606, 1504.0664, 1515.415, 3037.1044, 3038.4508, 3045.239, 3049.5332, 3098.6085, 3101.2893, 3108.4609, 3113.8191, 3119.2866, 3125.9615

Compound: $MeCHCMe_2 + O_3$ TS_{ANTI}	**Energy (kJ mol^{-1}):** -421.558157771816
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.782165 0.236012 -1.091068 6 -0.874306 -0.264360 0.043812 6 0.770417 0.551827 -0.431907 6 0.913304 1.994077 -0.058972 1 1.031170 2.113714 1.015917 1 0.039549 2.556114 -0.383758 1 1.784635 2.425011 -0.556244 1 0.730017 0.300814 -1.486883 6 -1.223231 0.268505 1.435859 1 -2.154761 -0.200205 1.757749 1 -0.448886 -0.004383 2.150151 1 -1.370033 1.348374 1.450396 1 -2.801214 -0.093587 -0.882391 1 -1.794218 1.323344 -1.170786 1 -1.474364 -0.199688 -2.039316 8 1.572185 -0.263284 0.268364 8 1.440624 -1.510683 -0.157766 8 -0.558560 -1.511767 -0.015746	-466.3525, 89.6845, 176.2857, 193.9454, 222.5575, 235.3344, 247.1831, 296.438, 339.7262, 376.8853, 412.9267, 485.6561, 524.767, 559.3632, 627.6716, 770.2026, 905.2958, 910.0071, 981.8117, 1009.4561, 1014.5526, 1064.8005, 1118.5438, 1146.5144, 1161.7471, 1189.4767, 1261.1009, 1373.0331, 1384.6445, 1390.8201, 1403.6407, 1422.5666, 1473.3562, 1479.8921, 1488.9339, 1490.883, 1497.2512, 1505.5882, 3030.8364, 3035.6217, 3038.8522, 3089.1983, 3093.7419, 3099.8496, 3119.6383, 3121.0775, 3124.4951, 3136.2108
IRC:  	

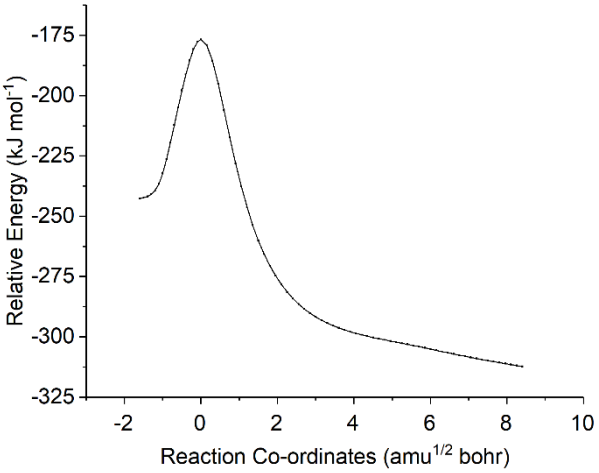
Compound: $MeCHCMe_2 + O_3$ C_{ANTI}	**Energy (kJ mol^{-1}):** -421.605132678016
Reaction Coordinates: 6 3.226302 -0.638153 0.168365 6 1.818787 -0.129682 -0.048385 6 -1.866763 -0.375132 -0.350313 6 -2.204602 -1.731438 0.121341 1 -2.588917 -1.708894 1.138098 1 -1.307388 -2.352057 0.076703 1 -2.947171 -2.182390 -0.542049 1 -1.475935 -0.168670 -1.340142 6 1.621460 1.363727 -0.029196 1 2.119112 1.796186 -0.902129 1 0.564229 1.627452 -0.046492 1 2.105787 1.798500 0.847730 1 3.926210 -0.129741 -0.497011 1 3.540601 -0.409141 1.189463 1 3.271565 -1.712188 0.009315 8 -2.044909 0.603692 0.408725 8 -1.700863 1.863783 -0.066705	**Frequencies (cm^{-1}):** 24.6817, 44.6322, 74.7078, 85.5727, 92.8105, 99.4911, 130.2591, 152.2036, 199.0116, 269.2797, 325.2901, 395.5072, 498.9114, 545.1685, 550.271, 791.9803, 863.5713, 875.7613, 891.1069, 904.2128, 960.206, 1074.031, 1093.1404, 1125.8131, 1162.7069, 1247.1089, 1348.7825, 1388.207, 1403.0531, 1408.7298, 1459.3169, 1462.5566, 1467.2691, 1468.5009, 1476.6733, 1494.4853, 1593.4248, 1756.1197, 3009.9083, 3026.5708, 3031.296, 3070.2546, 3077.4937, 3084.7504, 3103.7982, 3135.1382, 3137.0156, 3171.8886

8 0.898371 -0.904349 -0.230064	

Compound: $MeCHCMe_2 + O_3$ TS_{DMFO} 1	**Energy (kJ mol^{-1}):** -421.562412908607
Reaction Coordinates: 6 1.076547 1.726726 -0.342731 6 0.730735 0.306270 0.016816 6 -1.011017 0.107900 0.642501 6 -1.948613 1.044531 -0.104046 1 -1.965690 0.804259 -1.166031 1 -2.957663 0.903853 0.285678 1 -1.679995 2.092538 0.028470 1 -0.751714 0.436042 1.662253 6 1.588496 -0.348858 1.072799 1 1.737647 0.341480 1.901364 1 2.564046 -0.580680 0.638311 1 1.143043 -1.268510 1.435639 1 0.515339 2.064281 -1.210802 1 2.142979 1.806347 -0.563201 1 0.862091 2.387546 0.495748 8 -1.211069 -1.158836 0.524305 8 0.177948 -1.669761 -0.814101 8 0.504750 -0.422223 -1.112637	**Frequencies (cm^{-1}):** -464.4145, 125.8449, 178.4565, 182.8643, 209.148, 233.3068, 274.6675, 294.9501, 337.3068, 373.3082, 411.4326, 492.8246, 538.8472, 596.9151, 648.3781, 780.8192, 901.5617, 953.308, 967.1753, 989.2816, 1003.0883, 1041.5102, 1104.9221, 1127.7686, 1164.8217, 1276.1836, 1281.9841, 1299.9895, 1396.1905, 1403.5467, 1417.8383, 1422.9553, 1471.7498, 1477.4423, 1485.3375, 1492.333, 1500.7002, 1505.8269, 2922.4449, 3033.895, 3036.1349, 3039.1887, 3094.9116, 3098.7751, 3103.713, 3116.6291, 3131.9684, 3160.173
IRC:  	

Compound: $MeCHCMe_2 + O_3$ CPr_{DMFO} 1	**Energy (kJ mol^{-1}):** -421.612023626196
Reaction Coordinates: 6 -2.512406 -0.932241 -0.440998 6 -1.530899 0.069185 0.045685 6 -1.299755 0.363030 1.470542 1 -2.021213 -0.149676 2.101141 1 -1.330527 1.444666 1.618757 1 -0.285024 0.054362 1.730761 8 -0.885480 0.683163 -0.849624 8 0.083956 1.589891 -0.436400 1 -2.537007 -0.958109 -1.527163 1 -3.507651 -0.704282 -0.053081	**Frequencies (cm^{-1}):** 39.7403, 44.8699, 77.4796, 88.4943, 103.3423, 124.2875, 157.4773, 160.3839, 190.9702, 293.528, 309.4418, 367.8338, 480.8197, 512.8259, 594.2307, 782.8576, 812.6365, 891.1953, 913.9003, 930.4715, 988.146, 1073.3978, 1097.6353, 1127.3188, 1135.0153, 1306.0908, 1373.8141, 1387.5912, 1405.7322, 1426.6915, 1443.9167, 1458.5583,

1 -2.234761 -1.918664 -0.061764 6 1.898688 -0.597448 -0.407457 6 2.986679 0.186524 0.258868 1 3.032243 -0.030912 1.323698 1 3.943989 -0.056027 -0.210997 1 2.803941 1.249244 0.094482 1 1.786830 -0.415176 -1.491145 8 1.188441 -1.404269 0.150458	1459.9681, 1470.3089, 1471.2569, 1479.7331, 1570.7409, 1776.5179, 2926.9447, 3024.8398, 3027.0652, 3034.2594, 3075.4222, 3082.484, 3087.2993, 3131.4625, 3137.6628, 3139.0482

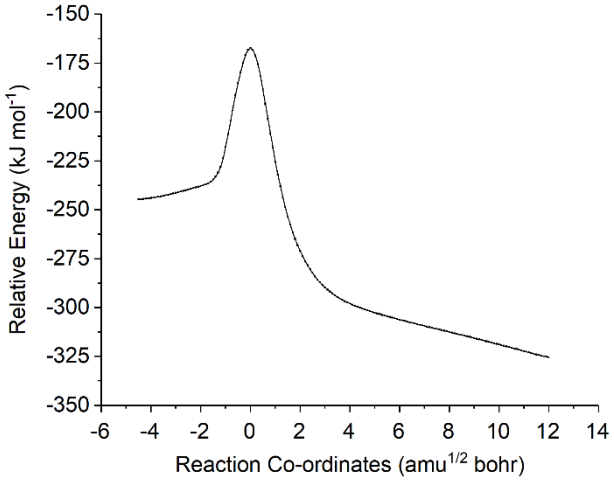
Compound: $MeCHCMe_2 + O_3$ TS_{DMFO} 2	**Energy (kJ mol^{-1}):** -421.559064397801
Reaction Coordinates: 6 -1.078887 -1.637625 -0.778188 6 -0.638144 -0.432392 0.006330 6 1.080095 0.130026 -0.545203 6 2.068641 -0.796198 0.164622 1 3.052246 -0.626531 -0.274908 1 2.130442 -0.565035 1.225123 1 1.819582 -1.848541 0.026164 1 0.981853 -0.091613 -1.620694 6 -0.584410 -0.562017 1.508062 1 -0.121712 -1.504135 1.790976 1 -1.611634 -0.559964 1.882476 1 -0.052056 0.264168 1.966030 1 -1.235095 -1.382760 -1.824629 1 -2.008582 -2.040172 -0.370960 1 -0.325814 -2.421720 -0.716426 8 1.109775 1.372783 -0.220251 8 -0.824805 1.764468 0.161602 8 -1.249095 0.683442 -0.468462	**Frequencies (cm^{-1}):** -480.2753, 104.3204, 172.4186, 197.7865, 216.2532, 239.2856, 264.4242, 318.009, 330.4402, 388.6542, 399.715, 487.3769, 527.8877, 571.8559, 644.806, 783.2927, 896.5886, 955.4545, 983.2999, 997.8347, 1009.8732, 1039.2419, 1084.9956, 1141.5825, 1189.7616, 1279.8408, 1282.5421, 1338.8266, 1389.5462, 1403.5466, 1418.9586, 1427.4506, 1468.2293, 1479.9942, 1486.0295, 1493.8978, 1497.1086, 1508.1341, 2914.3777, 3032.6749, 3036.2167, 3038.3616, 3093.7143, 3098.1012, 3112.5657, 3125.9276, 3131.3313, 3162.4647
IRC  	

Compound: $MeCHCMe_2 + O_3$ CPr_{DMFO} 2	**Energy (kJ mol^{-1}):** -421.610541650470
Reaction Coordinates: 6 -1.815272 -1.389891 -0.771255 6 -1.441415 -0.146777 -0.052760 6 -1.555028 0.022707 1.405656	**Frequencies (cm^{-1}):** 41.7998, 58.3635, 65.2839, 79.5834, 97.647, 107.534, 156.371, 164.1727, 180.0062, 289.4071, 308.5627, 366.8994,

1 -1.987703 -0.856512 1.874963 1 -2.145169 0.918819 1.613003 1 -0.563005 0.226740 1.812625 8 -1.011875 0.799063 -0.770647 8 -0.617315 1.967007 -0.124686 1 -1.692118 -1.270739 -1.844579 1 -2.849644 -1.658993 -0.545935 1 -1.178830 -2.205702 -0.421583 6 2.425014 -0.721681 0.072252 6 2.570316 0.750564 -0.141048 1 3.053892 0.920136 -1.107820 1 1.613643 1.271192 -0.101840 1 3.256042 1.149597 0.612563 1 3.370095 -1.302176 0.041676 8 1.381828 -1.301307 0.269065	479.8787, 527.1083, 593.4557, 780.6412, 812.1044, 894.3221, 911.6484, 928.9357, 989.0279, 1072.5462, 1096.7011, 1144.3467, 1147.9438, 1305.9462, 1387.7099, 1389.2479, 1403.6777, 1426.6526, 1441.7838, 1459.7322, 1467.0467, 1471.5204, 1477.1735, 1481.8101, 1570.2575, 1787.3611, 2873.1107, 3004.6472, 3027.9351, 3034.0048, 3060.2229, 3078.5874, 3081.0599, 3105.6982, 3136.5806, 3140.4641

Compound: $MeCHCMe_2 + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -421.556402140495
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.640357 -1.059582 -0.747861 6 -0.892864 -0.074825 0.157072 6 0.668581 0.362641 -0.777078 6 1.317464 1.558995 -0.139940 1 0.833672 2.473271 -0.474039 1 2.362047 1.588488 -0.460360 1 1.293506 1.500698 0.943107 1 0.406995 0.449195 -1.828386 6 -1.600396 1.285836 0.299757 1 -2.596214 1.092071 0.700883 1 -1.075455 1.930019 0.998567 1 -1.717911 1.791781 -0.658488 1 -2.572878 -1.341705 -0.255833 1 -1.052190 -1.962092 -0.895415 1 -1.889327 -0.625679 -1.717491 8 1.257998 -0.837343 -0.586005 8 1.507719 -1.019128 0.699676 8 -0.404068 -0.560334 1.248298	-467.3132, 103.2029, 195.4634, 200.243, 226.7866, 258.5396, 289.8417, 304.1453, 311.1064, 346.239, 420.7633, 487.8422, 547.1886, 571.5685, 695.4948, 789.0796, 897.3989, 910.6994, 956.8011, 991.5011, 1023.3904, 1061.597, 1077.3589, 1130.9944, 1163.9672, 1182.657, 1206.2704, 1364.2579, 1393.0693, 1395.4713, 1405.1096, 1424.8817, 1470.623, 1481.0968, 1485.2167, 1495.4393, 1498.6324, 1506.6639, 3029.7573, 3036.3222, 3038.0324, 3086.3059, 3094.9386, 3112.3149, 3121.9339, 3127.9074, 3143.1043, 3159.3044

IRC

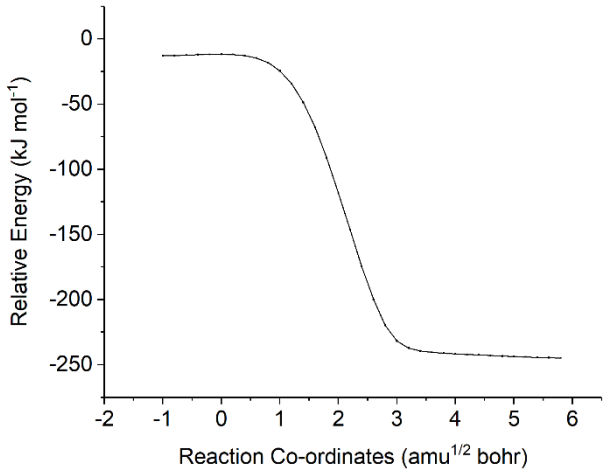


Compound: $MeCHCMe_2 + O_3$ CPr_{SYN}	**Energy (kJ mol^{-1}):** -421.608401293787
Reaction Coordinates: 6 -1.488448 1.338632 -0.286630 6 -1.854330 -0.096253 0.001738 6 1.889394 -0.664075 0.570923 6 2.128980 -1.238853 -0.755259 1 2.150474 -2.323929 -0.714141 1 3.064026 -0.835816 -1.154851 1 1.345868 -0.896240 -1.434895 1 1.729606 -1.246798 1.469673 6 -3.329642 -0.427465 0.047561 1 -3.761668 -0.303519 -0.948398 1 -3.477811 -1.451333 0.380144 1 -3.859087 0.262054 0.707601 1 -2.046749 1.708205 -1.149184 1 -0.418756 1.452958 -0.450077 1 -1.786502 1.958356 0.563704 8 1.865527 0.575688 0.780137 8 2.022237 1.403722 -0.314372 8 -1.014654 -0.953892 0.191788	**Frequencies (cm^{-1}):** 26.1022, 41.0813, 54.7406, 71.8994, 77.7347, 86.7309, 97.3139, 152.8184, 161.0665, 296.7717, 391.7577, 452.845, 497.3666, 540.9522, 669.6858, 764.0928, 788.3718, 876.3052, 888.2451, 900.9167, 986.1014, 1055.4851, 1089.8235, 1112.1629, 1123.7228, 1242.6301, 1354.1102, 1387.8518, 1396.6765, 1399.4392, 1440.0942, 1461.0493, 1462.1664, 1466.7276, 1475.5573, 1494.8781, 1576.2977, 1762.2427, 3019.0949, 3026.9161, 3030.9632, 3072.7577, 3073.0736, 3083.7923, 3122.6784, 3137.047, 3143.3993, 3183.1819

6.9 Ozonolysis of 2-methyl-2-pentene (Alkene 7)

Compound: $EtCHCMe_2 + O_3$ PRC1.1	**Energy (kJ mol^{-1}):** -460.747340455438
Reaction Coordinates: 6 -2.926431 -1.475814 -0.386089 6 -1.736522 -0.944110 0.425894 6 -0.801170 -0.123331 -0.402321 6 -0.412376 1.154885 -0.223088 6 0.556467 1.792245 -1.175016 6 -0.872458 2.040682 0.897410 1 1.490925 2.043468 -0.661643 1 0.159821 2.732333 -1.567837 1 0.795951 1.140772 -2.013611 1 -0.015520 2.387482 1.480770 1 -1.358724 2.934926 0.497538 1 -1.566088 1.553234 1.576623 1 -0.401677 -0.639481 -1.271131 1 -2.099906 -0.386042 1.287935 1 -1.175474 -1.795430 0.824746 1 -3.541740 -0.658781 -0.764871 1 -3.557798 -2.118530 0.228378 1 -2.587324 -2.061404 -1.242132 8 1.449466 -0.472725 1.081214 8 2.442836 -0.518140 0.299294 8 2.484260 -1.484121 -0.529947	**Frequencies (cm^{-1}):** 24.3772, 39.0395, 52.1489, 56.6795, 69.4759, 101.5354, 122.3423, 156.3385, 192.7105, 210.6896, 262.5123, 305.4494, 366.032, 418.5862, 482.2918, 512.7082, 731.7565, 752.2646, 826.8154, 869.7889, 920.3645, 962.6203, 1003.8852, 1015.6723, 1079.2643, 1094.4421, 1098.6073, 1143.5357, 1147.1185, 1167.0006, 1239.2296, 1290.7326, 1337.6765, 1393.3027, 1408.3391, 1414.3389, 1419.4656, 1469.915, 1475.9219, 1487.2231, 1491.0555, 1495.4187, 1498.928, 1506.5892, 1675.1502, 3001.9397, 3010.1237, 3017.1463, 3025.9382, 3043.6647, 3053.8741, 3069.224, 3090.55, 3091.6538, 3104.5644, 3119.7839, 3127.8807

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -460.744901381960
Reaction Coordinates: 6 3.070359 -0.360149 0.108386 6 1.660901 -0.888308 -0.207046 6 0.597663 -0.176813 0.568100	**Frequencies (cm^{-1}):** -148.1205, 54.1249, 65.1226, 107.6598, 126.0068, 153.4591, 169.4816, 179.9395,

6 -0.069520 0.960791 0.177542 6 -0.938176 1.682539 1.168994 6 0.244327 1.701946 -1.090320 1 -1.821607 2.104339 0.691028 1 -0.384251 2.514758 1.616030 1 -1.258309 1.027084 1.978052 1 0.672892 1.059699 -1.855002 1 -0.651203 2.168967 -1.498254 1 0.960536 2.503321 -0.883164 1 0.486292 -0.479461 1.602977 1 1.467298 -0.809970 -1.276691 1 1.615687 -1.950503 0.036204 1 3.175172 0.689398 -0.168216 1 3.821902 -0.929343 -0.439971 1 3.295278 -0.447932 1.172378 8 -1.812563 -0.211244 -0.916951 8 -2.026263 -1.076576 0.014105 8 -1.007801 -1.833479 0.236683	182.1914, 215.7886, 313.0412, 357.4286, 399.0068, 444.0117, 511.7577, 547.3871, 740.4461, 749.8615, 824.3318, 883.1431, 912.0016, 957.3278, 1005.8709, 1011.9397, 1065.3115, 1080.7093, 1086.6118, 1094.9507, 1115.5838, 1149.9181, 1237.5583, 1294.3723, 1337.9675, 1376.0062, 1406.7923, 1410.381, 1419.3049, 1472.8497, 1479.6381, 1481.9242, 1492.6201, 1498.4052, 1503.0607, 1511.6697, 1587.1901, 3008.281, 3016.5786, 3026.927, 3046.1347, 3072.6226, 3072.7756, 3081.6067, 3090.5786, 3096.0364, 3109.7847, 3128.8697, 3146.0254
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ1.1	**Energy (kJ mol^{-1}):** -460.844826485851
Reaction Coordinates: 6 1.726537 -0.747415 0.329396 6 0.356559 -0.595628 -0.315866 6 -0.532778 0.659786 0.031630 6 -0.722567 1.547477 -1.193997 1 -1.372356 2.389784 -0.958182 1 0.235710 1.939768 -1.539840 1 -1.172539 0.977958 -2.006301 6 -0.116607 1.455738 1.261655 1 0.017222 0.806456 2.124222 1 0.805906 2.005831 1.080125 1 -0.894427 2.180129 1.502940 8 -1.795585 0.047508 0.401689 8 -1.762202 -1.243175 -0.236261 8 -0.447294 -1.697684 0.106936 1 0.458280 -0.641425 -1.404884 1 2.016807 -1.793823 0.215279 1 1.659150 -0.561621 1.400877 6 2.797042 0.139066 -0.308735 1 2.569363 1.200482 -0.207539	**Frequencies (cm^{-1}):** 52.8853, 113.4263, 187.0898, 214.8036, 230.4054, 251.427, 291.0146, 303.4499, 331.9844, 382.0785, 419.3479, 466.621, 515.5523, 608.5525, 699.1929, 711.1992, 771.1634, 824.6508, 860.66, 933.7451, 938.7342, 940.1331, 963.0493, 1003.4908, 1023.3307, 1060.4343, 1110.9264, 1159.7843, 1182.9483, 1216.0754, 1255.0844, 1297.3725, 1334.5637, 1373.7122, 1402.6847, 1404.4904, 1420.5908, 1424.2249, 1478.7767, 1489.1409, 1493.9075, 1499.9695, 1502.3072, 1508.7366, 1515.988, 3003.7631, 3031.3114, 3032.5537, 3041.8825, 3046.379, 3075.619, 3094.2251, 3096.9861, 3098.0272, 3106.8693, 3111.6073, 3123.6411

1 3.764150 -0.033649 0.162782 1 2.904267 -0.077216 -1.372878	

Compound: $EtCHCMe_2 + O_3$ PRC1.2	**Energy (kJ mol^{-1}):** -460.747724375538
Reaction Coordinates: 6 1.514008 -1.269378 0.756672 6 0.622896 -0.070354 0.906175 6 0.513660 1.110020 0.260584 6 1.349596 1.607772 -0.883666 1 0.703695 1.887865 -1.719910 1 2.078691 0.894468 -1.243701 1 1.879330 2.517823 -0.586549 6 -0.549355 2.081412 0.692933 1 -1.074408 1.750442 1.586899 1 -1.288830 2.218113 -0.103830 1 -0.121667 3.068858 0.886398 1 -0.075941 -0.205984 1.727055 1 0.843025 -2.130363 0.661652 6 2.568339 -1.351450 -0.344308 1 3.324342 -0.571842 -0.251919 1 2.125811 -1.287109 -1.337879 1 3.082301 -2.311249 -0.278471 1 2.004921 -1.416429 1.726386 8 -1.171745 -0.677283 -1.036562 8 -2.321842 -0.404536 -0.583605 8 -2.705930 -1.051022 0.445608	**Frequencies (cm^{-1}):** 25.6604, 44.3871, 51.0711, 53.7853, 83.6472, 101.5725, 111.5851, 174.1157, 238.9903, 251.4035, 275.4482, 316.4937, 336.1399, 397.371, 462.9088, 619.2409, 730.9618, 740.3755, 776.6171, 885.0587, 895.453, 961.3383, 1007.8813, 1032.7309, 1079.2222, 1094.997, 1104.0563, 1140.7121, 1147.8444, 1163.6155, 1224.1557, 1312.257, 1382.8257, 1400.693, 1411.8033, 1420.3499, 1427.533, 1465.1825, 1470.8392, 1479.773, 1491.4561, 1497.5721, 1511.2134, 1515.2005, 1674.1797, 2987.5776, 3000.3032, 3006.8705, 3016.2611, 3033.5309, 3042.6471, 3050.6253, 3087.4138, 3100.844, 3105.5098, 3116.6265, 3184.6047

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -460.739786646692
Reaction Coordinates: 6 -2.517389 0.046252 -0.472549 6 -1.819378 -0.769219 0.628382 6 -0.377775 -0.441323 0.916786 6 0.702277 -0.883915 0.182516 6 2.082458 -0.753494 0.763092 6 0.556397 -1.802240 -0.996841 1 2.161339 0.114828 1.416673 1 2.839419 -0.674003 -0.015414 1 2.318912 -1.637634 1.364018 1 1.330991 -1.606804 -1.737146 1 -0.410924 -1.711338 -1.482297 1 0.675215 -2.841190 -0.671817 1 -0.164801 -0.022691 1.891504 1 -1.881728 -1.829795 0.365439 1 -2.384237 -0.656002 1.554830 1 -2.605922 1.091877 -0.190624 1 -3.517892 -0.353819 -0.641555 1 -1.968904 0.010457 -1.412243 8 0.877242 0.995325 -1.129709 8 0.866211 1.850904 -0.160878 8 -0.262328 1.871241 0.469377	**Frequencies (cm^{-1}):** -184.7692, 50.4835, 86.4092, 113.7601, 137.8623, 147.3028, 164.4755, 191.3028, 201.9791, 234.44, 285.7862, 343.2962, 394.391, 442.8648, 510.9799, 591.2409, 735.1897, 744.0848, 826.9125, 870.1603, 899.3584, 957.4594, 1007.6298, 1020.4367, 1058.9903, 1073.302, 1088.0406, 1100.7156, 1110.7763, 1134.2899, 1235.3982, 1302.7241, 1357.5725, 1373.2093, 1407.9464, 1413.5969, 1420.4798, 1472.6008, 1480.0011, 1480.8523, 1490.4083, 1492.8335, 1506.1366, 1512.2903, 1574.2953, 3006.6021, 3010.109, 3014.2479, 3042.1801, 3056.0302, 3074.7985, 3084.4545, 3104.1582, 3112.7303, 3129.7948, 3136.1839, 3163.6699
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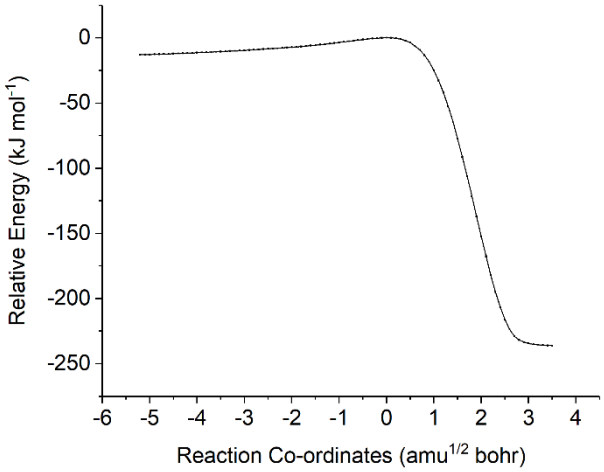
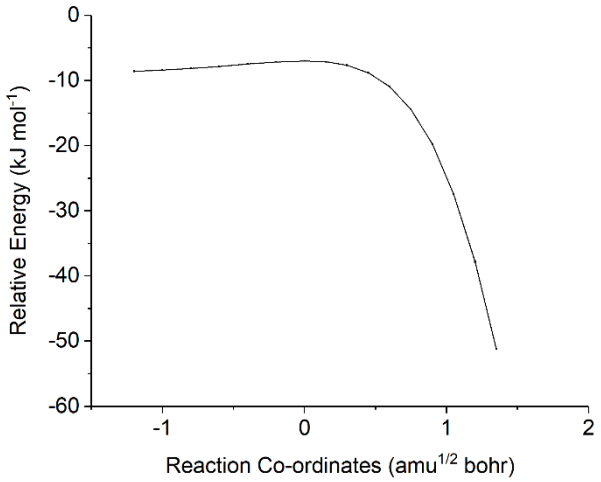


Compound: $EtCHCMe_2 + O_3$ POZ1.2	**Energy (kJ mol^{-1}):** -460.841474813509
Reaction Coordinates: 6 1.743490 -0.439424 0.783544 6 0.358621 0.214437 0.766326 6 -0.831376 -0.467249 -0.022909 6 -2.028609 -0.663614 0.905749 1 -2.870966 -1.080670 0.354598 1 -1.776029 -1.347694 1.718098 1 -2.331513 0.287350 1.341226 6 -0.514041 -1.742532 -0.789863 1 -1.398525 -2.068054 -1.336938 1 0.291958 -1.597387 -1.502786 1 -0.238514 -2.540709 -0.100893 8 -1.138444 0.528552 -1.021177 8 -0.850125 1.757360 -0.340904 8 0.476537 1.505535 0.160495 1 0.022033 0.340278 1.799141 1 1.606289 -1.499856 1.007186 1 2.285008 -0.026756 1.637272 6 2.605437 -0.260637 -0.468328 1 2.836668 0.789223 -0.635493 1 3.545488 -0.799746 -0.346243 1 2.123227 -0.633452 -1.369594	**Frequencies (cm^{-1}):** 31.4557, 97.9497, 173.3504, 211.4148, 236.1125, 259.6678, 264.073, 285.9836, 341.214, 357.6992, 406.0484, 501.7996, 564.0141, 627.5542, 699.0777, 717.6724, 761.8879, 808.9397, 860.4008, 917.9469, 930.4121, 934.0109, 954.1294, 975.5551, 1021.6561, 1086.9356, 1098.312, 1141.2577, 1186.327, 1206.6786, 1256.9978, 1305.117, 1346.9067, 1371.5275, 1398.596, 1405.4694, 1423.6047, 1428.4515, 1477.2474, 1488.2502, 1489.5688, 1496.7173, 1501.3657, 1506.1677, 1517.4918, 3008.5522, 3031.9684, 3034.1431, 3045.7197, 3050.0698, 3055.6507, 3094.7489, 3104.6311, 3104.9209, 3115.4515, 3120.6432, 3144.2798

Compound: $EtCHCMe_2 + O_3$ PRC1.3	**Energy (kJ mol^{-1}):** -460.747724375538
Reaction Coordinates: 6 -1.528255 -2.408615 -0.110197 6 -1.976308 -0.944957 -0.030330 6 -0.994301 -0.003626 -0.657275 6 -0.639514 1.231222 -0.250401 6 0.359265 2.031354 -1.032997 6 -1.199335 1.921692 0.958828 1 0.671289 1.520989 -1.942599 1 1.251486 2.230300 -0.429899 1 -0.049450 3.007845 -1.307121 1 -0.391776 2.295008 1.592614 1 -1.837492 1.281787 1.562039 1 -1.787859 2.792826 0.655777	**Frequencies (cm^{-1}):** 25.3411, 38.1564, 46.1916, 62.1397, 72.7198, 102.7148, 121.6829, 167.3478, 197.6592, 207.2022, 253.2639, 289.9318, 350.3514, 418.1852, 470.7755, 512.796, 730.7464, 746.4923, 824.0487, 865.476, 926.2027, 964.4243, 1001.8646, 1025.4569, 1086.8402, 1093.9333, 1098.4524, 1141.9493, 1146.0957, 1165.8577, 1237.7572, 1289.2825, 1338.3482, 1395.2342, 1409.9316,

1 -0.536041 -0.369073 -1.572324 1 -2.168225 -0.674373 1.007981 1 -2.936838 -0.844433 -0.550921 1 -0.588078 -2.557650 0.419014 1 -1.378789 -2.716079 -1.146597 1 -2.278585 -3.067411 0.327844 8 1.202822 -0.331289 1.065809 8 2.268628 -0.235307 0.390553 8 2.516181 -1.166173 -0.441559	1415.715, 1419.883, 1469.1078, 1474.3306, 1481.436, 1490.5559, 1494.4989, 1498.9472, 1507.7617, 1673.6631, 2981.2833, 3003.1462, 3016.5654, 3030.8419, 3043.5369, 3057.4094, 3062.1603, 3089.4291, 3103.5251, 3107.05, 3118.6057, 3125.6229

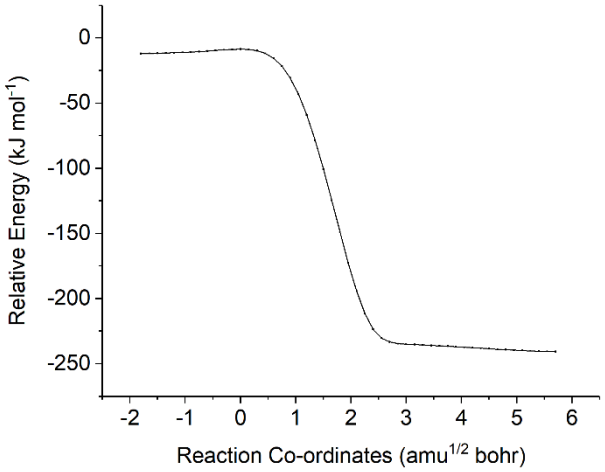
Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -460.745048402460
Reaction Coordinates: 6 -3.003459 -0.232966 0.218382 6 -1.693548 -0.748272 -0.373478 6 -0.510738 -0.521799 0.515472 6 0.779968 -0.883888 0.220106 6 1.844579 -0.788076 1.275002 6 1.125176 -1.655769 -1.020962 1 1.554590 -0.117395 2.082811 1 2.788974 -0.442421 0.855539 1 2.029012 -1.775108 1.711936 1 1.021286 -2.729528 -0.833369 1 2.157205 -1.476167 -1.318794 1 0.477770 -1.399694 -1.856163 1 -0.716644 -0.182554 1.523842 1 -1.507235 -0.267510 -1.338019 1 -1.782883 -1.819739 -0.587671 1 -2.951217 0.840414 0.399510 1 -3.227357 -0.723912 1.167379 1 -3.837776 -0.420843 -0.457380 8 1.275637 1.138352 -0.896046 8 0.794931 1.959291 -0.028715 8 -0.477767 1.839743 0.130167	**Frequencies (cm^{-1}):** -126.491, 68.9222, 76.5664, 112.5713, 123.5622, 150.6893, 156.4756, 181.0043, 193.376, 209.4068, 288.478, 329.1104, 421.1836, 430.5905, 492.2905, 517.4084, 738.6056, 752.5652, 814.2382, 869.5764, 930.2156, 958.748, 1009.0385, 1036.3133, 1070.9306, 1086.9033, 1089.5301, 1099.3898, 1114.1089, 1139.2754, 1232.4285, 1289.9454, 1340.3804, 1382.917, 1408.0571, 1416.1403, 1418.9474, 1461.1663, 1473.1831, 1480.6995, 1483.5446, 1500.625, 1501.5581, 1506.1808, 1589.6959, 2990.1223, 3008.1951, 3013.7395, 3026.3928, 3031.5984, 3071.7701, 3082.5418, 3087.4777, 3101.8727, 3109.1984, 3124.5935, 3149.3621
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ1.3	**Energy (kJ mol^{-1}):** -460.845901713431
Reaction Coordinates:	**Frequencies (cm^{-1}):**

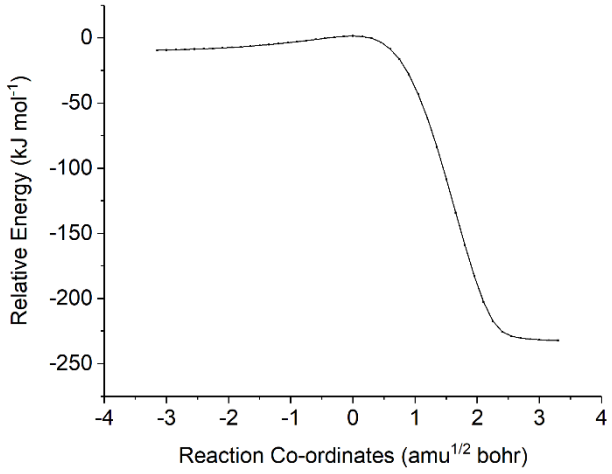
6 1.672473 -0.747777 -0.199550 6 0.513832 0.073422 0.339480 6 -0.953385 -0.413689 0.034679 6 -1.670419 -0.796857 1.325247 1 -2.693753 -1.107462 1.116577 1 -1.156306 -1.623029 1.820911 1 -1.695486 0.050545 2.009221 6 -1.087757 -1.488648 -1.035441 1 -0.574404 -1.202557 -1.950762 1 -0.685300 -2.437941 -0.682155 1 -2.141390 -1.639102 -1.270005 8 -1.557208 0.770646 -0.541564 8 -0.764883 1.852708 -0.017294 8 0.565550 1.373544 -0.252371 1 0.612346 0.183647 1.424295 1 1.556572 -1.770529 0.167259 1 1.609302 -0.790614 -1.287323 6 3.035988 -0.201019 0.225423 1 3.124432 -0.163640 1.312713 1 3.838966 -0.833866 -0.152727 1 3.192963 0.806770 -0.157191	50.885, 98.4154, 179.7514, 214.5487, 229.8212, 257.0531, 283.636, 299.8391, 321.321, 347.0321, 443.3669, 488.5574, 505.5981, 600.0054, 700.7677, 749.1161, 775.0452, 810.0957, 865.2591, 932.9256, 936.3662, 939.0062, 967.3431, 975.3204, 1019.3547, 1062.3722, 1117.8919, 1160.6095, 1184.1923, 1213.5223, 1259.1745, 1302.7511, 1344.2241, 1358.8357, 1403.7369, 1408.8623, 1418.4758, 1424.2717, 1473.9708, 1483.9326, 1490.184, 1498.2063, 1500.1633, 1507.6806, 1510.4988, 3002.5993, 3029.7136, 3030.8764, 3031.2636, 3044.2585, 3071.4208, 3092.1848, 3092.6604, 3103.6445, 3105.7702, 3112.4243, 3123.6743

Compound: $EtCHCMe_2 + O_3$ PRC 2.1	**Energy (kJ mol^{-1}):** -460.751783712005
Reaction Coordinates: 6 -3.001608 1.052763 0.198353 6 -1.637208 0.725716 -0.423354 6 -0.780670 -0.112455 0.471376 6 -0.134832 -1.259034 0.181313 6 0.713261 -1.936271 1.217679 6 -0.218846 -1.987250 -1.130137 1 0.376408 -2.963249 1.386052 1 1.750536 -1.995819 0.877005 1 0.699729 -1.404488 2.167021 1 0.781746 -2.173632 -1.525892 1 -0.786946 -1.454879 -1.887784 1 -0.682631 -2.966847 -0.981932 1 -0.679968 0.265061 1.484517 1 -1.777973 0.252435 -1.394376 1 -1.114039 1.669995 -0.621498 1 -3.583664 0.145733 0.365649 1 -3.578486 1.710073 -0.453067 1 -2.884327 1.554850 1.160039 8 1.925602 0.431374 -0.932292 8 1.700829 1.555159 -0.394783 8 1.603448 1.570962 0.868685	**Frequencies (cm^{-1}):** 29.2275, 39.6196, 48.3274, 66.479, 73.649, 92.3192, 148.0055, 161.3737, 201.1173, 211.2481, 273.1839, 304.5078, 363.7559, 421.248, 488.8513, 510.2296, 738.8918, 750.5936, 824.8152, 862.694, 922.278, 962.9471, 1006.5153, 1018.8988, 1081.1436, 1093.9354, 1099.5826, 1143.6492, 1154.4732, 1171.8565, 1236.5816, 1292.091, 1338.4629, 1391.6324, 1408.2846, 1413.6368, 1419.4938, 1469.3301, 1474.9754, 1484.1329, 1489.0941, 1495.9253, 1499.2529, 1505.2213, 1671.4855, 2977.5611, 3009.919, 3018.4747, 3026.53, 3051.2988, 3059.8369, 3068.5702, 3091.0571, 3091.4878, 3108.8168, 3125.3984, 3128.0445

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -460.742913889416
Reaction Coordinates: 6 3.013184 -0.288539 0.004775 6 1.611362 -0.913995 -0.095548 6 0.574447 -0.126895 0.648329 6 -0.101753 0.972647 0.160745 6 -0.922865 1.809094 1.094706	**Frequencies (cm^{-1}):** -181.1186, 54.02, 72.8453, 119.6983, 145.1096, 165.0871, 183.5146, 186.8669, 195.1584, 218.0639, 309.8123, 354.167, 401.5708, 454.3051, 522.7918, 562.4166,

6 0.190095 1.581615 -1.183780 1 -1.862578 2.105240 0.628123 1 -1.149367 1.277675 2.016799 1 -0.383173 2.727539 1.348147 1 -0.697255 2.058358 -1.596503 1 0.555686 0.856456 -1.906837 1 0.954092 2.358318 -1.075121 1 0.514424 -0.304809 1.714142 1 1.332293 -1.011486 -1.146224 1 1.643633 -1.924580 0.311238 1 3.040152 0.708789 -0.434403 1 3.743955 -0.906652 -0.518182 1 3.330296 -0.203388 1.045018 8 -1.990977 -0.186153 -0.636526 8 -1.552170 -1.397193 -0.533666 8 -1.107976 -1.659782 0.649996	740.3799, 749.1805, 825.8896, 884.8969, 910.7131, 958.3067, 1006.5499, 1012.1368, 1065.0227, 1075.7464, 1078.9228, 1094.3438, 1114.621, 1145.6073, 1237.9765, 1298.5338, 1339.7951, 1368.9063, 1407.6763, 1410.7949, 1419.6865, 1470.7354, 1478.4169, 1479.7185, 1492.5676, 1498.5335, 1502.571, 1511.2965, 1575.1834, 3008.7156, 3013.3935, 3028.8012, 3039.2506, 3071.7678, 3073.0656, 3083.7123, 3090.4455, 3098.6306, 3116.4479, 3124.0163, 3162.3047
IRC:  	

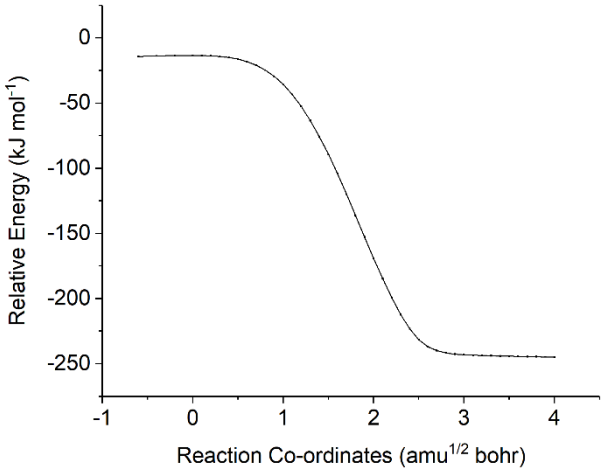
Compound: $EtCHCMe_2 + O_3$ POZ 2.1	**Energy (kJ mol^{-1}):** -460.843501343655
Reaction Coordinates: 6 1.667493 -0.828110 0.248072 6 0.364867 -0.541504 -0.492456 6 -0.521618 0.659809 -0.010703 6 -0.453937 1.856948 -0.948252 1 -1.173513 2.616647 -0.644264 1 0.539922 2.302516 -0.920321 1 -0.674248 1.557802 -1.971927 6 -0.321935 1.057974 1.448917 1 -1.041917 1.834302 1.706092 1 -0.481736 0.209219 2.110144 1 0.678056 1.452318 1.624326 8 -1.843077 0.102884 -0.179027 8 -1.674264 -1.216978 0.320601 8 -0.513746 -1.683048 -0.425510 1 0.577979 -0.405180 -1.556139 1 1.987376 -1.825477 -0.058793 1 1.482791 -0.882786 1.321102 6 2.784283 0.169736 -0.063184 1 2.545179 1.179939 0.270611 1 3.709224 -0.125741 0.431749 1 2.984664 0.214458 -1.135451	**Frequencies (cm^{-1}):** 47.4534, 126.4152, 192.5844, 207.5033, 219.7459, 254.4629, 273.7822, 299.043, 334.8363, 349.228, 429.6521, 481.6655, 507.1535, 616.1306, 684.515, 741.1934, 764.233, 832.789, 872.5007, 911.836, 934.2853, 943.4107, 964.3483, 989.8548, 1024.021, 1051.7533, 1097.6096, 1139.996, 1190.2706, 1228.5345, 1247.518, 1292.2529, 1329.372, 1363.5998, 1400.8704, 1404.7698, 1417.9464, 1423.8806, 1480.2859, 1489.7912, 1493.3749, 1501.5444, 1501.712, 1510.1692, 1515.7845, 3020.5767, 3028.9326, 3041.7889, 3043.3856, 3048.8662, 3071.5452, 3092.9159, 3095.1476, 3106.1513, 3112.3338, 3115.3751, 3125.813

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -460.739223263807
Reaction Coordinates: 6 2.471674 -0.371705 0.413611 6 1.565857 -1.194268 -0.516112 6 0.229373 -0.599878 -0.885614 6 -0.923128 -0.706495 -0.128596 6 -2.251413 -0.437599 -0.770653 6 -0.954805 -1.452280 1.177614 1 -2.149359 0.205804 -1.642041 1 -2.940437 0.034657 -0.071257 1 -2.704924 -1.381829 -1.090402 1 -1.749325 -1.078267 1.820557 1 -0.016942 -1.388890 1.722906 1 -1.160883 -2.511743 0.988926 1 0.100554 -0.317922 -1.920912 1 1.394114 -2.171246 -0.054085 1 2.111499 -1.388760 -1.440557 1 2.750496 0.571745 -0.050663 1 3.380587 -0.934139 0.629029 1 1.987581 -0.143141 1.362637 8 -0.943726 1.401001 0.806164 8 0.239578 1.811944 0.479121 8 0.475608 1.671689 -0.784740	**Frequencies (cm^{-1}):** -210.381, 64.1734, 78.7749, 144.4476, 152.7367, 168.0899, 178.485, 199.2285, 224.9638, 238.2085, 291.5851, 336.3554, 394.844, 458.776, 508.2422, 606.2353, 736.6651, 741.9745, 825.4385, 880.9332, 898.2541, 956.9904, 1010.4448, 1023.0714, 1057.7753, 1070.4666, 1088.8278, 1101.6903, 1111.7485, 1131.7605, 1235.1962, 1304.1358, 1356.3034, 1366.5303, 1409.1368, 1411.9132, 1420.3169, 1470.5815, 1474.4364, 1480.2292, 1490.1934, 1497.1972, 1506.0978, 1513.2282, 1562.894, 3004.8635, 3008.4611, 3010.6017, 3039.3617, 3056.5642, 3077.4097, 3087.8548, 3097.769, 3118.7522, 3119.9338, 3130.1692, 3175.0173
IRC:  	

Compound: $EtCHCMe_2 + O_3$ POZ 2.2	**Energy (kJ mol^{-1}):** -460.840392867891
Reaction Coordinates: 6 -1.629032 -0.759939 -0.705251 6 -0.322266 0.029848 -0.857520 6 0.920513 -0.342683 0.035470 6 2.037185 -0.970964 -0.789100 1 2.932028 -1.101438 -0.181324 1 1.728418 -1.953174 -1.148652 1 2.284552 -0.345550 -1.645490 6 0.622602 -1.160980 1.288302	**Frequencies (cm^{-1}):** 33.2038, 94.3935, 192.1587, 217.787, 227.7734, 266.1785, 278.2379, 287.9476, 312.593, 361.7135, 438.1265, 503.8548, 554.0692, 634.154, 683.3027, 747.6194, 773.2159, 807.8858, 859.3256, 902.9729, 929.6835, 941.4005, 949.6806, 969.7482, 1025.4588, 1083.6496, 1091.9296,

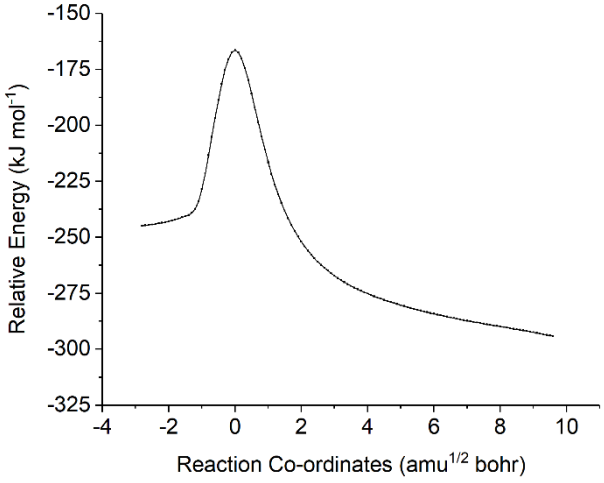
1 1.559527 -1.387722 1.796436 1 -0.009530 -0.603086 1.973249 1 0.133418 -2.104515 1.047289 8 1.396478 0.966349 0.419174 8 0.181882 1.684007 0.617377 8 -0.509332 1.438771 -0.634396 1 -0.006483 -0.041134 -1.899851 1 -1.388793 -1.826859 -0.722673 1 -2.205700 -0.575836 -1.614361 6 -2.515267 -0.422626 0.494516 1 -2.702283 0.648812 0.544259 1 -3.477021 -0.926320 0.392618 1 -2.082768 -0.732126 1.442758	1123.255, 1189.0178, 1221.0166, 1245.5609, 1297.0915, 1351.0727, 1359.2106, 1401.0082, 1404.5703, 1419.7757, 1426.7973, 1480.5737, 1483.3825, 1493.0461, 1498.3334, 1505.3499, 1511.8922, 1517.0094, 3018.5421, 3037.2543, 3039.2362, 3046.0323, 3047.9443, 3051.4913, 3099.815, 3102.2491, 3105.9589, 3114.9782, 3123.0568, 3139.602

Compound: $EtCHCMe_2 + O_3$ TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -460.744562310228
Reaction Coordinates: 6 -2.940131 -0.498997 0.192076 6 -1.580485 -0.804563 -0.430586 6 -0.431965 -0.610759 0.510496 6 0.889236 -0.809358 0.181562 6 1.942728 -0.756866 1.244621 6 1.303424 -1.395740 -1.140571 1 2.295133 -1.767314 1.475906 1 2.806458 -0.184736 0.904273 1 1.569521 -0.302992 2.160392 1 2.312160 -1.085961 -1.408047 1 0.634233 -1.118090 -1.951319 1 1.305209 -2.488907 -1.070018 1 -0.671360 -0.463757 1.555443 1 -1.568342 -1.833872 -0.807885 1 -1.428106 -0.176186 -1.315750 1 -3.130187 -1.139886 1.054960 1 -3.744101 -0.661319 -0.525717 1 -2.985733 0.537508 0.525673 8 1.306422 1.398360 -0.555729 8 0.106342 1.873917 -0.539670 8 -0.474230 1.720624 0.602462	**Frequencies (cm^{-1}):** -155.9795, 65.8628, 79.7094, 125.0189, 144.5644, 155.7207, 167.4377, 187.0588, 207.5286, 217.3186, 291.1199, 330.7988, 420.4388, 452.9391, 506.7389, 517.5295, 737.4264, 761.4205, 814.1708, 870.1303, 931.0773, 960.9485, 1008.0967, 1037.6528, 1067.2787, 1079.2626, 1086.3053, 1098.115, 1112.1505, 1138.5875, 1232.7408, 1287.0828, 1337.5211, 1377.4321, 1409.2684, 1415.9508, 1419.4432, 1466.0984, 1471.3071, 1477.6821, 1482.4807, 1499.4956, 1500.3425, 1507.9302, 1580.9457, 2986.8401, 3002.4501, 3006.8086, 3012.3662, 3030.4233, 3071.1719, 3083.8721, 3088.3992, 3102.507, 3115.8668, 3124.479, 3164.8054
IRC:	

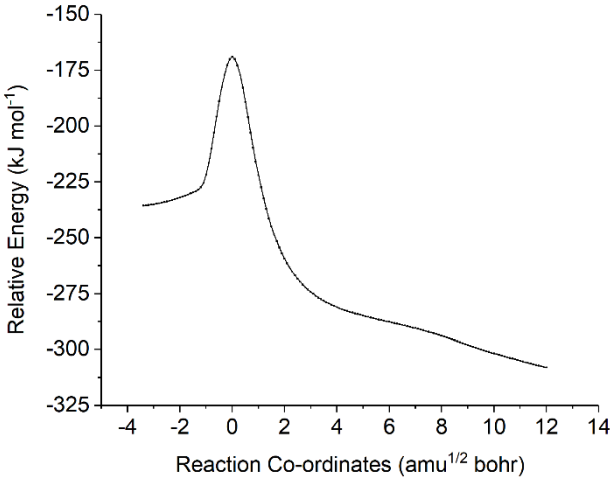


Compound: $EtCHCMe_2 + O_3$ POZ 2.3	**Energy (kJ mol^{-1}):** -460.844901066989
Reaction Coordinates: 6 -1.608994 -0.691290 0.381261 6 -0.506994 -0.049396 -0.451245 6 0.980740 -0.372674 -0.049653 6 1.711809 -1.158509 -1.129623 1 2.767087 -1.262012 -0.878330 1 1.286842 -2.158935 -1.217035 1 1.630206 -0.656781 -2.092727 6 1.150152 -1.006620 1.328265 1 2.213037 -1.132768 1.531758 1 0.726096 -0.373767 2.104785 1 0.676955 -1.986669 1.380867 8 1.572688 0.945357 -0.043607 8 0.514314 1.751675 0.470474 8 -0.576638 1.388640 -0.408813 1 -0.652831 -0.298266 -1.505013 1 -1.516220 -0.362457 1.417020 1 -1.462241 -1.774885 0.376739 6 -3.004380 -0.361941 -0.147967 1 -3.133577 -0.718363 -1.172004 1 -3.772830 -0.831357 0.466415 1 -3.179431 0.713459 -0.143127	**Frequencies (cm^{-1}):** 37.7871, 105.7857, 190.8539, 219.5431, 222.7744, 258.1937, 285.9021, 290.4856, 321.0124, 341.2438, 464.8371, 490.2754, 506.3945, 610.0883, 703.2477, 740.3268, 769.374, 835.4526, 874.2226, 910.4849, 931.7367, 942.3624, 964.0713, 974.8783, 1023.5637, 1059.0311, 1099.5441, 1138.8188, 1188.8782, 1221.8449, 1244.8372, 1296.7898, 1322.7599, 1354.1272, 1402.6848, 1404.9084, 1416.2299, 1422.515, 1473.8661, 1483.5697, 1490.9123, 1499.5985, 1501.3279, 1508.9773, 1512.1057, 3021.9935, 3027.8837, 3033.3401, 3038.2292, 3047.0145, 3069.1242, 3089.9786, 3100.9758, 3103.4849, 3108.3195, 3113.9712, 3124.397

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -460.811539072716
Reaction Coordinates: 6 2.761296 0.142974 -0.273923 6 1.730179 -0.815328 0.320875 6 0.355126 -0.733891 -0.293151 6 -0.727340 0.828886 0.053570 6 -0.292233 1.786076 -1.065222 6 -0.353458 1.257299 1.475071 1 -0.582893 1.382800 -2.033404 1 -0.818916 2.731962 -0.925774 1 0.775882 1.993371 -1.061481 1 0.693505 1.544724 1.568555	**Frequencies (cm^{-1}):** -479.1659, 74.237, 84.0426, 187.0363, 194.4555, 209.3752, 225.7804, 263.1228, 272.7625, 288.9553, 354.1889, 403.9203, 444.9637, 483.4066, 515.2923, 566.7698, 617.3961, 766.3513, 789.4478, 910.0444, 924.2431, 979.7504, 1000.2722, 1039.4269, 1061.2736, 1070.1991, 1117.0657, 1150.1401, 1163.1063,

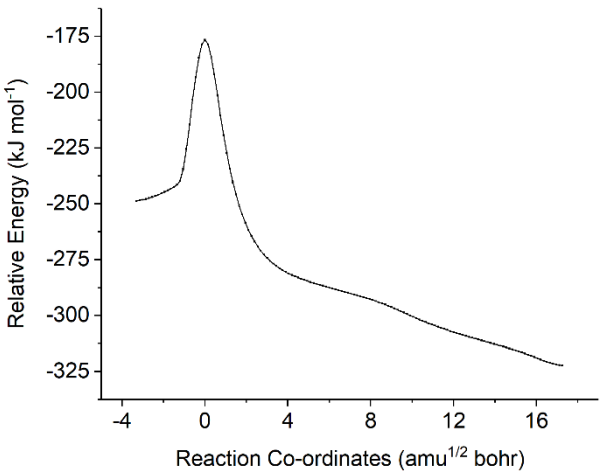
1 -0.962657 2.122327 1.743400 1 -0.578011 0.460195 2.181322 1 0.287241 -0.669948 -1.375421 1 2.075802 -1.842114 0.166635 1 1.656004 -0.680008 1.400193 1 2.548232 1.181808 -0.028932 1 3.750159 -0.089653 0.119490 1 2.808765 0.055607 -1.360181 8 -1.915600 0.349406 -0.083706 8 -1.661477 -1.590896 -0.366806 8 -0.484739 -1.631906 0.238297	1189.3258, 1243.9402, 1302.3482, 1329.4567, 1375.6091, 1387.3813, 1403.5334, 1411.8623, 1425.2802, 1474.0566, 1482.9939, 1489.0423, 1493.334, 1501.6197, 1505.9289, 1513.7988, 3017.9122, 3032.4811, 3037.6761, 3040.1015, 3071.491, 3090.9851, 3099.6783, 3099.7627, 3110.531, 3116.7395, 3119.5251, 3128.892
IRC:  	

Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 1	**Energy (kJ mol^{-1}):** -460.864209176868
Reaction Coordinates: 6 -2.746572 -1.436900 -0.022976 6 -2.698950 0.093773 0.107491 6 -1.421595 0.658712 -0.382478 6 1.702731 -0.666516 0.009300 6 2.229291 -0.354244 1.389015 6 2.576816 -0.267518 -1.153963 1 1.628590 -0.853930 2.144791 1 3.274886 -0.652361 1.484713 1 2.175828 0.725306 1.538179 1 2.866290 0.779073 -1.065490 1 3.491250 -0.866794 -1.141119 1 2.054689 -0.428275 -2.093123 1 -1.008064 0.434117 -1.360372 1 -3.503362 0.530905 -0.496221 1 -2.855358 0.413215 1.137389 1 -1.957731 -1.900600 0.564735 1 -3.712220 -1.803948 0.322173 1 -2.615627 -1.748006 -1.059184 8 0.641492 -1.240803 -0.153890 8 0.420770 1.947482 -0.148486 8 -0.773448 1.444254 0.345526	**Frequencies (cm^{-1}):** 33.6457, 46.2326, 64.6811, 68.837, 80.8736, 93.4359, 105.0318, 139.3042, 145.6334, 200.6471, 227.2482, 321.4662, 384.8229, 421.2239, 485.633, 533.207, 536.2094, 773.9371, 788.5223, 891.6848, 901.2894, 902.674, 915.2185, 938.0514, 1022.5082, 1087.011, 1097.0075, 1117.6295, 1180.9584, 1242.8227, 1275.5046, 1325.1152, 1373.467, 1380.7905, 1388.5091, 1420.9052, 1458.2684, 1467.1285, 1468.123, 1470.9394, 1488.6784, 1496.2215, 1505.25, 1581.4933, 1749.075, 2996.7655, 3027.7843, 3035.9727, 3045.1524, 3084.8294, 3092.3543, 3097.7201, 3108.5523, 3128.7554, 3132.9936, 3140.2787, 3160.1392

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -460.813267916166
Reaction Coordinates: 6 -2.658095 -0.438840 0.413683 6 -1.672636 -0.577437 -0.747518 6 -0.443365 0.295819 -0.685945 6 1.090682 -0.423924 0.134999 6 1.625603 -1.325198 -0.989511 6 0.627738 -1.174306 1.386509 1 1.959700 -0.721056 -1.830512 1 2.484894 -1.878200 -0.607272 1 0.885475 -2.050850 -1.328766 1 0.174912 -0.484580 2.095225 1 1.504707 -1.615617 1.863715 1 -0.069551 -1.981349 1.161706 1 0.036369 0.521708 -1.633061 1 -2.184905 -0.346862 -1.686364 1 -1.344368 -1.614215 -0.846498 1 -2.199718 -0.675262 1.371508 1 -3.054642 0.573268 0.476457 1 -3.495551 -1.119701 0.264124 8 1.783162 0.644963 0.353707 8 0.521620 2.130115 0.004566 8 -0.569393 1.381928 0.095031	**Frequencies (cm^{-1}):** -466.3664, 82.1596, 98.5159, 184.1872, 199.4772, 212.44, 239.6671, 244.564, 249.7741, 306.4548, 362.9335, 410.1543, 442.0656, 484.479, 559.8324, 582.5296, 646.4352, 766.794, 786.865, 895.9897, 911.6849, 977.9318, 997.4033, 1044.8329, 1065.1108, 1076.9716, 1109.593, 1129.4466, 1168.9152, 1193.1954, 1249.9746, 1295.5509, 1367.2143, 1374.785, 1388.2109, 1393.1462, 1403.0975, 1427.864, 1474.7754, 1479.9962, 1488.7833, 1491.8261, 1503.0639, 1505.4831, 1510.3453, 3019.634, 3029.9611, 3034.704, 3049.6204, 3053.0351, 3087.0973, 3093.0151, 3108.7163, 3118.4941, 3122.2832, 3124.1391, 3125.5211
IRC:  	

Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 2	**Energy (kJ mol^{-1}):** -460.861089237022
Reaction Coordinates: 6 -3.351808 -1.417482 -0.306008 6 -2.149754 -0.889328 0.493746 6 -1.483951 0.244468 -0.185015 6 2.176266 -0.407651 -0.020780 6 3.445724 -1.229661 -0.013609 6 2.331722 1.089590 0.039143 1 3.212973 -2.288251 0.064721 1 4.000555 -1.047661 -0.937139 1 4.096235 -0.925974 0.808424 1 2.729623 1.363638 1.020551 1 3.067427 1.424067 -0.695437 1 1.379951 1.596996 -0.116866	**Frequencies (cm^{-1}):** 23.9309, 35.6761, 46.5341, 69.9858, 77.4838, 94.4675, 98.5761, 142.0988, 155.4303, 205.0905, 221.0893, 331.0307, 395.5124, 417.9723, 498.7341, 534.2013, 545.5193, 777.4413, 791.8485, 889.4822, 893.0189, 904.4087, 910.6318, 940.0194, 1018.4545, 1092.5708, 1093.5578, 1125.6242, 1181.2031, 1246.6976, 1276.2185, 1324.046, 1373.2371, 1387.8472, 1402.1745, 1415.8393, 1462.5369, 1466.7706, 1472.8464,

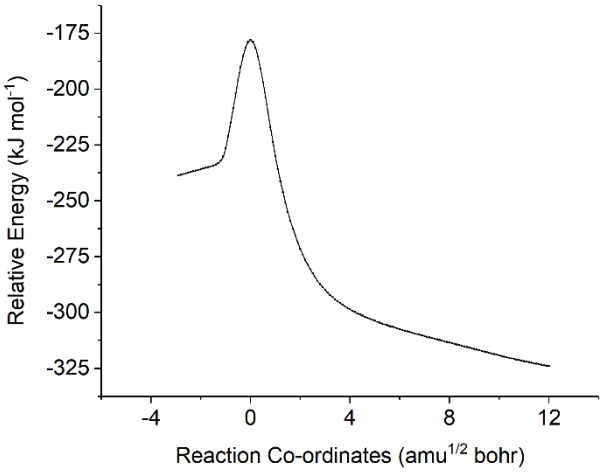
1 -1.083099 0.179235 -1.191020 1 -2.446748 -0.580228 1.495372 1 -1.401021 -1.680251 0.592891 1 -3.055857 -1.723214 -1.309867 1 -3.777666 -2.285516 0.195668 1 -4.130316 -0.660561 -0.396249 8 1.086472 -0.946040 -0.070669 8 -0.748029 2.383866 -0.273575 8 -1.388598 1.348187 0.397255	1476.8279, 1496.5605, 1500.5129, 1505.5468, 1582.7457, 1756.4078, 3009.952, 3031.1276, 3031.3437, 3037.8114, 3069.9628, 3084.5503, 3086.4508, 3103.3832, 3106.1436, 3108.5046, 3136.8146, 3162.6793

Compound: $EtCHCMe_2 + O_3$ TS_{ANTI} 3	**Energy (kJ mol^{-1}):** -460.815150365172
Reaction Coordinates: 6 -3.044257 -0.388912 -0.206862 6 -1.641666 -0.726048 0.316530 6 -0.586348 0.173317 -0.257533 6 1.208680 -0.382996 -0.023896 6 1.336254 -1.427883 -1.143975 6 1.297574 -0.944140 1.397884 1 1.276785 -0.945506 -2.117389 1 2.316476 -1.899817 -1.059722 1 0.581952 -2.212035 -1.073665 1 0.654244 -1.810476 1.550768 1 2.327827 -1.255570 1.578871 1 1.049927 -0.172990 2.124634 1 -0.545417 0.274780 -1.338291 1 -1.616308 -0.656224 1.404187 1 -1.393005 -1.755535 0.055297 1 -3.091941 -0.469447 -1.293537 1 -3.779588 -1.075585 0.212346 1 -3.331603 0.625274 0.069131 8 1.841179 0.720631 -0.230354 8 0.408585 2.121097 -0.224276 8 -0.483610 1.349908 0.378940	**Frequencies (cm^{-1}):** -457.3233, 71.7136, 88.4465, 163.3415, 198.7008, 207.7597, 223.3457, 239.4381, 264.134, 296.7229, 353.4822, 409.9526, 470.2056, 485.5686, 527.8649, 582.21, 622.0962, 770.3444, 784.3912, 910.532, 920.1128, 978.157, 994.6453, 1025.2795, 1055.252, 1066.4819, 1125.1303, 1152.2629, 1161.0383, 1189.0801, 1241.532, 1305.2837, 1339.3799, 1376.2074, 1390.4667, 1404.4123, 1406.2823, 1423.7964, 1473.6081, 1479.0223, 1490.3864, 1493.175, 1499.4556, 1503.9026, 1506.5505, 3030.8716, 3033.8539, 3035.5343, 3048.1488, 3080.4791, 3089.4359, 3094.3687, 3098.6311, 3106.8316, 3117.101, 3121.3381, 3122.8082
IRC:  	

Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 3	**Energy (kJ mol^{-1}):** -460.861089255396

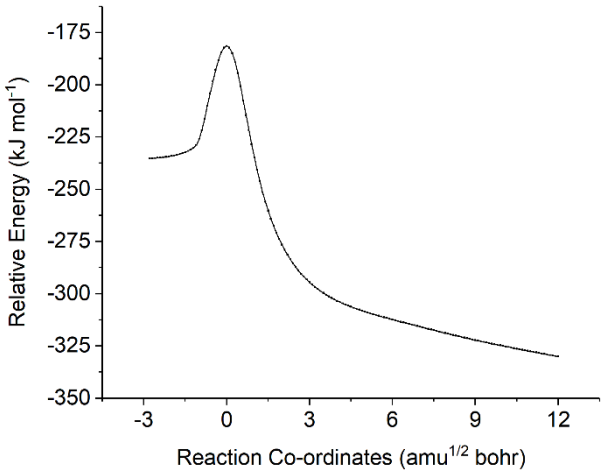
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.351813 -1.417477 -0.305998 6 -2.149736 -0.889338 0.493730 6 -1.483949 0.244470 -0.185023 6 2.176261 -0.407650 -0.020787 6 3.445719 -1.229662 -0.013571 6 2.331718 1.089592 0.039120 1 3.212962 -2.288251 0.064756 1 4.000582 -1.047668 -0.937082 1 4.096202 -0.925975 0.808484 1 2.729623 1.363653 1.020522 1 3.067421 1.424058 -0.695468 1 1.379947 1.596995 -0.116893 1 -1.083112 0.179262 -1.191036 1 -2.446701 -0.580257 1.495370 1 -1.401001 -1.680264 0.592843 1 -3.055893 -1.723189 -1.309872 1 -3.777653 -2.285522 0.195675 1 -4.130325 -0.660556 -0.396200 8 1.086469 -0.946039 -0.070698 8 -0.748036 2.383873 -0.273557 8 -1.388590 1.348179 0.397264	23.9286, 35.6741, 46.5332, 69.9871, 77.4824, 94.4603, 98.5729, 142.0974, 155.4277, 205.0889, 221.0885, 331.0311, 395.5133, 417.9716, 498.7342, 534.202, 545.5198, 777.4416, 791.849, 889.4825, 893.019, 904.4071, 910.6328, 940.021, 1018.4558, 1092.5708, 1093.5582, 1125.624, 1181.2031, 1246.6977, 1276.2193, 1324.0474, 1373.2389, 1387.8484, 1402.1758, 1415.8404, 1462.5368, 1466.7707, 1472.8474, 1476.828, 1496.5594, 1500.5123, 1505.5467, 1582.747, 1756.4072, 3009.954, 3031.1301, 3031.3461, 3037.8137, 3069.9643, 3084.5529, 3086.4509, 3103.3856, 3106.1455, 3108.5063, 3136.8158, 3162.6752

Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 1.1	**Energy (kJ mol^{-1}):** -460.816959471184
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.901085 0.305717 0.163324 6 1.774784 -0.577887 -0.370812 6 0.531142 -0.612527 0.525616 6 -0.730164 0.665562 0.005819 6 -1.671779 0.763298 1.182401 6 -0.134478 1.960941 -0.478165 1 -1.892354 -0.212801 1.599566 1 -2.606461 1.219490 0.846748 1 -1.234615 1.402020 1.947899 1 0.472551 2.409846 0.304950 1 -0.933776 2.664214 -0.721681 1 0.477696 1.815707 -1.365057 1 0.674958 -0.156917 1.520388 1 2.119367 -1.610622 -0.439598 1 1.499112 -0.289120 -1.386766 1 3.784935 0.230017 -0.470464 1 3.192816 0.000922 1.170406 1 2.620864 1.358569 0.205994 8 -1.164787 -0.071166 -1.054583 8 -1.689613 -1.218826 -0.650348 8 -0.170430 -1.692752 0.532246	-471.0743, 81.6386, 105.4888, 168.6498, 180.2379, 210.585, 225.8014, 257.8719, 276.5099, 318.6966, 352.7581, 383.2011, 413.3991, 492.6395, 543.5212, 622.5578, 656.414, 774.7803, 797.3925, 881.9389, 953.2105, 969.8193, 990.7369, 1008.2743, 1031.8374, 1080.8487, 1113.3007, 1129.4713, 1161.8987, 1275.4081, 1280.812, 1282.7783, 1304.4924, 1331.83, 1403.1779, 1409.8112, 1418.9948, 1423.5344, 1470.9732, 1480.7155, 1487.7482, 1496.6431, 1503.4551, 1506.004, 1507.362, 2908.6421, 3028.2587, 3033.7609, 3039.3049, 3041.2397, 3065.4527, 3087.3637, 3094.1067, 3101.7185, 3105.7787, 3136.6371, 3161.8636
IRC:	

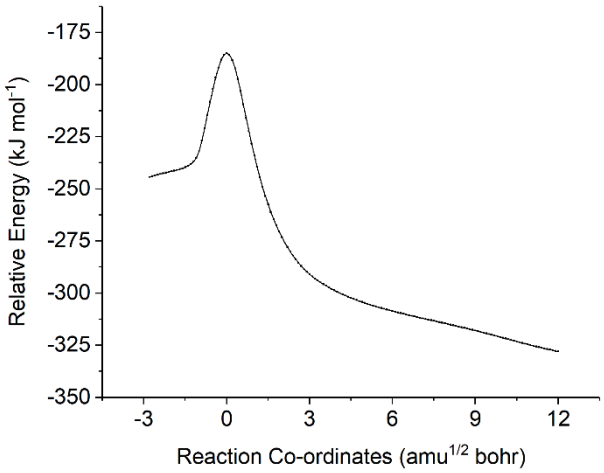


Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 1.1	**Energy (kJ mol^{-1}):** -460.867934905695
Reaction Coordinates: 6 -3.860828 0.009408 -0.201594 6 -2.484954 0.188240 0.451376 6 -1.419492 -0.589281 -0.267965 6 2.036072 0.062166 -0.002279 6 1.890844 0.356893 1.433660 6 2.967888 -0.957952 -0.544586 1 0.885814 0.069186 1.749641 1 1.952682 1.437238 1.581681 1 2.635139 -0.172647 2.022421 1 2.689492 -1.939727 -0.153941 1 3.987489 -0.753232 -0.210793 1 2.932745 -0.979827 -1.630559 1 -1.359773 -0.396613 -1.355782 1 -2.494664 -0.111798 1.499261 1 -2.184831 1.238131 0.397528 1 -4.601675 0.639258 0.289721 1 -4.201922 -1.024429 -0.134572 1 -3.836715 0.288896 -1.256078 8 1.353300 0.690848 -0.858834 8 0.427084 1.615774 -0.390671 8 -0.678004 -1.395532 0.248231	**Frequencies (cm^{-1}):** 27.8053, 37.1247, 44.6573, 75.4092, 86.3917, 92.1706, 148.1384, 158.2367, 160.2278, 213.9424, 292.7054, 308.851, 345.7128, 367.8171, 480.7424, 511.2775, 594.1502, 761.2436, 812.6567, 875.9366, 913.8521, 919.1078, 930.4521, 988.1959, 1007.2752, 1073.3832, 1097.5459, 1129.2985, 1162.7426, 1271.5519, 1306.0831, 1327.8363, 1387.813, 1405.6697, 1409.7397, 1427.9857, 1443.8341, 1458.6885, 1469.9351, 1470.432, 1479.5184, 1501.8644, 1505.3573, 1570.5704, 1773.3791, 2910.3032, 3026.9668, 3029.736, 3033.954, 3034.6784, 3075.3711, 3077.3872, 3082.2355, 3097.806, 3098.6158, 3137.4983, 3138.8749

Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 1.2	**Energy (kJ mol^{-1}):** -460.818460392725
Reaction Coordinates: 6 -2.482014 0.195109 -0.616668 6 -1.765611 0.611426 0.665055 6 -0.474827 -0.155666 0.969705 6 0.948746 0.432245 -0.056953 6 2.172628 -0.047299 0.689677 6 0.899750 1.903822 -0.372714 1 3.024931 -0.040831 0.005930 1 2.039876 -1.054190 1.069659 1 2.387783 0.632272 1.512548 1 0.076604 2.140958 -1.042518	**Frequencies (cm^{-1}):** -454.0009, 77.2587, 109.644, 181.412, 188.1209, 213.2111, 243.3287, 248.0009, 276.7827, 317.0274, 342.2381, 376.3952, 420.8202, 537.4465, 547.0684, 641.5719, 686.8183, 776.8888, 792.7865, 855.6644, 954.351, 970.9598, 991.9732, 1006.9882, 1033.3206, 1072.4483, 1104.3095, 1128.8541, 1168.0884, 1274.614,

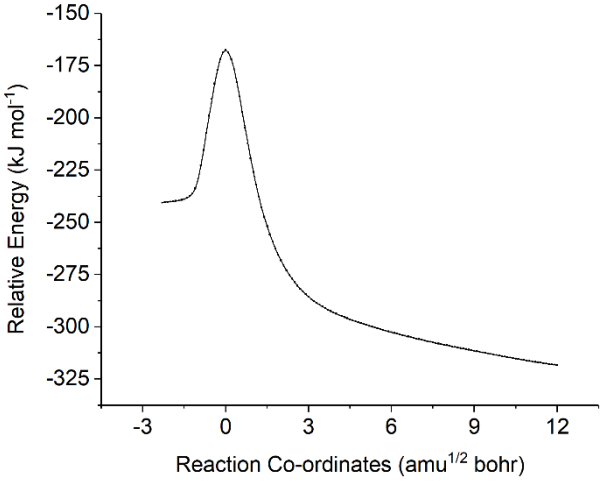
1 1.834369 2.214248 -0.844098 1 0.785292 2.479088 0.544599 1 -0.005626 0.159922 1.917110 1 -2.422140 0.422336 1.520232 1 -1.570342 1.685863 0.676726 1 -1.905006 0.448058 -1.505661 1 -2.648089 -0.880716 -0.629143 1 -3.449286 0.692895 -0.690222 8 0.600410 -0.295432 -1.158244 8 0.617203 -1.591063 -0.889689 8 -0.460163 -1.430721 0.772462	1277.5031, 1290.9043, 1301.1546, 1346.6058, 1402.8714, 1404.6547, 1419.2349, 1436.3834, 1472.1008, 1476.9934, 1492.1135, 1494.358, 1496.4221, 1506.543, 1510.7876, 2907.6912, 3014.0588, 3034.5399, 3039.5029, 3040.2522, 3049.2946, 3096.7606, 3099.0988, 3104.4754, 3113.962, 3131.967, 3160.1674
IRC:  	

Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 1.2	**Energy (kJ mol^{-1}):** -460.869579166621
Reaction Coordinates: 6 3.094760 -0.026109 0.958873 6 2.628573 0.208301 -0.470480 6 1.407488 -0.565369 -0.878563 6 -1.907478 0.055573 0.160776 6 -1.474003 0.271010 1.551733 6 -2.937231 -0.936399 -0.237909 1 -1.492487 1.341455 1.767465 1 -0.429138 -0.034337 1.641431 1 -2.090183 -0.290583 2.248848 1 -3.119725 -0.900022 -1.308646 1 -3.868120 -0.751728 0.302736 1 -2.595661 -1.937172 0.037322 1 1.059744 -0.363464 -1.908113 1 3.412017 -0.047966 -1.194710 1 2.397571 1.260964 -0.656543 1 2.332832 0.287166 1.671906 1 3.301313 -1.080478 1.139912 1 4.002086 0.541643 1.164166 8 -1.405804 0.732593 -0.780139 8 -0.398443 1.635168 -0.458308 8 0.831383 -1.376202 -0.188097	**Frequencies (cm^{-1}):** 32.5771, 36.0513, 52.0089, 87.0383, 91.2122, 96.6722, 156.7307, 161.4639, 170.7772, 243.2004, 254.8985, 292.5509, 309.469, 367.7152, 481.215, 593.934, 666.6772, 676.7098, 812.8249, 851.4518, 909.0247, 913.0981, 930.7797, 988.1837, 1006.2303, 1073.2807, 1097.6846, 1110.2357, 1142.8199, 1285.0888, 1306.0627, 1368.4862, 1387.7171, 1405.7078, 1410.4635, 1423.8994, 1443.6497, 1449.0725, 1458.7549, 1470.4144, 1479.5275, 1494.4236, 1501.1051, 1570.2078, 1774.5573, 2918.3955, 2999.3505, 3026.8341, 3033.706, 3040.5998, 3046.8548, 3075.1883, 3081.4609, 3101.0818, 3104.2373, 3137.3909, 3138.6957

Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 1.3	**Energy (kJ mol^{-1}):** -460.819507452064
Reaction Coordinates: 6 3.119465 0.176826 0.127878 6 1.711089 0.576835 -0.321015 6 0.652339 -0.122017 0.525816 6 -1.054162 0.443223 0.043124 6 -1.931376 0.009719 1.193558 6 -1.121954 1.898147 -0.338379 1 -2.969687 -0.013578 0.853531 1 -1.661510 -0.977346 1.552174 1 -1.851911 0.732009 2.004272 1 -0.588252 2.090867 -1.265873 1 -2.163325 2.201506 -0.464576 1 -0.691657 2.512299 0.451093 1 0.565807 0.266576 1.555238 1 1.598611 1.660425 -0.246825 1 1.561585 0.295866 -1.364586 1 3.256243 -0.900581 0.042897 1 3.876571 0.668840 -0.483497 1 3.297697 0.457271 1.168124 8 -1.097852 -0.337085 -1.073576 8 -1.024456 -1.620126 -0.757813 8 0.561985 -1.404109 0.432906	**Frequencies (cm^{-1}):** -451.6284, 74.3251, 117.8385, 166.8116, 183.6887, 208.2467, 237.6444, 255.616, 275.2332, 309.65, 351.0906, 372.9184, 410.0775, 512.6074, 540.196, 643.8212, 651.8946, 780.6727, 807.6634, 880.5007, 953.9002, 970.4386, 992.6413, 1006.3586, 1016.2658, 1076.6189, 1117.7308, 1138.0936, 1165.0822, 1275.7393, 1279.0241, 1290.0328, 1295.6164, 1351.53, 1403.6186, 1406.1474, 1416.8627, 1432.5928, 1472.0785, 1478.636, 1484.565, 1493.9877, 1498.3776, 1504.5138, 1506.6789, 2907.9268, 3026.3595, 3030.4917, 3034.2701, 3039.1643, 3070.8277, 3087.6606, 3098.7651, 3104.4819, 3106.063, 3132.6655, 3162.141
IRC:  	

Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 1.3	**Energy (kJ mol^{-1}):** -460.866786927255
Reaction Coordinates: 6 3.185611 0.672167 0.637887 6 2.236185 0.217307 -0.478639 6 1.839433 -1.220027 -0.316682 1 2.685884 -1.929675 -0.194829 8 0.706502 -1.643333 -0.307602 1 2.760119 0.285191 -1.440239 1 1.346357 0.846252 -0.527436 1 3.528903 1.687757 0.447627 1 4.064740 0.028801 0.709845 1 2.680786 0.668516 1.603938 6 -1.834425 0.019159 0.163504 6 -2.149032 0.018241 -1.275153	**Frequencies (cm^{-1}):** 26.4289, 39.7216, 59.5485, 66.1879, 77.3031, 92.8913, 103.0281, 156.5794, 161.8554, 208.2951, 287.8481, 308.3365, 330.22, 366.9893, 480.2665, 521.0254, 593.4122, 763.9939, 812.1858, 881.7843, 911.1396, 924.4177, 929.0942, 989.0809, 1007.9408, 1072.5339, 1096.726, 1135.8189, 1170.3004, 1281.2302, 1305.8977, 1350.1376, 1388.1302, 1403.5358, 1410.5875, 1428.4456, 1442.0338, 1459.5666, 1471.3934,

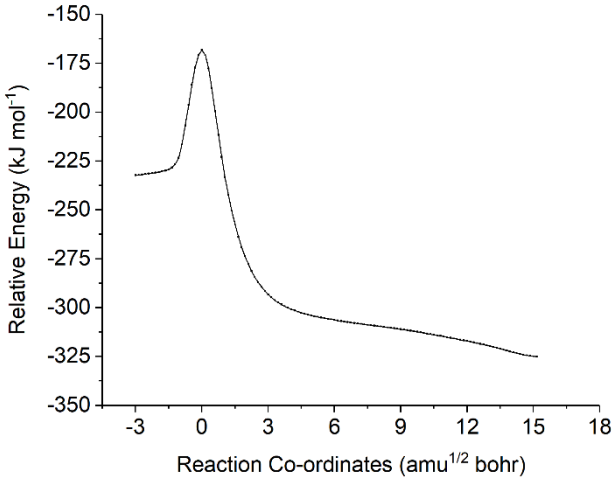
1 -1.213972 0.003420 -1.838064 1 -2.629602 0.965232 -1.533147 1 -2.771266 -0.830635 -1.544799 6 -2.265024 -1.044677 1.103741 1 -1.810694 -1.990298 0.799945 1 -3.349182 -1.170199 1.060147 1 -1.962993 -0.810073 2.121165 8 -1.166437 0.965286 0.666931 8 -0.715761 1.962133 -0.193340	1477.1977, 1478.5579, 1500.5376, 1505.715, 1569.6299, 1782.4593, 2857.0609, 2992.1677, 3028.0053, 3029.7568, 3033.8826, 3070.3747, 3078.8762, 3080.9003, 3092.6217, 3107.1726, 3136.3707, 3140.5222

Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -460.812591422153
Reaction Coordinates: 6 2.761406 0.290513 -0.053894 6 1.769555 -0.824458 0.267236 6 0.449639 -0.810641 -0.525072 6 -0.603053 0.711152 0.014606 6 -0.266192 1.944545 -0.781369 6 -0.472474 0.791800 1.514324 1 -0.522015 1.806018 -1.830068 1 -0.821312 2.803365 -0.396984 1 0.793094 2.173044 -0.706880 1 0.480620 1.234730 1.791603 1 -1.269745 1.442067 1.885382 1 -0.578599 -0.179946 1.983484 1 0.579386 -0.513781 -1.580150 1 1.554544 -0.875021 1.333552 1 2.226887 -1.782774 0.011426 1 3.740797 0.053727 0.362478 1 2.888478 0.412426 -1.131570 1 2.462825 1.254010 0.358735 8 -1.763005 0.185681 -0.449485 8 -2.067728 -0.941366 0.169193 8 -0.340298 -1.799982 -0.306708	**Frequencies (cm^{-1}):** -488.0994, 76.6912, 104.4884, 151.4119, 201.2416, 218.3989, 231.0198, 244.0531, 274.444, 327.3185, 351.3859, 398.7746, 416.0491, 489.5555, 530.7337, 580.5624, 646.675, 763.2517, 799.302, 874.7799, 953.0059, 988.0134, 998.2711, 1022.0807, 1035.2307, 1060.9173, 1103.8592, 1141.844, 1182.1691, 1272.8841, 1279.5604, 1289.5145, 1332.9465, 1348.1638, 1401.7346, 1410.7662, 1421.1893, 1424.2433, 1470.5881, 1479.8346, 1485.5512, 1495.2903, 1500.362, 1507.3689, 1511.3193, 2902.4321, 3028.7355, 3029.9501, 3036.9281, 3037.8088, 3077.539, 3091.106, 3098.2902, 3106.4894, 3113.6332, 3146.3587, 3162.8553
IRC:  	

Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -460.868574244763

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 3.130956 -0.790899 -0.262324 6 2.448340 0.561704 -0.456522 6 1.422964 0.884328 0.598264 6 -1.842686 -0.177379 -0.159311 6 -2.614315 0.573285 -1.181012 6 -2.155216 -0.155974 1.279937 1 -2.227703 0.384012 -2.178843 1 -3.670114 0.297588 -1.133746 1 -2.547522 1.641981 -0.964073 1 -3.089740 0.364271 1.472483 1 -2.179144 -1.181848 1.653331 1 -1.335366 0.337646 1.805770 1 1.611010 0.438478 1.593666 1 1.970844 0.646007 -1.433268 1 3.189959 1.369230 -0.402901 1 3.897941 -0.947004 -1.020712 1 3.616313 -0.849961 0.713840 1 2.401327 -1.596253 -0.326432 8 -0.880128 -0.867605 -0.598291 8 -0.093994 -1.538536 0.330724 8 0.476864 1.621824 0.430903	31.3421, 45.6193, 47.5088, 83.8815, 87.7596, 95.8092, 153.9235, 158.7132, 178.3563, 218.3773, 297.1738, 312.566, 320.2917, 368.4028, 480.055, 522.6356, 595.0632, 692.6976, 812.7758, 882.5456, 914.2083, 917.6329, 930.3352, 988.2781, 1029.4331, 1073.8301, 1097.126, 1128.6589, 1155.8921, 1278.4194, 1306.4992, 1332.2185, 1385.3263, 1405.421, 1412.6147, 1427.8829, 1444.8958, 1450.4783, 1458.531, 1470.0813, 1479.6599, 1497.0407, 1513.8315, 1570.4154, 1768.2816, 2903.031, 2991.699, 3027.7864, 3030.7221, 3035.6716, 3071.0709, 3076.3986, 3085.1692, 3090.3481, 3115.0263, 3137.7983, 3139.246

Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -460.813275099648
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.696225 0.079311 0.531770 6 -1.764794 0.653589 -0.529954 6 -0.526831 -0.210149 -0.875449 6 0.935294 0.471211 0.088976 6 1.489255 1.689982 -0.598145 6 0.503046 0.632032 1.524650 1 1.916557 1.429147 -1.564470 1 2.262021 2.157796 0.014828 1 0.699523 2.424286 -0.751310 1 -0.158574 1.487499 1.633889 1 1.397655 0.818907 2.125071 1 0.018289 -0.261847 1.898151 1 -0.146412 0.014081 -1.885625 1 -1.465962 1.673831 -0.280777 1 -2.312092 0.732030 -1.473489 1 -3.577640 0.714136 0.631347 1 -3.021223 -0.922714 0.258517 1 -2.224235 0.011299 1.509731 8 1.722068 -0.607849 -0.169861 8 1.207434 -1.709203 0.351117 8 -0.557799 -1.454736 -0.552126	-479.53, 86.2827, 109.2833, 165.107, 181.3241, 210.3598, 233.15, 248.0362, 266.2619, 326.0068, 341.8753, 393.4658, 400.9406, 524.6673, 553.8027, 641.6015, 645.3993, 762.728, 794.6158, 846.5084, 950.1201, 985.7957, 994.1469, 1011.2631, 1055.6358, 1063.795, 1095.3492, 1139.5666, 1200.2413, 1274.3023, 1282.2251, 1294.8333, 1315.3799, 1355.1976, 1402.0768, 1409.5581, 1417.0971, 1443.3523, 1471.6155, 1478.9567, 1488.1808, 1491.1732, 1500.0457, 1506.9508, 1507.5315, 2908.4522, 3021.6706, 3032.0116, 3038.0869, 3044.8708, 3049.0216, 3097.8013, 3104.3348, 3114.3172, 3121.9948, 3124.9729, 3172.8571
IRC:	

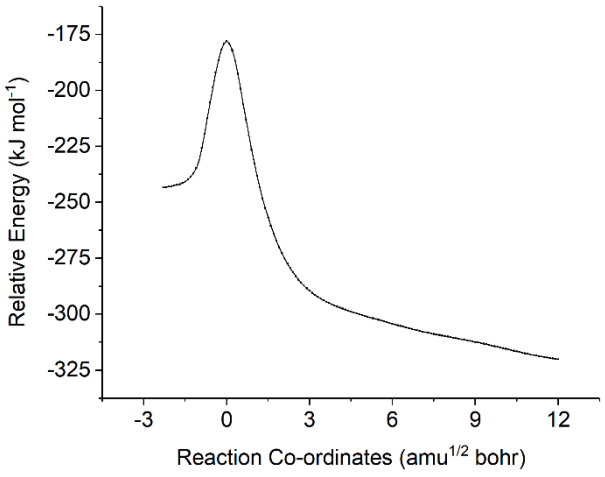


Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -460.869923564643
Reaction Coordinates: 6 -2.760207 1.174688 -0.310228 6 -2.567204 -0.332304 -0.220746 6 -1.503050 -0.781838 0.739179 6 1.785844 0.234548 -0.114556 6 2.214631 1.634680 0.128547 6 2.279746 -0.917619 0.658517 1 1.744004 2.314919 -0.576265 1 3.301190 1.714602 0.050387 1 1.941134 1.921790 1.146640 1 3.089198 -0.628483 1.323543 1 2.585592 -1.705379 -0.032954 1 1.448801 -1.328813 1.236108 1 -1.362554 -1.876950 0.788672 1 -2.299826 -0.765240 -1.189139 1 -3.492364 -0.839560 0.079785 1 -3.562405 1.417264 -1.006950 1 -3.009576 1.600201 0.661443 1 -1.850217 1.661386 -0.658912 8 0.954095 0.070986 -1.051274 8 0.485864 -1.217139 -1.279836 8 -0.843901 -0.048680 1.442781	**Frequencies (cm^{-1}):** 32.0791, 36.3885, 50.3062, 81.7583, 93.3164, 95.5359, 156.5819, 160.791, 176.1345, 247.3597, 254.8558, 294.8025, 311.7278, 367.6771, 481.1739, 594.3187, 669.5543, 673.4792, 812.6998, 851.1821, 906.6049, 914.6816, 930.349, 988.0072, 1006.3988, 1073.25, 1097.1092, 1110.4828, 1141.317, 1286.5316, 1306.504, 1368.703, 1385.7386, 1405.8651, 1410.897, 1424.3268, 1444.4487, 1449.4016, 1458.8081, 1470.1997, 1479.4604, 1494.4387, 1501.5803, 1569.3955, 1772.4071, 2917.6717, 3000.3105, 3027.1148, 3034.623, 3040.7016, 3044.8829, 3075.2249, 3083.146, 3101.118, 3105.2648, 3137.4639, 3138.933

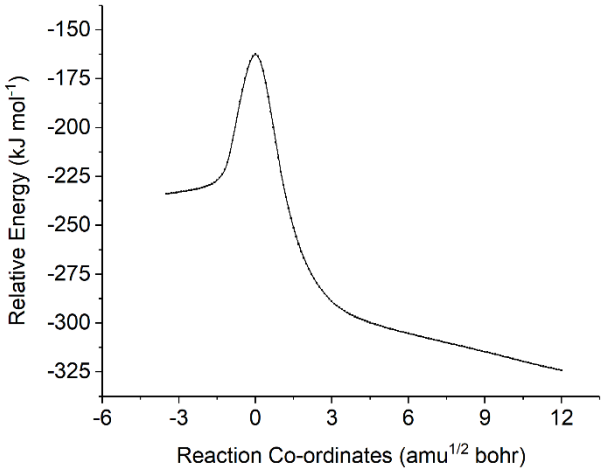
Compound: $EtCHCMe_2 + O_3$ TS_{DMFO} 2.3	**Energy (kJ mol^{-1}):** -460.816015668238
Reaction Coordinates: 6 -3.138942 0.095211 -0.113837 6 -1.736875 0.475855 0.368585 6 -0.675680 -0.292764 -0.432019 6 0.978314 0.515635 -0.015367 6 1.167989 1.780052 -0.808105 6 1.040514 0.622005 1.487917 1 1.262785 1.560811 -1.869863 1 2.064339 2.307843 -0.476128 1 0.319764 2.446664 -0.661366 1 0.468483 1.480248 1.831217	**Frequencies (cm^{-1}):** -464.5056, 85.9277, 100.2104, 167.2365, 187.1582, 201.5997, 233.4101, 246.1573, 281.9128, 319.6402, 338.0145, 387.4977, 398.206, 494.8809, 531.9622, 612.8663, 644.2466, 781.3726, 801.9247, 885.7056, 955.5296, 988.2384, 995.1731, 1004.9783, 1042.4614, 1069.6011, 1116.8607, 1142.4611, 1181.7165, 1276.7344,

1 2.085866 0.772627 1.770880 1 0.681899 -0.279619 1.971660 1 -0.705991 -0.055231 -1.509972 1 -1.629261 0.229970 1.423793 1 -1.591489 1.552132 0.250922 1 -3.897609 0.663143 0.426281 1 -3.262314 0.303515 -1.178121 1 -3.325894 -0.966306 0.044698 8 1.704217 -0.491510 -0.565947 8 1.506898 -1.629954 0.074677 8 -0.496427 -1.527506 -0.127111	1281.8838, 1289.3677, 1330.362, 1351.7667, 1402.8039, 1408.8579, 1418.3662, 1430.5735, 1469.4775, 1480.26, 1482.1232, 1494.279, 1495.7028, 1502.6158, 1504.6885, 2897.2873, 3026.8312, 3028.3065, 3032.2072, 3037.7245, 3079.0827, 3094.5078, 3098.6077, 3107.3115, 3113.2645, 3126.2524, 3163.1099

IRC:

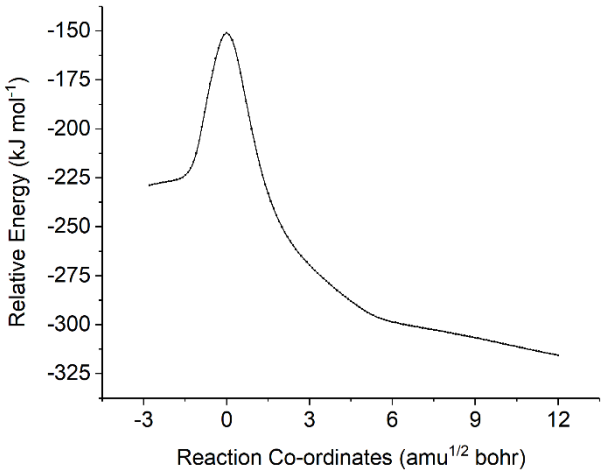


Compound: $EtCHCMe_2 + O_3$ CPr_{DMFO} 2.3	**Energy (kJ mol^{-1}):** -460.868053456462
Reaction Coordinates: 6 3.802266 0.065135 -0.156918 6 2.333210 -0.115135 -0.555308 6 1.448611 -0.349126 0.635888 6 -1.971417 0.017075 -0.158115 6 -2.638197 -1.052440 -0.942193 6 -2.243131 0.278430 1.265507 1 -2.303265 -1.044503 -1.976008 1 -3.722636 -0.927640 -0.903237 1 -2.407081 -2.021774 -0.494239 1 -3.079633 -0.316032 1.623138 1 -2.417668 1.347376 1.404090 1 -1.343211 0.043157 1.838307 1 1.572677 0.382251 1.456855 1 2.202535 -0.937626 -1.258574 1 1.962519 0.800181 -1.025893 1 4.407781 0.309019 -1.029162 1 3.919362 0.876501 0.563295 1 4.208929 -0.843045 0.289950 8 -1.135107 0.720570 -0.791925 8 -0.448027 1.699177 -0.083508 8 0.659589 -1.261184 0.747723	**Frequencies (cm^{-1}):** 29.9627, 39.6791, 45.4127, 77.2831, 83.7118, 92.3951, 153.8323, 158.8319, 160.0159, 213.5014, 294.1901, 311.7773, 344.7388, 367.649, 481.4676, 513.1831, 594.1278, 754.5233, 812.7161, 875.1885, 913.7388, 918.2885, 930.2463, 988.1077, 1009.8716, 1073.2731, 1097.2736, 1128.7074, 1162.2264, 1273.7171, 1306.4198, 1329.8785, 1385.7028, 1405.8328, 1410.351, 1429.0087, 1444.4131, 1458.5106, 1469.8437, 1470.2111, 1479.2547, 1501.797, 1505.421, 1569.353, 1771.8207, 2907.6319, 3027.17, 3028.0697, 3031.0588, 3034.2387, 3075.5306, 3076.5069, 3082.4138, 3096.4445, 3098.4116, 3137.5747, 3138.999

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 1	**Energy (kJ mol^{-1}):** -460.811969201101
Reaction Coordinates: 6 -2.766294 0.656071 0.244958 6 -1.686819 -0.292571 -0.273798 6 -0.463627 -0.353130 0.616626 6 0.967812 0.574308 -0.139113 6 2.020934 0.671890 0.970137 6 0.361194 1.937839 -0.517259 1 2.368213 -0.318482 1.253711 1 1.647090 1.192033 1.853386 1 2.875803 1.231887 0.586721 1 -0.369883 1.843504 -1.314475 1 -0.083965 2.438595 0.341508 1 1.177379 2.562253 -0.883015 1 -0.584166 0.007879 1.635698 1 -1.405411 -0.055842 -1.296933 1 -2.072976 -1.315500 -0.311077 1 -2.431885 1.692819 0.257461 1 -3.648659 0.603925 -0.392684 1 -3.075949 0.390956 1.257376 8 1.261356 -0.192352 -1.137221 8 0.422866 -1.951663 -0.573251 8 0.191430 -1.536043 0.660850	**Frequencies (cm^{-1}):** -468.7864, 91.5167, 107.1496, 186.3395, 193.1488, 223.8092, 232.0664, 257.3948, 275.8856, 315.3557, 350.5433, 378.4904, 426.0326, 487.3212, 550.8395, 575.6686, 703.5794, 777.721, 809.4047, 909.9975, 915.2302, 970.4371, 991.9742, 1026.3256, 1057.2693, 1069.8646, 1080.6486, 1130.8532, 1163.854, 1183.4241, 1186.8126, 1281.7509, 1334.7916, 1363.9778, 1393.4132, 1405.54, 1416.2593, 1425.6041, 1475.7756, 1479.1219, 1490.1092, 1494.3606, 1503.032, 1507.7117, 1508.6434, 3027.8691, 3030.0223, 3033.1197, 3040.9776, 3084.9336, 3086.0788, 3097.6576, 3102.0145, 3107.0016, 3113.9528, 3129.3519, 3142.0922
IRC  	

Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -460.865444864793
Reaction Coordinates: 6 2.313223 -2.059251 -0.283387 6 2.056536 -0.571305 -0.497913 6 1.649440 0.138040 0.722103 1 1.570697 -0.333872 1.695478 8 1.372699 1.364057 0.748030 8 1.412859 2.046732 -0.454403 1 2.930792 -0.041116 -0.896041 1 1.279028 -0.384930 -1.244577 1 1.411920 -2.562737 0.065213 1 2.619799 -2.528879 -1.216862 1 3.105965 -2.229536 0.446756 6 -2.077242 -0.222504 0.018359	**Frequencies (cm^{-1}):** 25.9622, 34.5316, 46.2082, 70.1313, 71.1642, 84.5992, 99.073, 111.5629, 152.662, 209.0405, 222.5433, 361.4854, 392.1321, 455.9351, 497.2504, 540.9262, 684.3924, 702.1492, 788.2835, 843.9204, 868.0986, 887.9738, 902.0967, 936.558, 1048.0589, 1089.2291, 1103.9213, 1123.3178, 1142.0878, 1242.569, 1253.6461, 1324.53, 1377.723, 1387.8906, 1399.5746, 1421.5018, 1424.9074, 1462.305, 1466.199, 1475.8167, 1494.869,

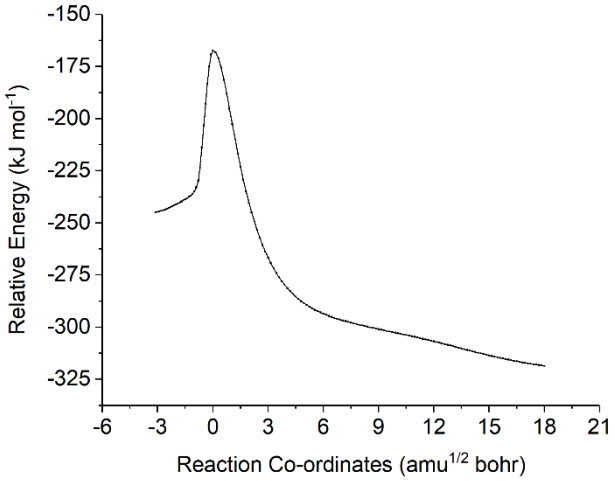
6 -2.000176 1.209916 -0.448212 1 -0.971658 1.521747 -0.618596 1 -2.443742 1.854512 0.315914 1 -2.594761 1.349164 -1.353278 6 -3.453803 -0.846706 0.077326 1 -4.146322 -0.202821 0.622435 1 -3.850234 -0.948346 -0.935845 1 -3.406178 -1.826154 0.545627 8 -1.089705 -0.855311 0.336888	1502.9655, 1508.8689, 1577.3807, 1761.5253, 3002.9158, 3018.9968, 3030.9491, 3034.897, 3040.7278, 3073.2313, 3083.9126, 3095.6327, 3108.6934, 3122.1549, 3137.0069, 3164.5409

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 2	**Energy (kJ mol^{-1}):** -460.807123410423
Reaction Coordinates: 6 2.296440 0.740451 -0.498059 6 1.545684 0.644466 0.830353 6 0.308918 -0.222550 0.964218 6 -1.085418 0.288186 -0.212874 6 -2.348219 -0.303185 0.426079 6 -1.043272 1.825474 -0.167163 1 -2.276054 -1.386996 0.477108 1 -3.202816 -0.051792 -0.204675 1 -2.537008 0.096709 1.423345 1 -0.162819 2.216389 -0.667533 1 -1.923265 2.186912 -0.701710 1 -1.092603 2.208665 0.851772 1 -0.125798 -0.187020 1.960980 1 2.227707 0.265120 1.601401 1 1.257334 1.639029 1.172700 1 2.761801 -0.204886 -0.760665 1 1.639401 1.017360 -1.318281 1 3.079390 1.495159 -0.406351 8 -0.704661 -0.252372 -1.318021 8 0.672407 -1.627328 -0.694219 8 0.320996 -1.511761 0.576813	**Frequencies (cm^{-1}):** -466.2744, 87.1898, 119.8976, 184.6315, 203.936, 243.855, 252.2109, 267.7604, 282.2899, 297.1045, 316.3958, 388.2188, 428.6042, 489.3294, 547.0559, 563.4913, 721.8044, 786.3065, 810.7037, 850.1438, 907.977, 976.7008, 989.6317, 1008.422, 1051.8707, 1068.6455, 1087.3559, 1129.5116, 1159.2621, 1180.4836, 1215.4094, 1304.4489, 1367.5289, 1374.1183, 1395.399, 1408.2357, 1418.8115, 1440.8961, 1470.094, 1481.6797, 1487.1251, 1491.9741, 1498.449, 1504.6923, 1512.3972, 2992.1801, 3030.2445, 3038.5553, 3042.9547, 3064.8386, 3086.9193, 3094.8031, 3109.3773, 3114.7553, 3127.5551, 3141.2108, 3146.3303
IRC  	

Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -460.862748738498
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 1.767600 -1.416121 1.100665 6 2.502338 -0.881574 -0.147928 6 1.646632 -0.059934 -1.022496 6 -2.139357 -0.146426 -0.022942 6 -1.802637 0.997537 0.903038 6 -3.608179 -0.398606 -0.283023 1 -0.737827 1.216115 0.898148 1 -2.113572 0.733728 1.917795 1 -2.365846 1.891438 0.628641 1 -3.740105 -1.317633 -0.847704 1 -4.163758 -0.450915 0.655055 1 -4.025097 0.437621 -0.849551 1 1.221544 -0.413499 -1.954300 1 3.325217 -0.240760 0.179797 1 2.894719 -1.711512 -0.735837 1 1.417513 -0.587607 1.710041 1 0.917032 -2.033476 0.819828 1 2.460195 -2.017161 1.688768 8 -1.283676 -0.838567 -0.536191 8 1.780618 1.693167 0.405984 8 1.342008 1.135950 -0.779113	23.7473, 34.5367, 40.1218, 53.3533, 75.3019, 76.0034, 93.7949, 112.6496, 140.6921, 198.2996, 243.1058, 317.524, 389.5487, 496.0073, 530.7907, 538.6688, 650.005, 786.2135, 810.9969, 843.0581, 870.3721, 888.3579, 898.5125, 906.5406, 1018.6502, 1086.9217, 1087.1552, 1122.5299, 1147.4445, 1239.7194, 1291.7765, 1335.0154, 1376.8092, 1387.6644, 1398.0328, 1403.2297, 1460.7673, 1462.1854, 1466.1347, 1474.692, 1490.9435, 1491.9057, 1514.3318, 1573.5704, 1765.6965, 3022.5206, 3027.9573, 3031.1668, 3050.2596, 3075.4424, 3083.8373, 3083.9844, 3116.5354, 3136.1728, 3137.0479, 3140.4147, 3177.0273

Compound: $EtCHCMe_2 + O_3$ TS_{SYN} 3	**Energy (kJ mol^{-1}):** -460.812859521795
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.894842 0.528923 0.215677 6 -1.448353 0.874680 -0.164163 6 -0.466543 0.059363 0.640370 6 1.252531 0.208094 -0.106273 6 2.196983 -0.324172 0.977091 6 1.399673 1.719280 -0.359981 1 1.981166 -1.368369 1.190210 1 2.138234 0.254693 1.900040 1 3.220937 -0.260908 0.604414 1 1.187775 2.311187 0.530337 1 2.438176 1.899166 -0.642121 1 0.767129 2.042486 -1.181168 1 -0.387095 0.306381 1.696775 1 -1.283901 0.701721 -1.224275 1 -1.259403 1.927502 0.039396 1 -3.085048 0.705076 1.275500 1 -3.584487 1.150298 -0.355561 1 -3.120853 -0.513340 -0.003528 8 1.132282 -0.519531 -1.164770 8 -0.515864 -1.639559 -0.745219 8 -0.522584 -1.285023 0.529195	-463.4298, 72.9943, 112.9906, 177.5762, 199.7273, 220.3099, 230.072, 267.5653, 276.9306, 304.3164, 347.9416, 388.5291, 438.8609, 486.0667, 553.9463, 595.6396, 675.0687, 786.7642, 817.9969, 896.219, 911.0528, 970.4132, 986.6603, 995.2966, 1054.9554, 1062.8364, 1082.8149, 1125.3399, 1171.5634, 1181.9626, 1199.8501, 1304.4136, 1344.1312, 1371.2267, 1392.7722, 1404.9442, 1407.3881, 1430.2224, 1476.4057, 1482.1159, 1489.7158, 1497.0901, 1498.6225, 1505.3896, 1506.6735, 3029.3874, 3033.7466, 3037.0537, 3070.4136, 3086.0046, 3090.3532, 3094.1983, 3108.4188, 3111.8246, 3127.1662, 3131.5909, 3142.4878
IRC	



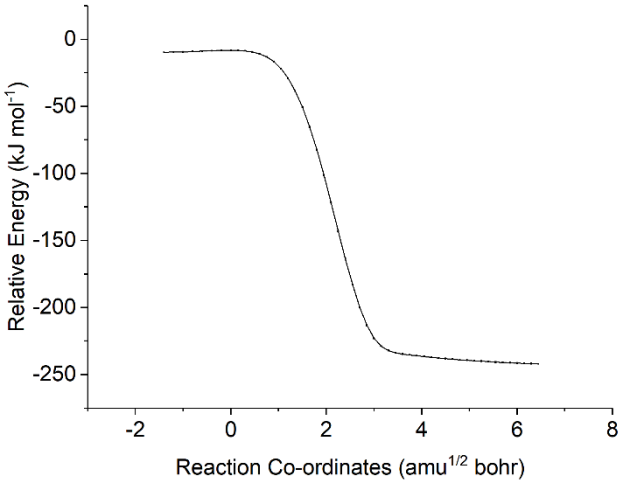
Compound: $EtCHCMe_2 + O_3$ CPr_{SYN} 3	**Energy (kJ mol^{-1}):** -460.863846029253
Reaction Coordinates: 6 3.310736 -0.890412 -0.598063 6 1.794289 -0.994246 -0.326007 6 1.406572 -0.224853 0.868737 6 -2.238351 -0.207423 -0.029653 6 -1.994924 1.192657 -0.535701 6 -3.666151 -0.705674 -0.065598 1 -0.932232 1.410371 -0.622199 1 -2.446903 1.903936 0.161341 1 -2.492805 1.342282 -1.495867 1 -4.338213 0.016067 0.402107 1 -3.989019 -0.808814 -1.104381 1 -3.744462 -1.667709 0.433597 1 1.226561 -0.674734 1.838371 1 1.251145 -0.575540 -1.173041 1 1.496242 -2.031356 -0.180234 1 3.892779 -1.309414 0.222793 1 3.552946 -1.447602 -1.502202 1 3.596879 0.148662 -0.742777 8 -1.341792 -0.911586 0.391444 8 1.463499 1.719162 -0.296210 8 1.285050 1.026618 0.889790	**Frequencies (cm^{-1}):** 26.1077, 35.0579, 54.5098, 69.0616, 72.9627, 78.7581, 96.8273, 111.5316, 152.656, 203.8266, 247.9063, 327.4773, 392.5347, 497.4806, 531.3288, 541.8035, 646.2076, 788.4496, 808.9049, 847.2536, 868.9046, 888.3579, 901.4048, 907.0536, 1008.7598, 1083.7553, 1089.5371, 1123.4939, 1150.8493, 1242.4352, 1283.8716, 1329.8784, 1376.6785, 1387.7664, 1399.7869, 1401.8019, 1462.1527, 1463.8635, 1466.6525, 1475.9937, 1494.975, 1496.6873, 1511.2746, 1575.4999, 1761.322, 3018.824, 3030.9988, 3040.9223, 3057.0563, 3073.0566, 3083.9463, 3098.2405, 3109.5749, 3121.5949, 3130.4695, 3137.1968, 3171.3473

6.10 Ozonolysis of 2,4-dimethyl-2-pentene (Alkene 8)

Compound: $iPrCHCMe_2 + O_3$ PRC1.1	**Energy (kJ mol^{-1}):** -500.007113422271
Reaction Coordinates: 6 1.789066 -0.540930 0.209110 6 0.691449 0.188997 -0.510722 6 0.072421 1.333862 -0.162440 6 -0.984184 1.926673 -1.047708 1 -0.738110 2.958755 -1.312374 1 -1.947715 1.964452 -0.528697	**Frequencies (cm^{-1}):** 27.8278, 29.2216, 45.9838, 65.3306, 75.6581, 100.4951, 121.7797, 150.9946, 192.9192, 198.7622, 225.6153, 247.5404, 258.0208, 304.2647, 394.2712, 406.0228, 450.0984, 492.5071, 519.9401, 731.3498,

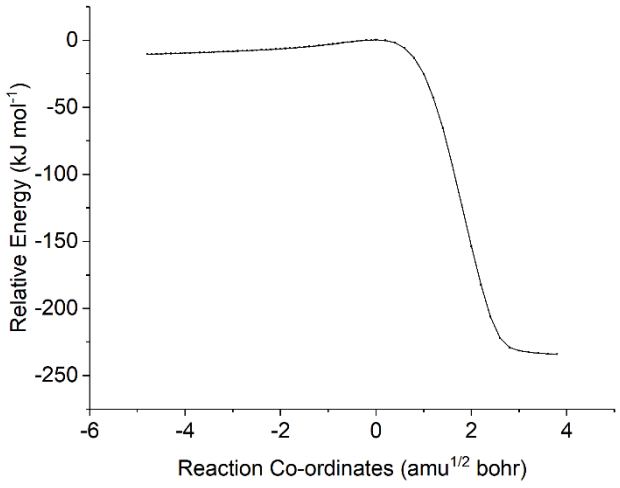
1 -1.115377 1.357790 -1.966598 6 0.374635 2.123768 1.078151 1 -0.540095 2.299762 1.648949 1 0.770648 3.107827 0.810908 1 1.094297 1.639131 1.732249 1 0.397567 -0.261315 -1.455879 1 1.827149 -0.207269 1.247501 6 3.150653 -0.223281 -0.436954 1 3.373438 0.843012 -0.392070 1 3.161334 -0.523623 -1.486853 1 3.951292 -0.762288 0.072998 6 1.529884 -2.053945 0.207590 1 0.577787 -2.292084 0.678838 1 2.322619 -2.579291 0.742499 1 1.503787 -2.441055 -0.813594 8 -1.606325 -0.525700 1.009654 8 -2.596484 -0.611275 0.227196 8 -2.594962 -1.567358 -0.611854	810.2753, 856.3753, 878.1828, 933.4397, 954.9176, 963.794, 967.212, 1005.536, 1088.8867, 1096.3883, 1108.2361, 1143.9595, 1147.8041, 1167.9505, 1193.7938, 1242.7709, 1329.6569, 1338.4878, 1393.5271, 1398.3223, 1410.2661, 1419.2407, 1421.0412, 1470.5019, 1480.9241, 1489.1324, 1489.5877, 1490.9299, 1494.0547, 1502.5791, 1511.9795, 1672.5912, 3003.5462, 3017.0545, 3018.2329, 3023.3437, 3036.1177, 3043.5051, 3057.1064, 3075.7103, 3083.3054, 3089.9149, 3102.7315, 3109.162, 3111.5439, 3124.6474

Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -500.002540642203
Reaction Coordinates: 6 1.652522 -0.123063 -0.232942 6 0.397910 0.123429 0.559559 6 -0.613245 0.998264 0.234188 6 -0.579277 1.876934 -0.983838 1 -1.585538 2.047879 -1.363889 1 0.021240 1.453718 -1.785075 1 -0.160601 2.854966 -0.727730 6 -1.652512 1.334790 1.267529 1 -1.759586 0.539729 2.004774 1 -2.623864 1.521251 0.811658 1 -1.364585 2.244973 1.803977 1 0.389200 -0.282884 1.565219 1 1.379312 -0.209606 -1.287922 6 2.624432 1.066466 -0.086852 1 2.927376 1.191294 0.954585 1 2.181987 2.003230 -0.422060 1 3.525114 0.888526 -0.676692 6 2.350254 -1.418992 0.191797 1 1.706602 -2.284379 0.053586 1 2.639121 -1.374458 1.244752 1 3.258361 -1.571853 -0.392682 8 -1.934213 -0.548831 -0.926881 8 -1.858444 -1.511919 -0.075220 8 -0.659174 -1.960418 0.067209	**Frequencies (cm^{-1}):** -140.3775, 55.1427, 60.9761, 113.6625, 142.4228, 148.0175, 175.2576, 178.9401, 187.3695, 207.1642, 221.1691, 258.7806, 320.992, 357.0901, 403.2545, 432.4468, 449.2924, 514.6342, 547.5262, 742.3748, 808.5065, 852.412, 873.6855, 933.1688, 950.9906, 962.0323, 967.4818, 1012.0507, 1071.7007, 1079.9289, 1088.7246, 1107.2123, 1118.4429, 1144.2462, 1195.7415, 1239.2319, 1314.5562, 1339.6123, 1381.8199, 1398.498, 1405.6976, 1418.397, 1419.5167, 1473.3818, 1480.9278, 1481.6195, 1489.0515, 1493.1165, 1498.8006, 1504.7293, 1514.1185, 1580.1926, 3008.8715, 3018.2182, 3020.2265, 3023.4512, 3029.3938, 3073.3521, 3077.9048, 3082.5571, 3085.1281, 3103.2035, 3110.6042, 3124.8174, 3126.4142, 3138.9563
IRC:	



Compound: $iPrCHCMe_2 + O_3$ POZ1.1	**Energy (kJ mol^{-1}):** -500.103746557038
Reaction Coordinates: 6 -1.603222 0.137923 -0.282162 6 -0.268423 -0.295439 0.327009 6 1.047886 0.490716 -0.044729 6 1.566968 1.286676 1.148293 1 2.500289 1.788293 0.893985 1 0.843779 2.044035 1.455538 1 1.748756 0.623658 1.993298 6 0.999528 1.322803 -1.320747 1 0.604907 0.743331 -2.152706 1 0.396046 2.219440 -1.189189 1 2.010417 1.637342 -1.580237 8 1.971942 -0.586522 -0.356533 8 1.398479 -1.747305 0.277168 8 0.023037 -1.628724 -0.096052 1 -0.358710 -0.298481 1.418918 6 -2.065444 1.472128 0.315512 1 -3.008005 1.778112 -0.139003 1 -2.233584 1.377082 1.390432 1 -1.349526 2.277985 0.159672 1 -1.466709 0.260216 -1.358278 6 -2.674225 -0.937656 -0.058471 1 -2.825894 -1.121644 1.007537 1 -3.626131 -0.610360 -0.478630 1 -2.401698 -1.881508 -0.526237	**Frequencies (cm^{-1}):** 63.6589, 86.5072, 177.0466, 208.9956, 220.2053, 232.3028, 248.8889, 257.8465, 291.9742, 314.8425, 327.3908, 362.761, 426.6376, 455.3196, 478.5584, 507.0613, 607.2296, 702.6973, 774.7755, 784.1627, 854.0398, 882.5222, 936.0491, 938.3434, 942.2629, 945.7903, 968.7018, 997.2557, 1015.0405, 1036.869, 1124.0657, 1161.8836, 1180.7941, 1198.7893, 1217.8898, 1257.2328, 1321.2756, 1346.6698, 1358.0091, 1401.9258, 1403.9789, 1406.197, 1423.4607, 1429.2298, 1480.633, 1487.9205, 1492.1182, 1493.901, 1498.5589, 1505.0623, 1511.8973, 1515.1472, 2994.9806, 3024.8671, 3028.6253, 3033.7306, 3042.8795, 3047.8159, 3081.1784, 3089.7995, 3096.6685, 3100.8306, 3108.5891, 3111.0904, 3114.0488, 3125.2335

Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -499.999722430240
Reaction Coordinates: 6 -1.703144 -0.459322 -0.075252 6 -0.357254 -0.394851 0.608653 6 0.809859 -0.969072 0.150276 6 0.875651 -1.783654 -1.109930 1 1.851275 -1.683168 -1.583583 1 0.114547 -1.503913 -1.832178 1 0.740680 -2.843630 -0.870458	**Frequencies (cm^{-1}):** -181.9004, 40.6923, 84.8475, 111.0838, 137.3917, 147.3002, 163.0879, 179.3852, 192.9297, 213.4243, 238.5445, 259.973, 309.013, 342.5862, 401.2038, 445.2885, 454.5781, 522.1027, 576.1944, 735.5201, 807.7162, 844.0254, 877.2215, 936.658,

6 1.972489 -1.105333 1.093699 1 1.988422 -0.300628 1.828194 1 2.922294 -1.110850 0.561483 1 1.896988 -2.048845 1.643928 1 -0.366421 -0.074408 1.643113 1 -1.796345 -1.472922 -0.481927 6 -1.878085 0.512112 -1.256805 1 -1.057946 0.445957 -1.968948 1 -1.920540 1.541717 -0.908606 1 -2.809563 0.283861 -1.777383 6 -2.828457 -0.267756 0.947785 1 -2.781800 0.730064 1.388413 1 -2.763620 -0.997094 1.756842 1 -3.804458 -0.378250 0.474034 8 1.618578 0.923209 -0.860878 8 1.465230 1.711600 0.152125 8 0.221209 1.892612 0.455818	957.8157, 963.8347, 969.2325, 1011.4797, 1062.1522, 1071.9462, 1083.6464, 1111.7856, 1116.981, 1135.0843, 1205.9489, 1236.5869, 1327.2139, 1343.211, 1381.0615, 1402.1624, 1408.1371, 1419.7364, 1423.2549, 1471.3536, 1480.2638, 1482.8981, 1487.6355, 1493.5459, 1501.2248, 1503.927, 1512.6591, 1571.9391, 2981.7844, 3010.299, 3014.4989, 3022.5091, 3037.597, 3075.0265, 3082.9765, 3084.406, 3089.5256, 3103.6992, 3112.9175, 3122.3164, 3137.4358, 3152.3962
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ POZ1.2	**Energy (kJ mol^{-1}):** -500.100633245354
Reaction Coordinates: 6 -1.579866 -0.488964 -0.147913 6 -0.252033 0.195836 -0.517318 6 1.121406 -0.456400 -0.079655 6 2.052393 -0.569653 -1.286569 1 3.022802 -0.959020 -0.979808 1 1.630679 -1.244647 -2.033460 1 2.196557 0.405343 -1.749080 6 1.059819 -1.769307 0.687110 1 2.065341 -2.056200 0.993992 1 0.440112 -1.697577 1.575670 1 0.670373 -2.561535 0.048192 8 1.633398 0.522032 0.847804 8 1.180982 1.755304 0.277922 8 -0.225112 1.493110 0.090875 1 -0.213898 0.317082 -1.603752 6 -2.697674 -0.022361 -1.090566 1 -3.632188 -0.536259 -0.862079 1 -2.872785 1.049660 -0.986785 1 -2.451704 -0.224012 -2.134326 1 -1.428952 -1.557767 -0.324103	**Frequencies (cm^{-1}):** 31.6172, 84.6341, 173.9468, 198.7875, 210.498, 245.1068, 251.1748, 261.6889, 268.9748, 297.7303, 330.7913, 356.335, 408.5799, 446.2319, 524.1109, 560.2077, 627.1684, 698.6341, 760.4209, 789.4613, 849.0477, 882.6398, 928.4741, 933.1168, 934.3884, 951.6687, 965.5118, 983.2591, 1015.4834, 1036.9377, 1118.2199, 1136.3719, 1185.6572, 1203.7652, 1207.6023, 1258.6658, 1320.0919, 1337.9736, 1372.5351, 1395.0445, 1404.0821, 1407.8154, 1424.3239, 1432.4554, 1480.4201, 1487.2623, 1489.6693, 1494.3251, 1500.0487, 1505.3406, 1509.8258, 1518.2389, 3007.5589, 3016.628, 3024.9876, 3033.4966, 3041.5448, 3050.5396, 3086.3557, 3089.7461, 3095.4829,

6 -2.001167 -0.288295 1.313406 1 -2.297405 0.744506 1.490603 1 -2.853872 -0.929083 1.541759 1 -1.206478 -0.519184 2.019399	3101.7082, 3105.7937, 3116.4162, 3117.0179, 3144.8173

Compound: iPrCHCMe$_2$ + O$_3$ PRC1.3	**Energy (kJ mol^{-1}):** -500.000279409791
Reaction Coordinates: 6 -1.581704 -0.853239 -0.074931 6 -0.501052 0.044195 -0.621235 6 -0.024825 1.264297 -0.294607 6 -0.497222 2.170694 0.805981 1 0.339661 2.429376 1.460213 1 -1.288449 1.755620 1.415307 1 -0.854377 3.112141 0.378269 6 1.111824 1.839523 -1.094025 1 1.373260 1.218469 -1.948580 1 2.003745 1.946860 -0.466960 1 0.868464 2.842564 -1.454595 1 -0.027500 -0.408139 -1.488867 1 -1.091962 -1.828882 0.026150 6 -2.198247 -0.532966 1.287533 1 -2.827605 0.357236 1.255442 1 -1.439136 -0.396251 2.056628 1 -2.834974 -1.363650 1.596115 6 -2.682702 -1.026288 -1.140101 1 -3.227057 -0.091949 -1.289197 1 -3.398077 -1.789421 -0.829474 1 -2.265302 -1.328050 -2.101395 8 1.495968 -0.624229 1.100531 8 2.551814 -0.730428 0.411051 8 2.566327 -1.631996 -0.489174	**Frequencies (cm^{-1}):** 26.3037, 33.5148, 48.9675, 52.7549, 67.208, 94.4654, 106.116, 152.5217, 194.4247, 224.8505, 260.011, 266.1376, 311.202, 330.8835, 361.1903, 411.0278, 428.6266, 502.324, 612.6817, 731.7053, 772.6249, 845.6366, 883.3978, 933.6116, 956.1644, 961.2719, 976.7021, 1009.8951, 1083.7224, 1095.3977, 1101.8301, 1141.7438, 1143.4608, 1164.4526, 1212.8486, 1234.8538, 1316.17, 1381.0462, 1396.671, 1403.5019, 1411.7191, 1422.049, 1429.6012, 1471.0963, 1478.8542, 1489.0387, 1494.1607, 1496.4895, 1498.495, 1513.0226, 1517.1128, 1669.2032, 2985.4365, 3000.8004, 3016.683, 3021.0501, 3029.4016, 3043.0184, 3050.0982, 3079.4505, 3085.22, 3088.2076, 3102.2087, 3104.1973, 3112.3794, 3186.0958

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{OZO}$ 1.3	**Energy (kJ mol^{-1}):** -499.997549805376
Reaction Coordinates: 6 -1.659128 -0.515511 -0.280310 6 -0.375304 0.147878 -0.714132 6 0.441881 1.055031 -0.080558 6 0.191077 1.655128 1.276569 1 1.102049 2.108589 1.664377 1 -0.156326 0.925521 1.998965 1 -0.561593 2.446237 1.207057 6 1.511490 1.733931 -0.893758 1 1.736673 1.189227 -1.809527 1 2.430726 1.850025 -0.320587 1 1.180957 2.738915 -1.177735 1 -0.190358 0.032111 -1.776572 1 -1.688261 -1.455265 -0.838086 6 -1.810009 -0.882316 1.199227 1 -2.032465 -0.014332 1.819222 1 -0.913847 -1.366476 1.582326 1 -2.643622 -1.577227 1.311920 6 -2.855817 0.325531 -0.768453 1 -2.797887 0.524172 -1.839446 1 -2.898802 1.284757 -0.249669 1 -3.790938 -0.202724 -0.574769	**Frequencies (cm^{-1}):** -135.7049, 45.1373, 63.3076, 80.9731, 108.6585, 135.3715, 153.5909, 173.9194, 182.8777, 215.4375, 257.6404, 300.3867, 310.67, 351.9971, 403.3407, 414.3216, 442.3494, 547.2437, 620.2243, 739.3489, 768.9937, 842.0089, 887.1343, 936.3834, 956.3107, 959.1164, 972.7979, 1014.2406, 1067.9408, 1082.6807, 1087.5722, 1100.2618, 1114.8221, 1145.2171, 1212.8139, 1234.3849, 1325.8879, 1383.1348, 1393.1328, 1401.4308, 1407.1826, 1419.4109, 1420.3396, 1476.0525, 1480.0688, 1484.0549, 1492.233, 1495.6422, 1501.5882, 1511.4496, 1521.7091, 1584.1, 3006.1583, 3015.2255, 3019.3736, 3021.4137, 3035.7223, 3072.2013, 3082.0836, 3086.0162, 3087.2944, 3089.444,

8 1.874765 -0.605230 0.886236 8 2.024209 -1.294142 -0.192312 8 0.920844 -1.800824 -0.622547	3110.5665, 3117.0969, 3134.3315, 3158.5257

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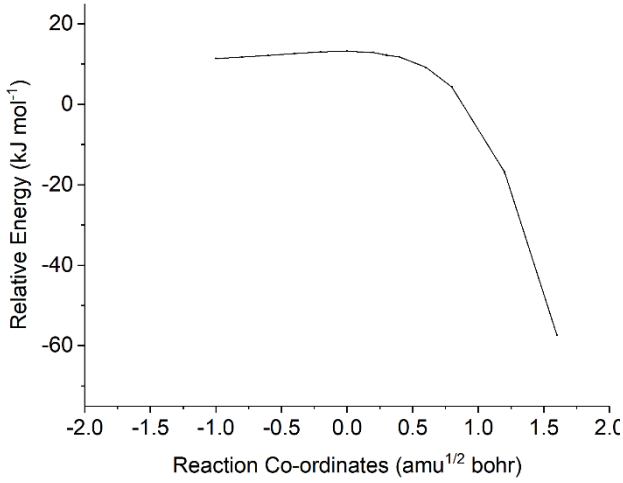

Compound: iPrCHCMe$_2$ + O$_3$ POZ1.3	**Energy (kJ mol^{-1}):** -500.100633245354
Reaction Coordinates: 6 1.671337 -0.359944 -0.363183 6 0.154212 -0.342494 -0.612159 6 -0.862847 0.595918 0.156085 6 -1.463616 1.615129 -0.809602 1 -2.207219 2.227837 -0.301001 1 -0.688875 2.274072 -1.206307 1 -1.943414 1.108428 -1.645895 6 -0.408015 1.255759 1.452114 1 -1.256387 1.771364 1.902932 1 -0.043997 0.521584 2.163971 1 0.368210 1.996224 1.266525 8 -1.882651 -0.346614 0.577434 8 -1.757831 -1.439340 -0.350854 8 -0.341461 -1.655682 -0.348177 1 0.010590 -0.138213 -1.677799 6 2.327888 0.941390 -0.836801 1 3.413445 0.848311 -0.794591 1 2.055942 1.178301 -1.866650 1 2.050707 1.790366 -0.210976 1 2.019293 -1.149047 -1.037420 6 2.129599 -0.757133 1.044713 1 1.559499 -1.602421 1.426668 1 3.180108 -1.049721 1.012380 1 2.046287 0.064251 1.753940	**Frequencies (cm^{-1}):** 46.4824, 89.9275, 187.4685, 201.508, 219.6827, 228.3401, 247.01, 261.9967, 293.8336, 316.7897, 347.0211, 368.982, 388.1407, 454.8979, 480.5243, 576.9602, 611.1634, 700.3137, 745.449, 772.236, 846.5201, 875.432, 931.4424, 937.4582, 939.944, 953.6238, 968.3482, 996.9119, 1025.6649, 1040.2321, 1107.7954, 1168.5579, 1175.8131, 1205.877, 1226.6813, 1259.1471, 1337.5697, 1365.9729, 1372.4108, 1402.7308, 1404.7239, 1409.7452, 1426.8378, 1433.9203, 1480.6848, 1488.4707, 1493.6447, 1496.9913, 1500.3666, 1510.8525, 1513.4241, 1522.0331, 2996.7406, 3008.1548, 3029.0776, 3032.3352, 3040.3454, 3049.9615, 3087.8367, 3091.1481, 3094.9858, 3096.154, 3107.1995, 3112.8581, 3118.0372, 3147.2337

Compound: iPrCHCMe$_2$ + O$_3$ PRC 2.1	**Energy (kJ mol^{-1}):** -500.009406834231
Reaction Coordinates: 6 1.788255 -0.403335 -0.247965 6 0.696610 0.305405 0.504068	**Frequencies (cm^{-1}):** 18.981, 26.1882, 43.2357, 56.759, 71.7588, 82.1701, 133.2563, 153.8705,

6 -0.039400 1.365684 0.124722 6 -1.044615 1.974826 1.059001 1 -0.809113 3.027230 1.243330 1 -2.044454 1.945835 0.618280 1 -1.081588 1.454670 2.014012 6 0.088630 2.071376 -1.195952 1 -0.888187 2.149436 -1.678736 1 0.441762 3.095264 -1.041948 1 0.769404 1.581309 -1.886752 1 0.525757 -0.077805 1.507342 1 1.846199 -0.012087 -1.264662 6 3.145324 -0.149222 0.431575 1 3.380503 0.914935 0.460471 1 3.139914 -0.518414 1.459554 1 3.946892 -0.662299 -0.103164 6 1.509290 -1.911502 -0.340578 1 0.590149 -2.115256 -0.889419 1 2.325645 -2.422672 -0.853664 1 1.411762 -2.351909 0.653977 8 -2.117246 -0.407449 -0.977107 8 -2.109078 -1.460781 -0.280099 8 -2.076078 -1.322723 0.976225	197.3768, 202.9195, 221.6348, 226.0821, 255.998, 305.9665, 400.4669, 404.5636, 449.2833, 503.9504, 516.1791, 737.9668, 808.5246, 856.8971, 874.3888, 930.4028, 951.6773, 962.0714, 964.7791, 1009.0885, 1089.3386, 1099.5493, 1108.4234, 1141.2138, 1163.7013, 1181.7893, 1191.5402, 1240.8429, 1331.9012, 1337.6577, 1392.1902, 1396.439, 1409.2418, 1418.4163, 1420.0185, 1469.5077, 1482.2037, 1487.8275, 1488.7227, 1490.3843, 1494.6795, 1502.9823, 1510.9899, 1675.7558, 3009.2858, 3016.8792, 3017.7218, 3022.8519, 3041.0768, 3051.5577, 3056.8417, 3075.2803, 3083.7303, 3090.0323, 3095.4343, 3106.6313, 3112.3412, 3123.0306

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{OZO}$ 2.1	**Energy (kJ mol^{-1}):** -500.002253312432
Reaction Coordinates: 6 -1.608263 0.029661 -0.224264 6 -0.364743 -0.183322 0.596962 6 0.726083 -0.948687 0.231877 6 0.781749 -1.741291 -1.046546 1 1.809187 -1.855607 -1.387040 1 0.204116 -1.288910 -1.849278 1 0.384116 -2.746395 -0.873661 6 1.751719 -1.304045 1.266434 1 1.710601 -0.630633 2.120096 1 2.757464 -1.269332 0.847894 1 1.582877 -2.325347 1.623634 1 -0.432586 0.102863 1.639466 1 -1.311533 0.209328 -1.262280 6 -2.489461 -1.237972 -0.202733 1 -2.815583 -1.460756 0.814943 1 -1.965337 -2.111486 -0.586603 1 -3.381025 -1.084147 -0.812614 6 -2.419237 1.235104 0.260264 1 -2.736088 1.095028 1.296648 1 -3.317802 1.359422 -0.345269 1 -1.835144 2.151120 0.208219 8 2.056531 0.739913 -0.637969 8 1.200940 1.708639 -0.672658 8 0.627486 1.896219 0.469861	**Frequencies (cm^{-1}):** -180.9287, 56.2153, 62.8728, 128.8376, 153.9729, 164.2228, 184.5153, 193.0556, 204.0999, 218.4721, 229.1815, 263.4276, 323.3701, 359.1357, 404.3638, 446.5766, 456.5301, 522.6237, 563.1585, 740.0163, 807.5006, 853.439, 880.6008, 935.5041, 954.7114, 962.3628, 966.6474, 1012.6059, 1068.2445, 1074.4047, 1079.7941, 1108.1044, 1117.4222, 1143.1772, 1192.7951, 1240.5507, 1316.7084, 1336.3124, 1375.2911, 1398.7555, 1409.361, 1420.5825, 1421.0733, 1471.6174, 1478.5808, 1482.2321, 1489.8056, 1491.9585, 1499.8325, 1503.5811, 1515.58, 1567.7408, 3006.4669, 3009.0039, 3014.7146, 3023.2432, 3028.4457, 3074.6233, 3078.4428, 3084.4401, 3085.6671, 3106.3357, 3117.3085, 3120.1299, 3123.327, 3152.0532
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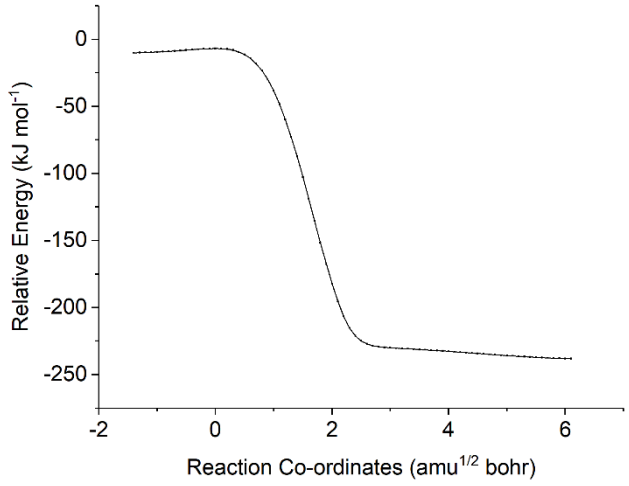
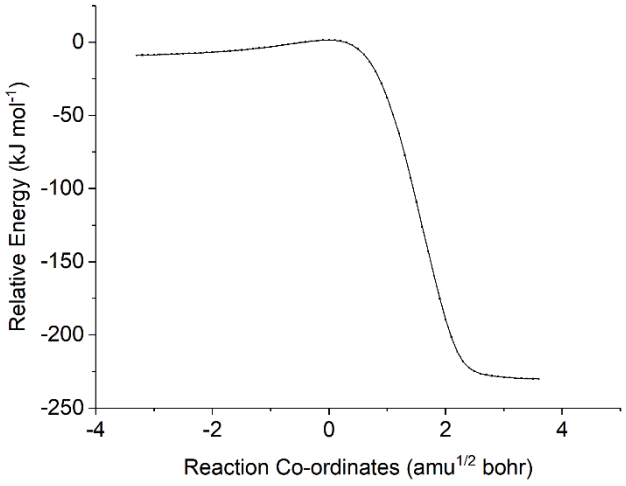


Compound: iPrCHCMe$_2$ + O$_3$ POZ 2.1	**Energy (kJ mol^{-1}):** -500.100633245354
Reaction Coordinates: 6 1.574337 0.089491 0.304225 6 0.281080 -0.250497 -0.447646 6 -1.045484 0.475715 -0.031317 6 -1.447157 1.584092 -0.994170 1 -2.434937 1.965380 -0.736718 1 -0.740911 2.411024 -0.938929 1 -1.472784 1.214323 -2.018140 6 -1.107218 0.923040 1.427250 1 -2.104643 1.309439 1.635104 1 -0.915766 0.089424 2.099038 1 -0.388138 1.712352 1.638984 8 -2.002832 -0.584264 -0.243244 8 -1.336044 -1.701431 0.324712 8 -0.033516 -1.654471 -0.328195 1 0.441693 -0.080458 -1.516901 6 2.684698 -0.899357 -0.071372 1 3.599001 -0.665783 0.475772 1 2.400762 -1.924110 0.158570 1 2.913263 -0.842818 -1.138561 1 1.382779 -0.009236 1.374967 6 2.029428 1.523191 0.006245 1 1.306735 2.274449 0.322202 1 2.966516 1.734163 0.522303 1 2.207469 1.659128 -1.063170	**Frequencies (cm^{-1}):** 50.4531, 93.3355, 179.8159, 200.6646, 215.7982, 226.5486, 242.3165, 265.6575, 281.1236, 304.078, 329.7536, 351.7206, 403.0925, 463.2806, 487.6588, 512.3638, 614.9535, 702.4236, 752.3579, 812.375, 857.4392, 885.2058, 918.9238, 937.7959, 939.3218, 946.3204, 967.9881, 997.2897, 1001.0016, 1027.6671, 1116.0032, 1152.7003, 1190.2494, 1192.783, 1228.5787, 1248.1367, 1320.9337, 1335.2542, 1350.7611, 1400.2939, 1402.532, 1405.7611, 1422.4386, 1427.3866, 1482.003, 1488.0895, 1491.664, 1495.7339, 1500.2557, 1505.0807, 1513.854, 1516.7735, 3007.0368, 3021.5804, 3025.0275, 3039.2277, 3044.2819, 3050.4058, 3077.969, 3086.0478, 3098.0634, 3108.6054, 3113.9024, 3115.6127, 3118.8761, 3127.8143

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{OZO}$ 2.2	**Energy (kJ mol^{-1}):** -499.998901097346
Reaction Coordinates: 6 -1.647352 -0.491510 -0.187702 6 -0.328037 -0.510170 0.554178 6 0.879437 -0.942757 0.036709 6 1.014188 -1.453737 -1.372024 1 2.032540 -1.328350 -1.735174	**Frequencies (cm^{-1}):** -206.2337, 48.3375, 77.2884, 143.3548, 147.4371, 164.0839, 169.6774, 199.1707, 203.7144, 220.6669, 243.8215, 277.3659, 310.8946, 337.0919, 403.2166, 446.2786,

1 0.341062 -0.960908 -2.067971 1 0.791151 -2.526243 -1.394060 6 1.992789 -1.299732 0.976582 1 1.882687 -0.795399 1.934244 1 2.963527 -1.037255 0.557388 1 1.993641 -2.380470 1.154001 1 -0.392999 -0.448772 1.632114 1 -1.657371 -1.376817 -0.833778 6 -1.866060 0.726996 -1.100905 1 -1.052159 0.869029 -1.810700 1 -1.952533 1.637873 -0.510448 1 -2.787479 0.594579 -1.669582 6 -2.809321 -0.627542 0.802713 1 -2.707644 -1.522449 1.418504 1 -3.761822 -0.689420 0.275314 1 -2.850277 0.237103 1.468032 8 1.865598 1.101511 -0.351266 8 0.853410 1.889982 -0.178046 8 0.248968 1.673284 0.944912	463.2756, 517.6724, 596.0347, 736.8243, 807.1903, 847.1062, 883.3437, 935.2766, 956.7314, 964.2363, 970.0326, 1013.747, 1062.2978, 1069.8668, 1083.085, 1111.5553, 1118.5845, 1133.7831, 1205.6172, 1235.7641, 1328.5416, 1341.2537, 1374.9208, 1401.2988, 1408.8557, 1419.3688, 1422.6629, 1470.007, 1473.9273, 1482.0141, 1491.0436, 1493.6054, 1500.6361, 1505.419, 1514.308, 1560.722, 2983.0405, 3005.1057, 3010.5308, 3023.0533, 3035.3184, 3077.3005, 3084.1586, 3088.1752, 3089.6386, 3096.4546, 3110.6873, 3120.0723, 3132.9801, 3164.4379
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ POZ 2.2	**Energy (kJ mol^{-1}):** -500.099560637349
Reaction Coordinates: 6 1.511226 0.541820 0.208904 6 0.236883 0.191002 -0.586858 6 -1.181507 0.391005 0.080941 6 -2.044347 1.357910 -0.723975 1 -3.065988 1.361543 -0.344586 1 -1.650488 2.371569 -0.641457 1 -2.065075 1.071532 -1.774355 6 -1.185916 0.754121 1.562760 1 -2.217875 0.854166 1.897963 1 -0.709791 -0.015737 2.162803 1 -0.681759 1.702839 1.745642 8 -1.786352 -0.912297 -0.098992 8 -0.667687 -1.799552 -0.062133 8 0.216302 -1.176976 -1.020841 1 0.248233 0.763110 -1.515969 6 1.951610 -0.536631 1.205267 1 2.842258 -0.201214 1.738036 1 1.190859 -0.774050 1.944216	**Frequencies (cm^{-1}):** 19.7529, 66.68, 184.6829, 201.3522, 217.0809, 235.7174, 241.2649, 261.5466, 284.4967, 311.8119, 325.9465, 357.2385, 406.5973, 480.7434, 496.2725, 570.0217, 645.4632, 706.6525, 751.4539, 811.9241, 843.4929, 888.7217, 920.7518, 930.026, 938.2038, 941.1205, 964.2786, 973.9224, 1015.3362, 1030.6448, 1113.2067, 1120.435, 1182.7668, 1200.7552, 1218.7763, 1243.0849, 1311.1311, 1325.0125, 1365.515, 1391.1997, 1403.3744, 1406.4317, 1422.8857, 1429.6434, 1480.1074, 1487.5858, 1489.2818, 1497.0927, 1500.165, 1507.0239, 1510.4919, 1517.8574, 3016.3181, 3021.9496, 3036.3651,

1 2.200934 -1.459144 0.682124 1 1.301660 1.463763 0.758617 6 2.655344 0.839774 -0.770554 1 2.401460 1.656463 -1.448704 1 3.561309 1.121365 -0.232816 1 2.886402 -0.039611 -1.374698	3042.7333, 3047.0783, 3050.7718, 3082.8316, 3088.7794, 3098.5789, 3099.8779, 3105.7524, 3114.1895, 3124.4814, 3143.1334

Compound: $iPrCHCMe_2 + O_3$ PRC 2.3	**Energy (kJ mol^{-1}):** -500.005090090309
Reaction Coordinates: 6 -1.623834 -0.854408 -0.484766 6 -0.579881 0.196663 -0.819377 6 -0.155354 1.257177 -0.105273 6 0.847048 2.210841 -0.691280 1 0.423649 3.217763 -0.756724 1 1.731981 2.279413 -0.054002 1 1.168544 1.905268 -1.684706 6 -0.650258 1.651402 1.259145 1 0.191459 1.795822 1.939958 1 -1.170550 2.612213 1.201408 1 -1.326818 0.930277 1.704588 1 -0.153600 0.099368 -1.811710 1 -1.650124 -1.521284 -1.350314 6 -1.274529 -1.741300 0.722059 1 -0.309826 -2.229514 0.587277 1 -1.233538 -1.177658 1.653133 1 -2.027085 -2.523138 0.840649 6 -3.038696 -0.261137 -0.358557 1 -3.298879 0.322316 -1.242278 1 -3.775402 -1.059990 -0.252939 1 -3.130134 0.392160 0.508915 8 2.186168 -0.250005 1.003876 8 2.274712 -1.235036 0.216485 8 2.215790 -0.989764 -1.022231	**Frequencies (cm^{-1}):** 30.4237, 36.3336, 45.8848, 57.6055, 74.3464, 100.6906, 139.6606, 159.5093, 195.2367, 203.4711, 225.0322, 233.2679, 239.1553, 313.096, 378.2277, 397.2372, 407.2777, 501.8941, 621.163, 737.5982, 768.0594, 838.4163, 854.8978, 930.7721, 958.6408, 962.4473, 975.9139, 1007.3822, 1074.562, 1099.2991, 1117.797, 1131.6367, 1162.1776, 1179.6282, 1205.4712, 1230.8193, 1356.1323, 1382.7233, 1385.4314, 1398.9969, 1411.0293, 1418.5159, 1423.9129, 1470.1953, 1480.7417, 1486.2552, 1490.0982, 1491.2978, 1500.0878, 1505.2301, 1513.1099, 1665.6227, 3009.2798, 3012.868, 3017.8091, 3025.4197, 3032.412, 3053.4266, 3058.8581, 3083.0867, 3088.8068, 3097.3399, 3105.1244, 3111.407, 3135.9647, 3148.2124

Compound: $iPrCHCMe_2 + O_3$ TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -499.996366433202
Reaction Coordinates: 6 -1.665814 -0.441125 -0.342935 6 -0.364275 0.229217 -0.728482 6 0.479681 1.050826 -0.009683 6 0.281690 1.445193 1.430372 1 1.214227 1.812606 1.855395 1 -0.073292 0.630344 2.051069 1 -0.447766 2.259059 1.496489 6 1.479690 1.880723 -0.763808 1 1.647782 1.498212 -1.768368 1 2.436014 1.913101 -0.242255 1 1.119094 2.911907 -0.844348 1 -0.220796 0.264138 -1.801304 1 -1.790563 -1.251322 -1.064738 6 -1.767432 -1.078144 1.048365 1 -1.896621 -0.336531 1.835558 1 -0.896806 -1.687049 1.285744 1 -2.642096 -1.729680 1.077364	**Frequencies (cm^{-1}):** -162.6441, 42.626, 53.8993, 117.6566, 126.5366, 151.4485, 155.1816, 181.475, 195.1166, 209.3387, 252.6882, 298.5906, 309.7401, 347.7951, 405.1941, 414.0097, 446.3455, 563.2313, 619.9793, 738.1627, 768.0798, 840.8062, 893.259, 936.158, 954.8705, 959.3061, 971.7796, 1016.0146, 1064.7336, 1081.7593, 1082.2415, 1099.6062, 1115.3371, 1144.5755, 1212.0356, 1233.3561, 1332.3875, 1381.1193, 1393.2182, 1401.5779, 1409.4948, 1420.3684, 1422.739, 1473.0324, 1479.0256, 1482.0782, 1491.3118, 1494.5322, 1500.3068, 1511.5857, 1519.5704, 1571.4045,

6 -2.827505 0.545098 -0.578511 1 -2.775075 1.386553 0.114418 1 -3.784815 0.043439 -0.425709 1 -2.815515 0.943379 -1.593769 8 2.166364 -0.558785 0.476619 8 1.501459 -1.631027 0.208765 8 0.985929 -1.616299 -0.973816	3006.3802, 3012.5716, 3020.8165, 3024.9599, 3038.0158, 3073.8912, 3082.3013, 3087.1173, 3088.4959, 3092.1226, 3114.3353, 3117.4812, 3149.9853, 3155.7495

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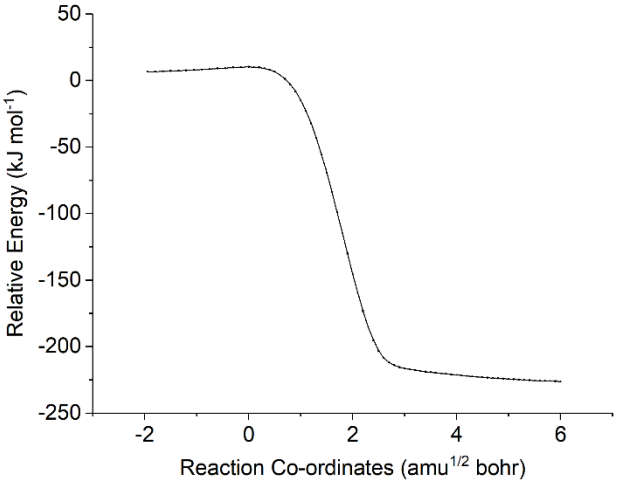
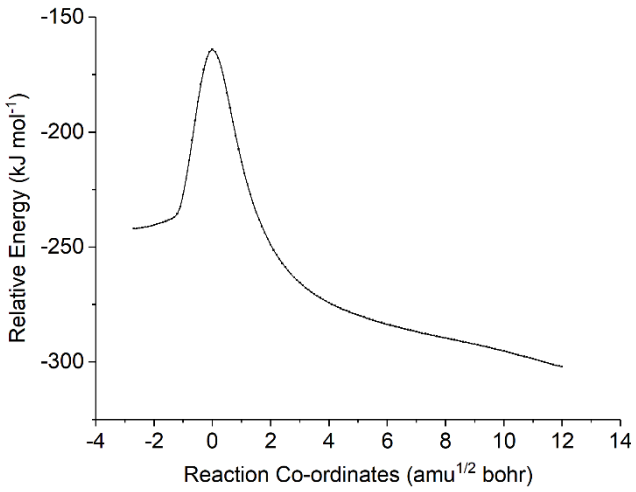


Compound: iPrCHCMe$_2$ + O$_3$ POZ 2.3	**Energy (kJ mol^{-1}):** -500.098143883523
Reaction Coordinates: 6 1.670392 -0.238455 -0.390414 6 0.170788 -0.185791 -0.742297 6 -0.883799 0.578490 0.130335 6 -1.238380 1.940238 -0.453036 1 -2.069761 2.379545 0.097310 1 -0.387829 2.616343 -0.376717 1 -1.522161 1.851419 -1.500526 6 -0.614874 0.661932 1.629794 1 -1.473104 1.130663 2.111274 1 -0.476068 -0.325168 2.060851 1 0.264310 1.266518 1.845256 8 -2.043338 -0.254419 -0.098331 8 -1.504717 -1.559558 0.045966 8 -0.349594 -1.526806 -0.847109 1 0.096510 0.234619 -1.749128 6 2.313800 1.151485 -0.446731 1 3.398379 1.066019 -0.373281 1 2.086864 1.664160 -1.383334 1 1.983000 1.788622 0.374822 1 2.094939 -0.812723 -1.220062 6 2.039035 -0.998356 0.887311 1 1.484689 -1.932695 0.962261 1 3.102214 -1.242573 0.868837 1 1.857444 -0.415743 1.788464	**Frequencies (cm^{-1}):** 44.6921, 104.3266, 189.4513, 210.6007, 217.1462, 239.7434, 249.0825, 269.3811, 277.9811, 296.3378, 324.534, 361.5894, 386.3785, 455.3301, 496.9549, 577.6385, 617.1396, 687.9109, 748.7095, 783.3638, 843.4096, 879.4662, 924.8332, 936.7227, 945.2614, 950.0748, 969.7543, 992.7414, 1011.2932, 1029.3371, 1108.2063, 1153.4811, 1183.502, 1220.285, 1229.7507, 1255.1683, 1333.6474, 1358.8002, 1368.6897, 1402.6724, 1404.9038, 1410.9872, 1426.1544, 1432.4832, 1481.3745, 1489.5617, 1493.3653, 1495.3651, 1502.8971, 1512.7125, 1512.9408, 1520.7649, 2997.9491, 3015.6902, 3025.9247, 3039.9615, 3043.7288, 3050.8246, 3083.4268, 3088.4833, 3094.6311, 3106.8354, 3112.9882, 3117.3468, 3118.8233, 3142.077

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{ANTI}$ 1	**Energy (kJ mol^{-1}):** -500.070492661337

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.621157 -0.207910 0.293868 6 -0.356163 0.380047 -0.297068 6 1.354416 -0.460175 0.052671 6 1.457646 -1.500084 -1.071548 1 0.638332 -2.215126 -1.074934 1 2.387821 -2.054518 -0.933896 1 1.509562 -0.999213 -2.036406 6 1.239055 -1.018898 1.473698 1 0.471697 -1.786104 1.568335 1 1.038562 -0.214324 2.178666 1 2.196495 -1.468145 1.743994 1 -0.260713 0.369224 -1.380034 1 -1.490448 -0.261313 1.376675 6 -1.928798 -1.610525 -0.238054 1 -2.893122 -1.942087 0.146779 1 -1.185803 -2.345229 0.063020 1 -1.990224 -1.616010 -1.328045 6 -2.802790 0.738111 0.003463 1 -2.631213 1.729664 0.417997 1 -2.965488 0.841778 -1.071202 1 -3.716031 0.334757 0.442195 8 -0.052772 1.567173 0.247708 8 0.999172 2.105251 -0.347528 8 2.158265 0.540481 -0.077095	-471.1801, 57.9601, 88.0866, 163.1743, 186.4835, 204.171, 216.8057, 222.3976, 242.3326, 265.1519, 281.4379, 294.9007, 349.5894, 426.1388, 453.9438, 479.3616, 484.7667, 539.3743, 585.7889, 617.239, 774.6216, 864.2835, 912.7329, 935.5245, 943.2124, 973.5274, 985.5904, 1005.1832, 1065.3997, 1088.4899, 1121.1091, 1151.9518, 1169.4564, 1187.5874, 1191.5036, 1243.1903, 1317.7933, 1336.8421, 1372.3582, 1388.2665, 1399.065, 1403.3356, 1409.9566, 1431.3369, 1477.4686, 1485.7221, 1489.726, 1494.6302, 1494.9663, 1502.8035, 1509.4269, 1518.3202, 3027.7162, 3032.8072, 3035.2257, 3039.9833, 3041.293, 3086.6453, 3093.9118, 3095.0956, 3101.2777, 3108.5995, 3114.3751, 3117.6017, 3122.5213, 3133.5451
IRC:  	

Compound: iPrCHCMe$_2$ + O_3 C_{ANTI} 1	**Energy (kJ mol^{-1}):** -500.123510392293
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.305770 -0.171141 -0.319203 6 -1.088537 0.505103 0.197996 1 -0.722785 0.370435 1.211703 8 -0.454580 1.292134 -0.540027 8 0.670377 1.912091 -0.013305 1 -2.373074 0.051551 -1.385397 6 -3.548971 0.400340 0.390957 1 -4.443148 -0.097686 0.015564 1 -3.653671 1.470524 0.215661 1 -3.498956 0.231606 1.467879 6 -2.191952 -1.691303 -0.117136	29.3556, 33.946, 63.9613, 67.1364, 77.8482, 90.4112, 102.9606, 122.2043, 139.4607, 204.9024, 209.7612, 224.9697, 267.4681, 320.0664, 384.9399, 429.9275, 477.4483, 485.446, 521.9341, 536.3316, 788.5174, 850.4705, 892.0988, 902.082, 910.6877, 939.6556, 948.7239, 957.6358, 970.5887, 1087.0823, 1100.6954, 1117.4863, 1184.0228, 1202.5914, 1242.708, 1326.0712, 1331.0379,

1 -1.307294 -2.090984 -0.607671 1 -2.126407 -1.939929 0.943082 1 -3.077873 -2.178657 -0.524714 6 2.164393 -0.577026 0.088517 6 2.922223 -0.024784 1.270626 1 3.128891 1.034726 1.123568 1 3.881997 -0.541295 1.357856 1 2.353142 -0.166571 2.185232 6 2.754277 -0.312600 -1.275612 1 2.627138 0.746795 -1.503384 1 2.245543 -0.908470 -2.029171 1 3.823930 -0.529839 -1.286627 8 1.147777 -1.232192 0.228275	1372.3638, 1380.6734, 1388.3722, 1402.6001, 1425.4602, 1458.1037, 1468.148, 1470.7619, 1487.9195, 1488.8987, 1489.4387, 1501.2361, 1511.0797, 1579.3058, 1749.793, 3027.4826, 3030.1211, 3035.5321, 3035.8033, 3052.7572, 3092.3544, 3092.733, 3097.739, 3099.0019, 3104.7283, 3125.1317, 3132.9509, 3140.2823, 3151.7939

Compound: $iPrCHCMe_2 + O_3$ TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -500.072336326532
Reaction Coordinates: 6 -1.552772 0.482412 0.024310 6 -0.304991 -0.278943 0.425705 6 1.361765 0.468572 -0.022401 6 1.495756 1.551813 1.060298 1 0.654724 2.246304 1.060609 1 2.402162 2.125597 0.861522 1 1.594547 1.093943 2.042323 6 1.258943 1.007423 -1.451484 1 0.488147 1.769782 -1.563233 1 1.075047 0.194244 -2.150053 1 2.216281 1.461794 -1.713435 1 -0.109340 -0.346865 1.491776 1 -1.270494 1.537878 -0.020608 6 -2.619975 0.341811 1.123163 1 -3.498072 0.938222 0.873627 1 -2.247865 0.680199 2.090715 1 -2.937322 -0.697022 1.226741 6 -2.114697 0.074893 -1.341937 1 -1.377587 0.163944 -2.136600 1 -2.465961 -0.956787 -1.327832 1 -2.961189 0.714380 -1.592134 8 -0.141384 -1.460464 -0.194501 8 0.911234 -2.089880 0.309753 8 2.141743 -0.551343 0.128579	**Frequencies (cm^{-1}):** -462.2543, 63.6016, 81.1371, 162.9494, 200.1402, 207.9409, 216.0407, 235.5798, 241.7963, 251.3711, 270.7694, 310.6758, 375.4883, 404.1233, 420.2776, 484.4743, 520.2483, 575.2814, 591.815, 630.2075, 776.0971, 847.7494, 910.8123, 929.6322, 958.5321, 967.7949, 992.1435, 1033.6567, 1060.0104, 1076.9625, 1121.3748, 1127.5066, 1169.9828, 1192.505, 1205.2895, 1252.9394, 1326.5249, 1352.5479, 1370.9894, 1388.061, 1390.1849, 1404.0971, 1406.6844, 1432.9231, 1475.8925, 1486.6406, 1491.2632, 1492.1053, 1495.8642, 1504.2979, 1506.603, 1514.073, 3019.175, 3027.3429, 3029.4878, 3035.1462, 3043.4231, 3087.347, 3091.8211, 3092.4273, 3093.7615, 3101.5168, 3113.3553, 3121.3541, 3122.3969, 3125.246
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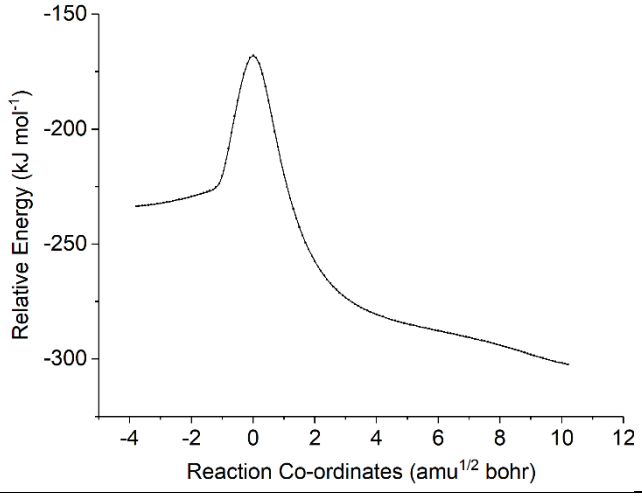
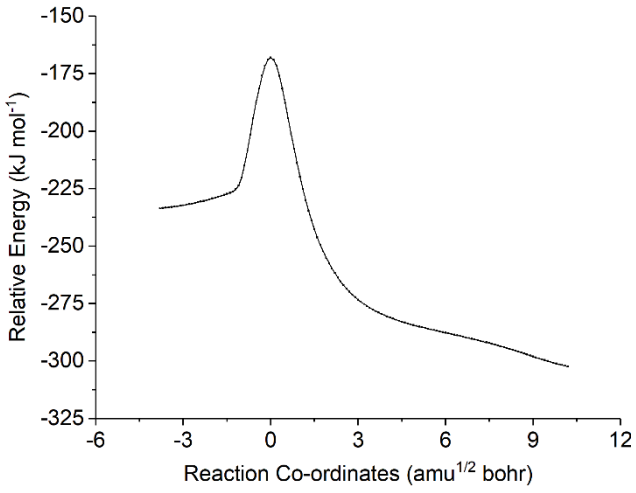


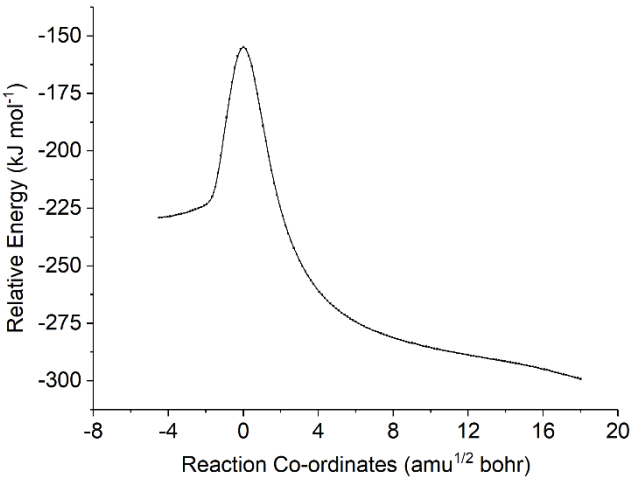
Compound: $iPrCHCMe_2 + O_3$ C_{ANTI} 2	**Energy (kJ mol^{-1}):** -500.120499876249
Reaction Coordinates: 6 -1.953916 -0.779032 0.036276 6 -1.177695 0.386127 -0.462423 6 2.440269 -0.441445 -0.015306 6 3.672341 -1.317526 0.031582 1 4.268530 -1.095985 0.918514 1 4.303938 -1.101715 -0.833500 1 3.392922 -2.367657 0.021310 6 2.649270 1.040898 0.153592 1 2.985806 1.235593 1.176059 1 1.731591 1.597712 -0.035401 1 3.448742 1.388134 -0.504542 1 -0.688610 0.381245 -1.431150 1 -1.230113 -1.602144 0.044249 6 -3.047186 -1.138466 -0.990205 1 -3.536986 -2.065680 -0.693818 1 -2.631532 -1.281929 -1.987934 1 -3.804408 -0.355455 -1.044340 6 -2.513759 -0.586934 1.444217 1 -1.723811 -0.365922 2.160238 1 -3.232192 0.232500 1.475436 1 -3.021736 -1.496249 1.764533 8 -1.083677 1.431909 0.215709 8 -0.338281 2.484565 -0.312113 8 1.337198 -0.926996 -0.180602	**Frequencies (cm^{-1}):** 20.882, 27.3247, 45.1603, 60.3496, 74.0044, 91.552, 97.7926, 138.3232, 156.8233, 193.0098, 217.9741, 224.1083, 257.4163, 336.2253, 395.5306, 439.0949, 445.7254, 498.7131, 545.3482, 601.4094, 791.7709, 826.622, 889.4105, 893.8463, 904.1785, 931.792, 946.4897, 971.6223, 975.1344, 1092.8839, 1111.693, 1125.7724, 1141.1876, 1205.4969, 1246.6721, 1303.8298, 1352.1113, 1378.8007, 1387.6804, 1402.3032, 1406.6338, 1427.9046, 1462.5708, 1467.0079, 1476.8716, 1489.0684, 1492.8779, 1496.8961, 1504.4592, 1511.4612, 1579.2211, 1756.6969, 3006.0507, 3009.1656, 3030.9345, 3031.4219, 3040.4566, 3069.4844, 3084.2886, 3096.5046, 3099.9138, 3102.178, 3103.6423, 3111.3342, 3136.5723, 3158.0452

Compound: $iPrCHCMe_2 + O_3$ TS_{ANTI} 3	**Energy (kJ mol^{-1}):** -500.066952645815
Reaction Coordinates: 6 1.713991 -0.264797 -0.393055 6 0.219904 -0.458719 -0.609011 6 -1.136865 0.636744 0.218607 6 -1.205039 1.849808 -0.721417 1 -0.265416 2.393961 -0.783511 1 -1.964443 2.531785 -0.334931 1 -1.515422 1.538181 -1.716951	**Frequencies (cm^{-1}):** -482.4731, 72.424, 84.1642, 181.1988, 190.084, 209.7179, 219.247, 241.3283, 250.125, 265.0202, 281.6505, 320.8835, 338.3924, 414.182, 425.3494, 465.3799, 483.6881, 566.3456, 594.4233, 644.3468, 771.4695, 838.2625, 911.7703, 935.9893,

6 -0.671689 0.944062 1.644410 1 0.244516 1.531503 1.673346 1 -0.534724 0.023476 2.206942 1 -1.455565 1.522708 2.137375 1 -0.125666 -0.261829 -1.620154 1 2.154859 -0.929015 -1.148058 6 2.242116 -0.729786 0.968285 1 1.920202 -0.073885 1.774657 1 1.916709 -1.741130 1.204054 1 3.332365 -0.723163 0.951098 6 2.188513 1.149720 -0.739064 1 1.859892 1.880346 -0.000923 1 3.278059 1.170874 -0.758551 1 1.833612 1.470769 -1.718741 8 -0.218576 -1.636266 -0.134683 8 -1.468648 -1.852334 -0.515298 8 -2.160847 -0.148496 0.140208	955.5541, 979.2762, 993.9721, 1025.6364, 1064.5484, 1092.1581, 1099.104, 1151.1831, 1163.1748, 1191.5638, 1220.3509, 1245.614, 1334.0414, 1352.5278, 1373.3171, 1381.3922, 1388.8319, 1403.9838, 1410.6919, 1432.8136, 1476.9238, 1487.406, 1488.8329, 1493.6328, 1502.7808, 1504.3049, 1512.258, 1518.5451, 2968.5141, 3033.6618, 3036.1891, 3040.0265, 3046.6242, 3092.8349, 3096.3311, 3100.7053, 3102.8949, 3106.1854, 3109.6152, 3124.1121, 3128.7563, 3131.9885
IRC:  	

Compound: iPrCHCMe$_2$ + O$_3$ C$_{ANTI}$ 3	**Energy (kJ mol^{-1}):** -500.124303990849
Reaction Coordinates: 6 -2.382824 -0.129443 -0.325221 6 -1.074251 0.432787 -0.751514 1 -0.543188 0.067282 -1.624800 8 -0.545806 1.371952 -0.117074 8 0.677653 1.851322 -0.570847 1 -3.077699 0.133670 -1.136237 6 -2.906238 0.460969 0.983052 1 -2.240562 0.217551 1.811105 1 -2.994263 1.545009 0.931188 1 -3.889438 0.046977 1.204245 6 -2.294814 -1.667732 -0.291939 1 -1.599147 -1.995787 0.478198 1 -3.280485 -2.082536 -0.083052 1 -1.950079 -2.069680 -1.244474 6 2.046895 -0.595206 0.208409 6 2.411775 0.005829 1.544183 1 2.288138 1.087741 1.475728 1 3.455593 -0.195639 1.791440 1 1.762267 -0.383898 2.323941 6 3.018452 -0.366376 -0.923120	**Frequencies (cm^{-1}):** 27.4213, 34.0516, 65.4931, 70.1959, 82.0788, 93.6496, 105.4779, 138.7385, 147.3152, 191.6971, 214.2501, 227.3651, 257.012, 336.7136, 384.9264, 441.1124, 447.3466, 486.0142, 536.2614, 596.0506, 788.3514, 828.4378, 891.9183, 902.5857, 904.9527, 931.8615, 939.7318, 975.3256, 978.1187, 1087.0022, 1110.7904, 1117.3594, 1146.4621, 1207.1281, 1242.5396, 1296.9603, 1347.2716, 1375.1951, 1380.6564, 1388.3723, 1410.0425, 1429.8317, 1458.2797, 1468.3225, 1470.9759, 1488.3255, 1488.8198, 1490.9387, 1502.6203, 1511.2647, 1576.4281, 1749.5251, 2957.4457, 3027.5773, 3035.8616, 3039.8724, 3042.7367, 3092.4506,

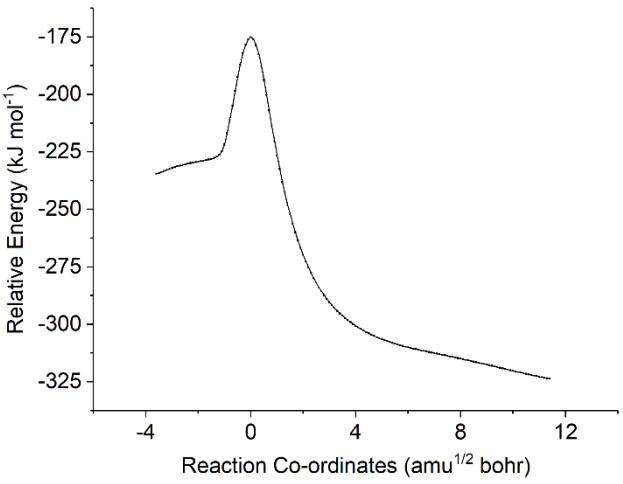
1 3.248923 0.694685 -1.012306 1 2.604985 -0.734401 -1.858054 1 3.952873 -0.892228 -0.708919 8 1.036667 -1.258738 0.061533	3097.7545, 3103.345, 3105.5396, 3111.7179, 3121.0061, 3132.6058, 3140.1532, 3156.321

Compound: iPrCHCMe$_2$ + O$_3$ TS$_{DMFO}$ 1.1	**Energy (kJ mol^{-1}):** -500.075670013921
Reaction Coordinates: 6 -1.602448 0.162377 -0.230437 6 -0.374052 -0.224118 0.625084 6 1.201839 0.497909 -0.064928 6 2.195689 0.382226 1.067093 1 3.205468 0.461226 0.656755 1 2.104403 -0.566201 1.584325 1 2.046471 1.201070 1.768749 6 1.059448 1.866798 -0.677118 1 0.704766 2.576102 0.067126 1 2.034825 2.213110 -1.025608 1 0.374551 1.863386 -1.521488 1 -0.295309 0.339946 1.570342 1 -1.267229 0.356233 -1.252408 6 -2.267054 1.427454 0.319742 1 -1.584963 2.277212 0.357886 1 -3.117619 1.716962 -0.298463 1 -2.640030 1.256131 1.332467 6 -2.602166 -0.997047 -0.295294 1 -3.444840 -0.730418 -0.935181 1 -2.135266 -1.896023 -0.690682 1 -2.992869 -1.234102 0.696358 8 1.300638 -0.440812 -1.050155 8 1.430554 -1.654665 -0.532006 8 -0.063679 -1.470552 0.735282	**Frequencies (cm^{-1}):** -462.8351, 49.0125, 95.177, 162.3988, 176.1447, 201.5902, 209.2841, 233.1641, 248.1251, 267.9689, 303.7398, 338.6916, 343.3215, 381.8714, 413.0056, 427.1393, 534.9081, 573.8174, 644.6694, 665.3672, 786.0754, 831.7373, 917.4204, 935.3415, 952.3717, 966.8606, 972.5306, 990.427, 1011.9406, 1097.5121, 1125.5317, 1138.4621, 1163.9922, 1195.2854, 1273.7237, 1280.8368, 1297.8542, 1326.0099, 1349.9759, 1397.2951, 1401.4685, 1403.89, 1419.3568, 1429.5839, 1470.9667, 1481.5396, 1488.7819, 1490.7186, 1494.1225, 1504.1951, 1505.7506, 1511.8159, 2907.5713, 3019.39, 3022.5946, 3028.7693, 3034.043, 3039.8467, 3077.5167, 3084.1178, 3091.1681, 3101.8077, 3106.2256, 3120.7541, 3137.6264, 3162.1852
IRC:  	

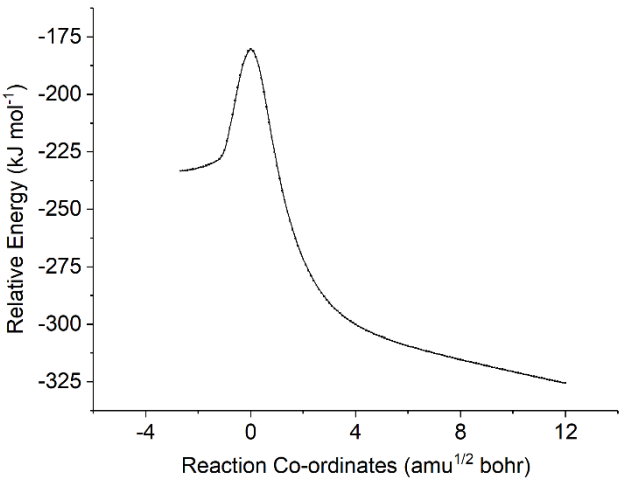
Compound: iPrCHCMe$_2$ + O$_3$ CPr$_{DMFO}$ 1.1	**Energy (kJ mol^{-1}):** -500.127738386250

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.280766 0.020421 0.243743 6 1.109599 0.555313 -0.543903 6 -2.323608 -0.021283 0.041788 6 -2.091733 -1.453139 0.296797 1 -2.172812 -1.640091 1.369793 1 -1.059885 -1.691467 0.029636 1 -2.779744 -2.072448 -0.272484 6 -3.261608 0.492055 -0.987693 1 -2.933548 0.150741 -1.972518 1 -4.262540 0.087818 -0.821339 1 -3.296468 1.578227 -0.976401 1 0.883849 1.621234 -0.352219 1 1.987305 0.163926 1.289487 6 3.509359 0.906887 -0.021959 1 3.290226 1.960692 0.156855 1 4.330060 0.621777 0.636141 1 3.853062 0.801596 -1.052817 6 2.550689 -1.456469 -0.017103 1 3.377788 -1.806660 0.601384 1 1.675390 -2.063341 0.210636 1 2.809138 -1.629282 -1.062549 8 -1.714356 0.856717 0.715048 8 -0.785716 0.419401 1.652778 8 0.457246 -0.069297 -1.349530	28.8479, 31.4456, 40.2345, 64.9932, 84.6148, 87.6478, 149.2758, 157.7152, 162.9258, 198.9538, 229.2595, 272.9603, 291.9476, 310.2365, 351.4906, 367.6751, 410.5925, 481.2188, 593.8979, 641.1227, 796.501, 812.8661, 913.0078, 913.9669, 926.0007, 930.5531, 946.387, 973.8385, 988.2613, 1073.135, 1097.5548, 1126.9288, 1152.0461, 1199.3392, 1305.2502, 1306.1502, 1362.7537, 1387.6256, 1401.6335, 1405.6884, 1412.1562, 1433.8316, 1443.9564, 1458.7778, 1470.4252, 1479.1982, 1486.9531, 1490.4176, 1504.6272, 1508.9443, 1570.0899, 1772.3351, 2909.4477, 3012.5999, 3024.1472, 3026.7341, 3033.9029, 3034.6161, 3075.0393, 3081.4913, 3084.128, 3091.8887, 3095.3449, 3103.1073, 3137.4614, 3138.7634

Compound: $iPrCHCMe_2 + O_3$ TS_{DMFO} 1.2	**Energy (kJ mol^{-1}):** -500.078148008237
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.605736 0.474029 0.043317 6 0.385443 -0.084251 -0.710002 6 -1.225552 0.483084 0.006953 6 -2.219779 0.283943 -1.114693 1 -3.227158 0.274591 -0.691494 1 -2.053057 -0.652487 -1.635364 1 -2.149961 1.113589 -1.816100 6 -1.175807 1.863190 0.607770 1 -0.772694 2.571100 -0.114530 1 -2.184533 2.191571 0.866272 1 -0.561661 1.886447 1.504761 1 0.214125 0.433561 -1.670200 1 1.434240 1.537709 0.229910 6 2.822926 0.363942 -0.888755 1 2.651465 0.875523 -1.837958 1 3.703652 0.809319 -0.423894 1 3.044068 -0.681997 -1.106136 6 1.870115 -0.235115 1.371458 1 2.778861 0.155098 1.831818 1 1.051085 -0.105210 2.077355 1 1.999388 -1.305084 1.212042 8 -1.249451 -0.457558 0.995545 8 -1.273338 -1.677557 0.483650 8 0.234499 -1.364468 -0.769540	-442.9627, 61.036, 103.4755, 167.1876, 185.9858, 204.0616, 217.6061, 243.5371, 248.6403, 262.369, 296.049, 310.3756, 343.0872, 377.9881, 402.0569, 425.3787, 538.9022, 630.5345, 648.3162, 683.9385, 775.6779, 820.9131, 919.8382, 936.3115, 955.6347, 969.0862, 983.068, 1000.8802, 1024.5609, 1092.9989, 1107.4285, 1133.5826, 1169.3909, 1197.6573, 1274.7883, 1278.8809, 1296.2285, 1342.4837, 1348.9773, 1399.4069, 1403.0968, 1404.8225, 1420.2185, 1436.5624, 1471.9546, 1483.5098, 1488.489, 1492.7339, 1495.0027, 1502.9817, 1506.0707, 1514.5336, 2897.3101, 3017.8808, 3020.8839, 3034.3892, 3037.3136, 3039.5797, 3079.7387, 3090.7534, 3096.6893, 3099.2351, 3104.6386, 3110.3456, 3132.5172, 3160.352
IRC:	

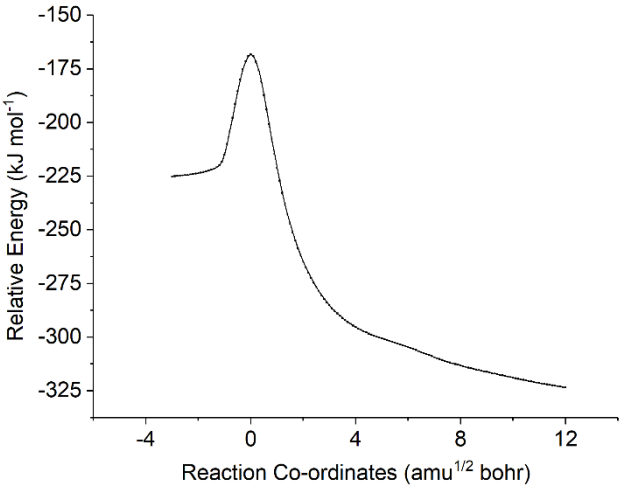


Compound: $iPrCHCMe_2 + O_3$ TS_{DMFO} 1.3	**Energy (kJ mol^{-1}):** -500.073453434399
Reaction Coordinates: 6 1.734063 -0.296988 -0.357009 6 0.282747 -0.293658 -0.887311 6 -0.989035 0.618985 0.134630 6 -2.142086 0.812244 -0.824865 1 -3.046172 1.013763 -0.245000 1 -2.310007 -0.067894 -1.435028 1 -1.945286 1.672872 -1.461833 6 -0.511315 1.869807 0.825928 1 -0.065558 2.551858 0.105963 1 -1.363800 2.378697 1.281564 1 0.214363 1.648250 1.603125 1 0.147663 0.378533 -1.752875 1 2.218581 -0.983042 -1.060353 6 1.894080 -0.916225 1.032220 1 1.340233 -1.850919 1.103271 1 2.946150 -1.127537 1.229111 1 1.539371 -0.252690 1.821363 6 2.453884 1.046786 -0.497991 1 2.167472 1.759633 0.274164 1 3.532058 0.902911 -0.416653 1 2.261301 1.506047 -1.470523 8 -1.133322 -0.387451 1.044675 8 -1.583379 -1.487204 0.461543 8 -0.279599 -1.447368 -1.022457	**Frequencies (cm^{-1}):** -461.1451, 75.975, 108.3295, 177.1786, 186.2279, 211.4554, 235.119, 235.7138, 249.4934, 262.2912, 279.2264, 326.1872, 342.5325, 376.6126, 410.2419, 483.624, 514.0737, 555.2316, 644.8178, 682.8027, 773.4254, 824.5874, 919.8837, 933.8156, 952.7748, 975.0733, 981.0583, 1000.1476, 1020.9794, 1094.8482, 1126.6398, 1140.4738, 1168.0175, 1208.2899, 1272.7923, 1278.3631, 1297.9258, 1343.92, 1350.6298, 1397.4681, 1401.2057, 1404.6278, 1420.1886, 1430.2874, 1471.4806, 1481.4577, 1487.9063, 1493.832, 1500.6531, 1504.4551, 1511.9914, 1512.9309, 2900.7525, 2995.3514, 3024.4398, 3034.3336, 3034.865, 3039.4472, 3078.1385, 3087.3881, 3099.2106, 3103.8642, 3110.2417, 3113.234, 3146.441, 3163.9564
IRC:	



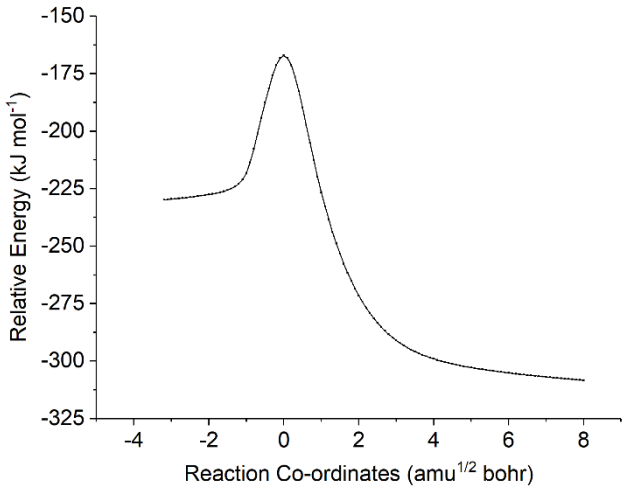
Compound: $iPrCHCMe_2 + O_3$ CPr_{DMFO} 1.3	**Energy (kJ mol^{-1}):** -500.122385192186
Reaction Coordinates: 6 2.889427 -0.222678 0.318605 6 1.423575 -0.529923 0.137027 6 -2.698685 0.038082 0.007238 6 -2.253383 -1.207135 -0.633565 1 -1.247238 -1.455295 -0.268305 1 -2.142969 -1.037853 -1.706513 1 -2.935681 -2.026214 -0.420887 6 -3.794291 0.107003 1.009267 1 -3.935214 1.124751 1.363960 1 -4.725248 -0.259020 0.569720 1 -3.564366 -0.546310 1.854439 1 0.829207 0.242319 -0.391357 1 3.338442 -1.066159 0.846056 6 3.036907 1.054000 1.159986 1 2.610241 0.927103 2.155411 1 4.091108 1.309281 1.274035 1 2.537333 1.898687 0.681829 6 3.546611 -0.062912 -1.060376 1 4.601856 0.188337 -0.947065 1 3.478387 -0.981521 -1.643795 1 3.071519 0.737405 -1.630975 8 -2.142739 1.141594 -0.265596 8 -1.101936 1.134838 -1.184170 8 0.881132 -1.540700 0.529059	**Frequencies (cm^{-1}):** 17.997, 23.7773, 43.5708, 48.9089, 84.7219, 92.7803, 99.8405, 157.2725, 207.0856, 228.2621, 241.1585, 285.0301, 312.6748, 332.7768, 349.2666, 362.086, 369.4749, 494.1998, 545.6884, 594.2158, 816.0457, 844.6458, 913.1819, 914.6117, 935.85, 938.2155, 970.6384, 989.0403, 996.4127, 1073.4082, 1099.1939, 1149.5405, 1180.5863, 1185.9172, 1307.1448, 1323.7547, 1345.8832, 1398.6401, 1400.3225, 1408.6369, 1416.4049, 1444.9111, 1450.7741, 1459.0266, 1470.5514, 1487.0453, 1489.8751, 1491.5541, 1504.8901, 1512.3676, 1562.2399, 1765.0888, 2899.4863, 2973.506, 3024.1812, 3025.2724, 3026.6817, 3046.436, 3059.7836, 3070.1193, 3085.7628, 3091.4801, 3092.5306, 3093.8049, 3132.7889, 3136.0249

Compound: $iPrCHCMe_2 + O_3$ TS_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -500.071981948728
Reaction Coordinates: 6 -1.650163 0.044057 0.296592 6 -0.423353 -0.471638 -0.495729 6 1.157578 0.524381 -0.001306 6 1.093945 0.682655 1.496852 1 2.087476 0.981104 1.843702 1 0.824783 -0.244818 1.989480 1 0.391746 1.464879 1.771911	**Frequencies (cm^{-1}):** -477.186, 77.0669, 86.0197, 141.6379, 177.6548, 195.4179, 223.4689, 234.2487, 248.98, 263.3514, 321.2703, 327.8648, 353.7062, 376.7076, 408.1218, 434.2736, 522.822, 535.4822, 623.1601, 649.2633, 787.2981, 837.2084, 908.9541, 934.957,

6 1.336346 1.768980 -0.830977 1 0.463711 2.411097 -0.761241 1 2.198545 2.336451 -0.473073 1 1.499432 1.511561 -1.875762 1 -0.443823 -0.169938 -1.558332 1 -1.433074 -0.070426 1.359211 6 -2.022743 1.496271 -0.004003 1 -2.095585 1.669482 -1.080488 1 -2.998064 1.727667 0.425870 1 -1.314176 2.214168 0.406394 6 -2.831016 -0.881077 -0.040443 1 -3.718206 -0.584006 0.521230 1 -3.076829 -0.828897 -1.103860 1 -2.592996 -1.915049 0.200712 8 2.007411 -0.429102 -0.455428 8 1.849702 -1.570224 0.191261 8 -0.076676 -1.686305 -0.259790	952.3219, 970.8741, 987.9967, 1000.7291, 1026.9948, 1097.2154, 1129.9278, 1143.8113, 1167.9972, 1189.9358, 1275.3809, 1279.429, 1310.961, 1333.9271, 1342.748, 1397.3151, 1402.6208, 1408.7535, 1420.3127, 1427.9879, 1473.5692, 1480.9665, 1490.1072, 1491.8858, 1496.0081, 1500.6997, 1509.197, 1515.6255, 2891.115, 3019.8263, 3024.863, 3028.6869, 3036.4295, 3051.1204, 3075.1273, 3084.4341, 3096.7447, 3106.233, 3114.7852, 3116.1087, 3148.1339, 3164.6568
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -500.127134953934
Reaction Coordinates: 6 2.213869 -0.111205 -0.354076 6 1.178814 -0.510876 0.669384 6 -2.254159 -0.021929 -0.179566 6 -2.596658 -0.025953 1.252760 1 -2.857170 0.989618 1.558577 1 -1.703214 -0.290453 1.822126 1 -3.398810 -0.727657 1.465191 6 -2.824124 -0.972011 -1.167018 1 -2.540254 -1.989351 -0.887330 1 -3.915109 -0.922808 -1.152332 1 -2.458560 -0.759600 -2.168156 1 1.268061 -0.001149 1.649468 1 1.819187 -0.396448 -1.331168 6 2.487466 1.394088 -0.311747 1 2.890625 1.688511 0.660272 1 3.224416 1.663960 -1.069332 1 1.573875 1.961184 -0.482713 6 3.488531 -0.930666 -0.077519 1 4.265152 -0.662764 -0.794812 1 3.878010 -0.727045 0.922582	**Frequencies (cm^{-1}):** 25.2482, 31.4077, 38.5771, 66.097, 78.0186, 87.1926, 150.1874, 153.6528, 157.9164, 214.2854, 233.2662, 293.6013, 311.2542, 320.0828, 339.6151, 364.8213, 367.6549, 480.2013, 546.5744, 595.1374, 812.7628, 845.8718, 903.8044, 916.0259, 929.3499, 939.0462, 964.0933, 978.7578, 988.4704, 1073.5852, 1096.7989, 1129.0417, 1181.8969, 1186.5562, 1306.4216, 1319.0425, 1338.494, 1385.5432, 1397.0523, 1405.3266, 1413.8224, 1428.9651, 1444.1218, 1458.589, 1470.2864, 1478.6056, 1488.7266, 1493.1665, 1502.2797, 1516.939, 1570.0738, 1772.238, 2889.4607, 3020.0885, 3023.0692, 3027.342, 3035.0695, 3043.9497, 3075.8787, 3077.4889, 3083.6251,

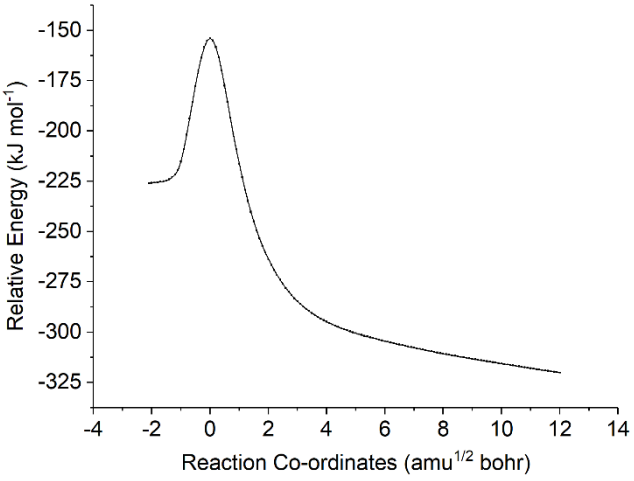
1 3.299357 -2.000933 -0.158947 8 -1.437062 0.823831 -0.640464 8 -0.835998 1.693746 0.260553 8 0.334561 -1.361796 0.501569	3085.0653, 3097.9716, 3111.7213, 3137.7133, 3139.0013

Compound: $iPrCHCMe_2 + O_3$ TS_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -500.072421952321
Reaction Coordinates: 6 -1.613862 0.303497 0.179073 6 -0.380571 -0.148710 -0.663744 6 1.161328 0.533138 0.161814 6 1.108762 0.169016 1.624537 1 2.094709 0.368056 2.053461 1 0.877228 -0.879548 1.767303 1 0.384131 0.784808 2.150706 6 1.328876 1.990711 -0.173515 1 0.431367 2.542825 0.101668 1 2.164484 2.418598 0.383618 1 1.510555 2.124881 -1.238108 1 -0.305507 0.424762 -1.602921 1 -1.345641 1.180993 0.772217 6 -2.709368 0.741931 -0.803418 1 -3.025451 -0.092765 -1.431161 1 -3.581841 1.104721 -0.257535 1 -2.367923 1.544804 -1.458308 6 -2.128346 -0.790023 1.112571 1 -1.369252 -1.135156 1.810575 1 -2.973940 -0.414224 1.690884 1 -2.459286 -1.656372 0.541144 8 2.003111 -0.219328 -0.597378 8 1.815657 -1.510737 -0.379644 8 -0.148086 -1.409152 -0.761409	**Frequencies (cm^{-1}):** -468.8294, 69.9601, 83.5466, 162.4342, 174.8974, 196.094, 202.543, 234.0363, 244.3457, 271.1151, 301.4603, 312.4394, 340.6927, 382.999, 395.7375, 425.2798, 529.4784, 608.7191, 629.581, 644.3865, 777.7042, 821.2586, 905.3799, 942.8821, 950.4471, 964.7296, 986.6206, 1003.016, 1047.9331, 1091.1513, 1118.0686, 1139.1364, 1191.9356, 1202.2983, 1276.6492, 1282.911, 1319.0373, 1343.1461, 1354.3946, 1401.2325, 1403.3469, 1409.6838, 1418.3709, 1435.0381, 1474.825, 1478.79, 1486.7251, 1488.8021, 1495.6582, 1499.7402, 1505.6081, 1509.6282, 2905.077, 3021.4644, 3023.2365, 3031.6685, 3038.1925, 3039.3135, 3085.0392, 3089.9928, 3097.9203, 3100.3187, 3114.7259, 3121.4946, 3125.064, 3173.2694
IRC:  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -500.124259822023
Reaction Coordinates:	**Frequencies (cm^{-1}):**

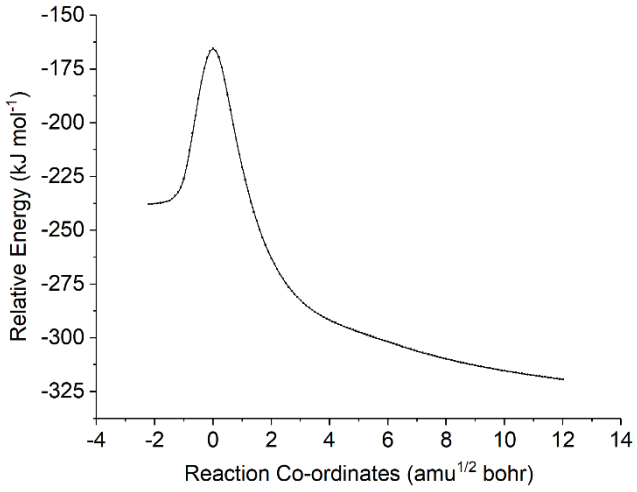
6 2.123726 -0.353472 0.069736 6 1.573618 0.816086 -0.704554 6 -2.364186 0.114129 0.001670 6 -3.532380 -0.758643 0.210934 1 -3.323993 -1.436757 1.043081 1 -3.647544 -1.412811 -0.657536 1 -4.435674 -0.182705 0.391451 6 -2.403284 1.598194 0.037296 1 -3.086317 1.969614 -0.731226 1 -2.798886 1.934455 0.998978 1 -1.412259 2.018154 -0.116874 1 1.481845 0.633903 -1.796124 1 1.349856 -1.126174 -0.042725 6 3.398473 -0.874216 -0.612387 1 4.214584 -0.154134 -0.524841 1 3.721243 -1.805307 -0.147297 1 3.233501 -1.073331 -1.672510 6 2.321988 -0.045625 1.549514 1 1.399292 0.310203 2.005092 1 2.644503 -0.940398 2.082456 1 3.078430 0.727865 1.691498 8 -1.232023 -0.400199 -0.225072 8 -1.139276 -1.782916 -0.263202 8 1.230509 1.877953 -0.241310	14.4891, 21.2726, 35.2289, 43.2848, 58.8272, 68.3785, 108.3498, 164.3416, 175.8775, 194.2761, 224.3244, 269.2932, 279.2299, 306.6837, 347.0984, 368.1928, 401.4177, 485.8981, 594.8197, 631.9608, 795.9861, 812.7106, 920.0257, 921.407, 931.9275, 932.1064, 948.4987, 975.5994, 989.3746, 1073.5879, 1097.6623, 1135.909, 1156.5968, 1203.8476, 1306.9287, 1323.7128, 1368.1208, 1392.7404, 1402.6293, 1410.9566, 1411.3325, 1432.5452, 1440.3432, 1457.4661, 1474.9388, 1476.2167, 1486.2944, 1490.8627, 1505.0435, 1508.7512, 1565.8231, 1781.2541, 2863.9563, 2973.5848, 3019.9088, 3023.4853, 3025.9787, 3034.2256, 3063.5348, 3065.6795, 3082.0888, 3090.9894, 3096.1639, 3106.9785, 3135.6667, 3140.3932

Compound: $iPrCHCMe_2 + O_3$ TS_{DMFO} 2.3	**Energy (kJ mol^{-1}):** -500.066795839265
Reaction Coordinates: 6 -1.766469 -0.217341 -0.394559 6 -0.288191 -0.411231 -0.855008 6 0.988521 0.607271 0.162316 6 0.671406 0.420317 1.624173 1 1.547158 0.741576 2.196303 1 0.467403 -0.615216 1.866160 1 -0.169125 1.042702 1.916852 6 1.109037 2.022144 -0.341169 1 0.160684 2.543584 -0.253740 1 1.846096 2.566879 0.253281 1 1.425108 2.036662 -1.382465 1 -0.110415 0.110985 -1.811761 1 -2.287256 -0.684552 -1.238326 6 -2.238497 1.235400 -0.358987 1 -1.934648 1.782558 -1.253315 1 -3.327961 1.269262 -0.313406 1 -1.865722 1.771589 0.514600 6 -2.177136 -1.005500 0.848499 1 -1.896765 -0.501951 1.772280 1 -3.261548 -1.124897 0.863687 1 -1.725465 -1.995714 0.845332 8 2.042665 -0.114589 -0.298365 8 1.955057 -1.382438 0.063344 8 0.169831 -1.609201 -0.775861	**Frequencies (cm^{-1}):** -495.6363, 69.6213, 100.52, 154.7337, 183.0207, 206.4045, 223.6152, 236.1763, 248.7624, 268.2419, 281.2969, 336.5263, 351.5232, 381.3227, 400.304, 490.8485, 507.3589, 539.8327, 638.715, 649.0084, 757.6566, 810.9272, 919.3114, 938.5082, 952.2078, 973.1992, 985.6012, 1003.7491, 1039.8187, 1088.8458, 1137.7089, 1143.521, 1185.7544, 1211.2596, 1273.1017, 1279.0107, 1320.7893, 1341.3197, 1358.4769, 1398.1285, 1402.113, 1410.5389, 1421.0847, 1436.3244, 1471.9642, 1481.1005, 1489.3929, 1493.5216, 1499.6349, 1508.8499, 1510.8068, 1518.8725, 2888.9119, 2986.0693, 3023.5227, 3024.8017, 3036.7874, 3040.0091, 3081.1475, 3084.6483, 3093.6675, 3105.4367, 3117.1616, 3122.8608, 3147.9095, 3177.8571
IRC:	



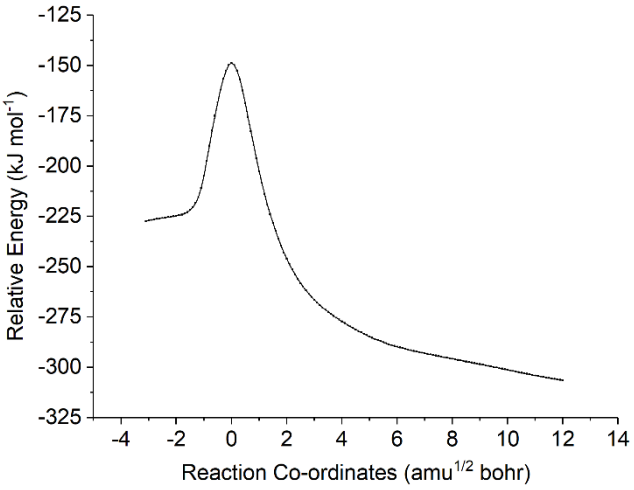
Compound: $iPrCHCMe_2 + O_3$ CPr_{DMFO} 2.3	**Energy (kJ mol^{-1}):** -500.125832022823
Reaction Coordinates: 6 -2.691871 0.167027 -0.332935 6 -1.189100 0.017371 -0.364028 6 2.391626 -0.188751 0.188959 6 2.701365 -0.416603 -1.232175 1 3.335421 0.396556 -1.592983 1 1.775056 -0.341577 -1.806043 1 3.166721 -1.386167 -1.386937 6 2.589509 -1.205604 1.251055 1 1.946897 -2.064344 1.041832 1 3.622242 -1.560576 1.248199 1 2.341439 -0.800898 2.228794 1 -0.621108 0.961250 -0.464188 1 -2.941520 0.633575 -1.295958 6 -3.073673 1.173724 0.766129 1 -2.521148 2.108407 0.664083 1 -4.137829 1.403389 0.715889 1 -2.864377 0.763618 1.755626 6 -3.425263 -1.162864 -0.205801 1 -3.192417 -1.644685 0.744465 1 -4.503804 -1.009950 -0.254195 1 -3.138252 -1.851524 -0.999343 8 1.916931 0.918817 0.566345 8 1.669774 1.878950 -0.410943 8 -0.597064 -1.036876 -0.283711	**Frequencies (cm^{-1}):** 17.274, 27.7281, 34.4582, 48.0621, 61.4965, 75.338, 115.0368, 153.3148, 158.6065, 199.5321, 229.3104, 274.4694, 284.3913, 308.6947, 345.338, 367.0033, 403.9287, 481.2934, 592.7389, 639.1293, 793.6342, 812.2531, 908.6225, 917.3767, 926.9215, 935.5493, 953.5336, 975.1232, 988.7548, 1071.9688, 1096.6657, 1131.518, 1164.3151, 1202.0956, 1303.3236, 1305.9453, 1358.0547, 1387.1315, 1403.5097, 1404.3155, 1419.3381, 1441.9909, 1451.8918, 1459.0231, 1470.9115, 1476.7442, 1486.8526, 1491.133, 1504.9349, 1509.7574, 1569.6274, 1765.8294, 2924.2893, 2973.5082, 3026.8061, 3027.6927, 3033.5845, 3035.715, 3076.2393, 3078.5658, 3089.2776, 3094.6394, 3098.2667, 3104.8448, 3136.7657, 3139.8181

Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 1	**Energy (kJ mol^{-1}):** -500.068262053231
Reaction Coordinates: 6 -1.461709 0.350608 -0.197709 6 -0.284725 -0.121977 0.649210 6 1.392419 0.302598 -0.159282 6 2.413962 0.106669 0.965845	**Frequencies (cm^{-1}):** -481.4162, 84.0977, 91.8708, 179.9365, 198.0151, 200.6185, 231.9471, 235.1189, 256.4753, 269.9332, 291.8698, 321.3273,

1 2.425423 -0.929758 1.293900 1 2.220397 0.756139 1.820707 1 3.405580 0.348078 0.578009 6 1.262599 1.764058 -0.615617 1 0.507377 1.878880 -1.387300 1 2.224545 2.048293 -1.044928 1 1.057617 2.436302 0.215569 1 -0.254526 0.259087 1.668174 1 -1.143583 0.414903 -1.237274 6 -2.618000 -0.662429 -0.124787 1 -2.975214 -0.779122 0.900135 1 -3.448816 -0.295765 -0.728307 1 -2.329505 -1.638062 -0.506128 6 -1.948660 1.722716 0.284002 1 -1.176838 2.487246 0.241914 1 -2.780523 2.058080 -0.335533 1 -2.309861 1.664220 1.313377 8 -0.012901 -1.443234 0.696773 8 0.091198 -1.932419 -0.528632 8 1.427029 -0.559594 -1.118427	370.2625, 383.5532, 411.2257, 465.745, 484.995, 565.2111, 596.8721, 697.8948, 804.197, 858.3296, 912.2048, 927.0302, 942.4135, 963.3563, 968.7725, 992.696, 1058.5784, 1065.9338, 1098.2219, 1127.1574, 1176.3397, 1183.4883, 1187.5908, 1198.4202, 1322.7995, 1342.3393, 1369.7385, 1393.4626, 1399.8376, 1406.0983, 1411.2366, 1432.2244, 1476.6139, 1486.0965, 1487.9644, 1495.923, 1497.4666, 1506.4185, 1509.3256, 1520.4549, 3028.2824, 3029.5043, 3032.2362, 3041.5389, 3067.5458, 3084.7733, 3085.1274, 3094.8, 3098.9383, 3108.1452, 3124.09, 3129.1503, 3130.6534, 3143.6853
IRC  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -500.123229909559
Reaction Coordinates: 6 -1.829302 0.554246 -0.292000 6 -1.290763 -0.127721 0.903600 1 -1.179673 0.364076 1.865085 8 -0.936726 -1.333440 0.939750 8 -1.004904 -2.072778 -0.228235 1 -1.223933 0.197944 -1.128764 6 -3.279604 0.079417 -0.541795 1 -3.940642 0.398049 0.265592 1 -3.643372 0.521749 -1.469343 1 -3.318727 -1.003519 -0.633536 6 -1.725664 2.073407 -0.152797 1 -2.099467 2.555386 -1.056140 1 -2.325115 2.436691 0.685188 1 -0.693308 2.384070 -0.000662 6 2.435591 0.211740 -0.062963 6 2.314071 -1.156732 -0.685406 1 1.287975 -1.518078 -0.657707	**Frequencies (cm^{-1}):** 15.6953, 33.0925, 47.6754, 62.3364, 69.5352, 77.8472, 84.4034, 114.2779, 150.9378, 201.1945, 214.6263, 234.6859, 278.4175, 337.0276, 392.8163, 409.5348, 498.1089, 538.604, 541.5551, 669.2494, 789.2977, 841.8158, 859.6544, 871.6625, 889.7857, 898.2679, 940.2435, 954.109, 975.4055, 1090.6197, 1112.3829, 1125.1761, 1175.5226, 1193.6934, 1243.1204, 1303.9092, 1320.9912, 1378.9565, 1387.8324, 1392.0116, 1400.487, 1420.567, 1462.0744, 1468.8427, 1474.8476, 1487.3731, 1494.524, 1499.6487, 1501.2636, 1517.6436, 1573.5063, 1762.1163,

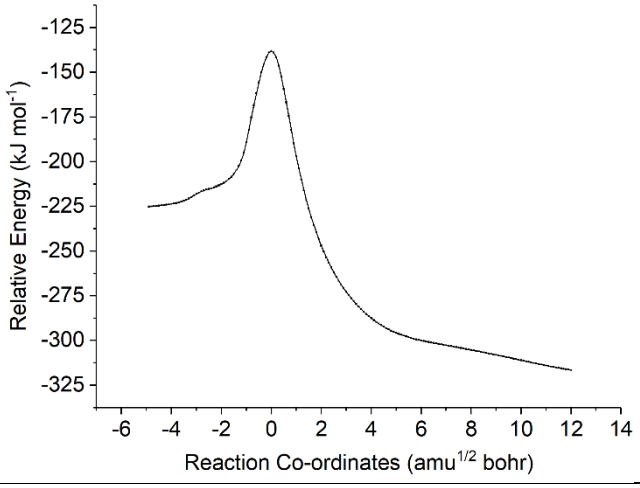
1 2.971051 -1.863227 -0.173358 1 2.659494 -1.110163 -1.721890 6 3.833341 0.771718 0.085094 1 3.795138 1.793175 0.453962 1 4.363418 0.737959 -0.868567 1 4.402936 0.153791 0.783202 8 1.466406 0.845674 0.305302	3017.3861, 3025.6979, 3031.1666, 3031.5407, 3044.5671, 3071.6854, 3083.9696, 3086.3412, 3094.1577, 3113.6004, 3120.6472, 3125.6497, 3136.6817, 3152.5093

Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 2	**Energy (kJ mol^{-1}):** -500.066213954739
Reaction Coordinates: 6 1.436251 0.615092 -0.229243 6 0.248396 -0.200428 -0.726430 6 -1.404894 0.305379 0.047577 6 -2.453156 -0.216640 -0.943383 1 -2.392409 -1.299229 -1.025331 1 -2.350527 0.229965 -1.933392 1 -3.443336 0.037159 -0.560575 6 -1.326204 1.841394 0.093551 1 -0.612395 2.184258 0.835798 1 -2.314007 2.204306 0.382270 1 -1.085725 2.270411 -0.878887 1 0.101437 -0.108859 -1.800999 1 1.219958 1.637100 -0.546835 6 2.675389 0.151657 -1.023195 1 3.529161 0.779875 -0.767361 1 2.520179 0.218192 -2.100912 1 2.930532 -0.879464 -0.777343 6 1.735296 0.630487 1.273162 1 0.850094 0.830950 1.869470 1 2.138630 -0.324057 1.602648 1 2.479811 1.403096 1.474680 8 0.122456 -1.505795 -0.418611 8 0.105803 -1.692404 0.891764 8 -1.357995 -0.294970 1.186165	**Frequencies (cm^{-1}):** -460.0688, 74.5295, 108.4249, 166.6766, 199.9193, 215.9657, 228.66, 251.9497, 256.6673, 261.7352, 272.0979, 316.1321, 367.4025, 387.5567, 416.4393, 456.1983, 488.3841, 556.2803, 601.8534, 726.8905, 801.9999, 823.3968, 907.9831, 918.129, 949.0882, 967.2588, 990.2745, 992.1108, 1058.5191, 1059.9501, 1097.3907, 1116.6333, 1160.0811, 1180.1905, 1200.8988, 1219.0603, 1330.3787, 1364.7292, 1370.4011, 1393.0153, 1404.639, 1406.3964, 1420.2337, 1443.4603, 1477.7713, 1485.3411, 1487.0939, 1493.6931, 1497.0142, 1501.2564, 1504.978, 1515.6145, 3027.7507, 3029.6423, 3034.8062, 3037.6912, 3040.4626, 3086.1254, 3090.465, 3093.8947, 3098.4555, 3103.9244, 3109.4, 3127.2386, 3139.4036, 3147.5646
IRC  	

Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -500.118357688853

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.080683 -0.879992 -0.149560 6 -1.229099 -0.032220 -1.026714 6 2.534282 -0.205632 -0.012512 6 2.242059 0.990637 0.860657 1 1.184172 1.241279 0.856123 1 2.829278 1.852858 0.539343 1 2.556063 0.764614 1.883670 6 3.991489 -0.506201 -0.286223 1 4.091352 -1.457032 -0.802790 1 4.564648 -0.520870 0.642563 1 4.415308 0.288446 -0.905102 1 -0.836662 -0.402449 -1.967625 1 -2.141851 -1.843095 -0.661628 6 -3.506835 -0.297320 -0.048988 1 -4.121780 -0.975472 0.543231 1 -3.968353 -0.195991 -1.031733 1 -3.485297 0.677318 0.431313 6 -1.459303 -1.121539 1.239560 1 -0.458062 -1.538944 1.151129 1 -1.405958 -0.192367 1.799596 1 -2.085873 -1.831960 1.780284 8 -0.893778 1.162494 -0.829532 8 -1.270497 1.795665 0.339763 8 1.653220 -0.902252 -0.474693	24.5521, 32.7713, 35.56, 54.5448, 71.4591, 76.68, 95.9597, 111.1639, 141.0605, 199.3674, 209.2241, 231.7209, 238.0842, 341.6722, 389.7899, 416.9106, 496.4191, 532.427, 539.0914, 740.6541, 786.2616, 797.8643, 855.4423, 866.6592, 888.5187, 899.4939, 944.1503, 966.4917, 973.7381, 1087.1571, 1101.7275, 1122.6367, 1126.2667, 1198.7375, 1239.9997, 1335.766, 1373.6813, 1387.2059, 1387.588, 1395.3244, 1398.7111, 1419.9976, 1462.2397, 1466.3041, 1474.9142, 1480.8502, 1491.884, 1493.3312, 1505.1668, 1526.0808, 1573.8247, 1764.6775, 3021.7578, 3030.8994, 3031.0287, 3036.2914, 3041.7423, 3075.2214, 3083.8592, 3093.0048, 3107.9704, 3134.4241, 3134.6034, 3136.9303, 3141.3789, 3162.5492

Compound: $iPrCHCMe_2 + O_3$ TS_{SYN} 3	**Energy (kJ mol^{-1}):** -500.062771247118
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.613477 -0.200771 -0.271594 6 0.180099 -0.219525 -0.821064 6 -1.170119 0.523144 0.234062 6 -2.381826 0.645234 -0.700128 1 -2.711636 -0.336514 -1.029528 1 -2.177890 1.271693 -1.569818 1 -3.197740 1.104780 -0.139222 6 -0.614079 1.899478 0.645907 1 0.207906 1.815722 1.346266 1 -1.427252 2.431039 1.142691 1 -0.309845 2.488494 -0.217718 1 0.088992 0.262931 -1.792189 1 2.027053 -1.100542 -0.746039 6 1.866153 -0.366214 1.232317 1 1.642350 0.538819 1.792694 1 1.283875 -1.178839 1.650554 1 2.926459 -0.580628 1.377790 6 2.387823 0.998648 -0.834821 1 2.060573 1.937620 -0.389685 1 3.449132 0.885360 -0.613364 1 2.283844 1.080639 -1.917967 8 -0.433703 -1.422164 -0.916930 8 -0.472784 -2.012441 0.265293 8 -1.272887 -0.352961 1.176320	-461.0477, 54.232, 93.7044, 178.5156, 183.9439, 199.0438, 211.2799, 232.687, 251.0008, 258.9887, 278.1869, 320.5225, 362.2752, 375.6822, 413.2658, 467.3043, 518.947, 545.3978, 580.8329, 685.7595, 806.4349, 851.2102, 906.3865, 931.1481, 942.9749, 966.7674, 988.0093, 991.944, 1055.0774, 1068.5416, 1085.375, 1146.8252, 1153.0952, 1178.855, 1194.295, 1212.1295, 1318.3241, 1346.433, 1367.5772, 1394.3539, 1405.7915, 1407.6633, 1409.6432, 1433.0077, 1476.4085, 1483.0153, 1490.1729, 1493.0785, 1497.4494, 1506.9714, 1509.3086, 1513.5409, 2973.1486, 3030.3957, 3032.0624, 3042.1619, 3044.864, 3085.9593, 3090.0437, 3098.5355, 3101.9952, 3105.609, 3107.068, 3132.7734, 3165.1651, 3173.0404
IRC	



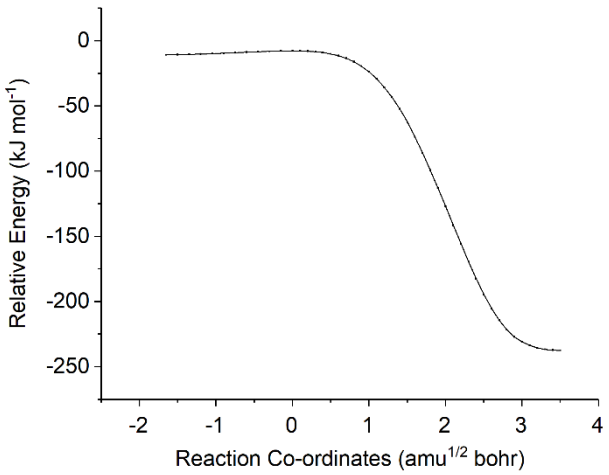
Compound: $iPrCHCMe_2 + O_3$ CPr_{SYN} 3	**Energy (kJ mol^{-1}):** -500.121175602241
Reaction Coordinates: 6 -2.292198 -0.277602 0.166078 6 -1.341785 0.182129 -0.869528 6 2.457346 -0.344803 -0.016746 6 2.374333 1.014816 0.634794 1 1.360888 1.406887 0.613758 1 3.053479 1.716397 0.146937 1 2.707734 0.929978 1.672866 6 3.845005 -0.895311 -0.261946 1 3.788341 -1.924512 -0.606058 1 4.450862 -0.834832 0.643978 1 4.347983 -0.287703 -1.018176 1 -1.017642 -0.440086 -1.696854 1 -2.934349 0.585946 0.368122 6 -1.551636 -0.602923 1.482700 1 -0.854053 -1.427364 1.342060 1 -1.006960 0.268181 1.836996 1 -2.285095 -0.888408 2.237202 6 -3.113671 -1.465095 -0.342019 1 -2.476356 -2.327642 -0.545948 1 -3.843074 -1.762732 0.410866 1 -3.658249 -1.220108 -1.254848 8 -0.832563 1.331219 -0.904949 8 -1.122493 2.211534 0.120086 8 1.467822 -0.975412 -0.328999	**Frequencies (cm^{-1}):** 21.6608, 25.8795, 31.0925, 47.0769, 71.8579, 72.7097, 91.4274, 103.0246, 137.507, 197.8939, 208.3724, 231.1948, 273.352, 338.7782, 388.7323, 409.3848, 495.659, 537.9287, 540.7916, 669.488, 785.7415, 842.0848, 851.4226, 877.785, 887.9959, 898.1869, 940.9245, 953.4296, 974.6768, 1086.3091, 1113.6974, 1122.2066, 1174.1187, 1193.3338, 1239.1454, 1307.6197, 1324.7563, 1379.9123, 1387.6935, 1393.8902, 1397.3693, 1422.1712, 1461.939, 1465.6463, 1474.4219, 1484.3829, 1490.9829, 1495.5498, 1502.6173, 1516.2136, 1572.5155, 1766.2766, 3015.9119, 3023.0509, 3027.6426, 3031.2524, 3040.6693, 3075.7965, 3084.0213, 3087.2277, 3098.523, 3105.9891, 3133.7071, 3137.0306, 3138.1189, 3163.4736

6.11 Ozonolysis of 2,4,4-trimethyl-2-pentene (Alkene 9)

Compound: $tBuCHCMe_2 + O_3$ PRC1	**Energy (kJ mol^{-1}):** -539.265745943092
Reaction Coordinates: 6 -1.644468 -0.549744 -0.088818 6 -0.420617 0.188677 -0.618756 6 0.114081 1.379140 -0.282475	**Frequencies (cm^{-1}):** 23.5497, 27.0865, 52.1706, 63.276, 72.898, 104.4801, 134.0495, 161.6554, 189.8, 202.7545, 224.1315, 236.5571,

6 1.316165 1.892010 -1.024629 1 1.110556 2.871959 -1.464366 1 2.162782 2.032168 -0.344745 1 1.626701 1.218470 -1.821171 6 -0.381028 2.307985 0.789253 1 0.388336 2.439636 1.555221 1 -0.569936 3.298882 0.367158 1 -1.288026 1.972026 1.278102 1 0.072809 -0.321908 -1.440114 6 -1.724088 -1.902765 -0.820978 1 -1.811237 -1.761134 -1.899900 1 -2.592682 -2.471402 -0.485859 1 -0.832585 -2.501918 -0.630543 6 -1.561776 -0.835886 1.424081 1 -0.670445 -1.415658 1.659053 1 -1.536053 0.072614 2.022315 1 -2.434648 -1.412482 1.737161 6 -2.929293 0.245965 -0.405762 1 -3.016770 0.433480 -1.476849 1 -3.807731 -0.321148 -0.090300 1 -2.952836 1.208261 0.103560 8 1.759711 -0.554546 1.054341 8 2.803442 -0.609437 0.343643 8 2.879086 -1.547785 -0.510512	253.3059, 289.6774, 309.8088, 326.7049, 355.0153, 377.5504, 429.1205, 447.8513, 501.0525, 564.4954, 732.6551, 763.1567, 823.6631, 860.1496, 927.5884, 931.6965, 948.1554, 960.3492, 964.695, 1003.8433, 1049.0301, 1052.8213, 1096.9679, 1102.3413, 1149.301, 1170.2271, 1183.4046, 1220.7054, 1254.0176, 1273.3372, 1392.2059, 1398.5246, 1402.5877, 1412.3159, 1422.2824, 1434.7596, 1471.6078, 1478.5623, 1481.6579, 1489.6815, 1491.5657, 1492.3093, 1497.0071, 1507.2385, 1509.4523, 1522.267, 1664.889, 3004.7658, 3017.4938, 3019.769, 3023.872, 3033.3399, 3043.5817, 3052.4394, 3078.9743, 3084.3854, 3089.2383, 3095.3166, 3101.4159, 3105.6899, 3116.2226, 3121.2693, 3155.803

Compound: $tBuCHCMe_2 + O_3$ TS_{OZO} 1	**Energy (kJ mol^{-1}):** -539.256954633627
Reaction Coordinates: 6 -1.578478 -0.037448 -0.043717 6 -0.200049 0.182165 -0.650181 6 0.834935 1.002310 -0.255201 6 1.966772 1.220213 -1.224944 1 2.105478 0.363613 -1.883512 1 2.903997 1.415912 -0.706039 1 1.754113 2.089105 -1.856357 6 0.805101 1.959815 0.902257 1 1.783128 2.011399 1.379618 1 0.070148 1.705844 1.656209 1 0.576513 2.964607 0.533081 1 -0.106372 -0.209681 -1.656563 6 -2.280728 -1.139599 -0.859240 1 -3.294985 -1.297283 -0.490410 1 -1.741709 -2.083541 -0.786438 1 -2.347321 -0.866829 -1.914349 6 -1.563130 -0.473808 1.433825 1 -1.181285 0.295823 2.100467 1 -0.956741 -1.365493 1.569280 1 -2.584099 -0.697602 1.748738 6 -2.393912 1.268389 -0.193261 1 -2.445768 1.585134 -1.236268 1 -1.964892 2.084314 0.386835 1 -3.414905 1.107243 0.158709 8 1.950971 -0.633630 0.974591 8 1.949601 -1.536339 0.053333 8 0.762132 -1.954379 -0.235453	**Frequencies (cm^{-1}):** -154.5626, 58.096, 79.6197, 102.6513, 126.5792, 146.5512, 161.3784, 173.9659, 186.2558, 193.7456, 231.4053, 247.0458, 283.054, 305.6357, 329.7352, 342.2766, 377.8088, 410.4105, 442.6905, 458.0767, 551.2908, 568.0049, 737.0809, 760.6, 817.6705, 874.633, 926.5463, 928.1873, 945.2539, 953.2571, 966.2232, 1009.3663, 1043.3984, 1051.4435, 1073.0755, 1079.2551, 1088.7215, 1119.9448, 1182.6554, 1215.25, 1253.7168, 1277.4695, 1388.6686, 1396.7039, 1402.3193, 1408.1939, 1421.2918, 1430.8371, 1470.6831, 1479.2151, 1482.9469, 1486.0857, 1490.4377, 1491.7719, 1498.3092, 1507.8178, 1509.6354, 1522.7248, 1572.9182, 3009.9294, 3018.1838, 3021.1309, 3025.9216, 3039.5454, 3074.9543, 3078.2198, 3081.9444, 3084.7541, 3099.7867, 3102.5979, 3105.4176, 3112.2188, 3133.7127, 3138.3895, 3167.4627
IRC:	

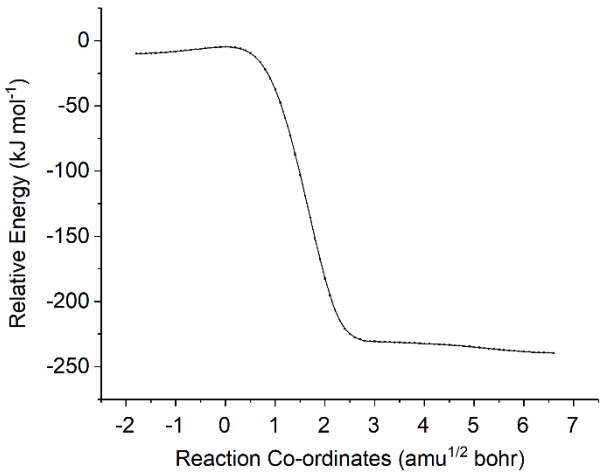


Compound: $tBuCHCMe_2 + O_3$ POZ1	**Energy (kJ mol^{-1}):** -539.357798672299
Reaction Coordinates: 6 1.520244 0.092091 -0.038106 6 0.075647 -0.330414 -0.402213 6 -1.226627 0.486443 -0.015529 6 -1.821614 1.140277 -1.261072 1 -2.751170 1.651817 -1.013596 1 -1.129770 1.871580 -1.682681 1 -2.031330 0.388663 -2.020945 6 -1.173441 1.461350 1.155244 1 -2.183913 1.817515 1.358093 1 -0.802195 0.980098 2.054665 1 -0.558080 2.329293 0.926328 1 0.048113 -0.428985 -1.492085 6 1.797584 0.160105 1.473078 1 1.446605 -0.736978 1.981334 1 2.873448 0.238285 1.637369 1 1.336163 1.024547 1.943469 6 2.457221 -0.969912 -0.652834 1 2.282605 -1.080615 -1.724565 1 3.497135 -0.672567 -0.511242 1 2.315580 -1.943919 -0.187004 6 1.831479 1.444131 -0.700163 1 1.679127 1.402793 -1.780324 1 2.876030 1.705575 -0.525298 1 1.221772 2.254257 -0.302348 8 -2.110851 -0.565604 0.457235 8 -1.573063 -1.775697 -0.111362 8 -0.176471 -1.621922 0.152676	**Frequencies (cm^{-1}):** 54.7313, 81.5257, 186.2241, 197.1281, 219.7587, 234.5228, 242.4183, 262.4339, 269.9165, 279.8438, 305.5961, 319.4592, 353.2745, 360.7425, 383.1867, 419.6713, 466.1317, 494.9815, 547.6901, 609.6174, 697.8755, 756.5622, 777.088, 811.5459, 856.9015, 928.4238, 932.8798, 939.0355, 943.6535, 952.5398, 969.0177, 991.3728, 1014.8152, 1023.7222, 1054.8785, 1082.9622, 1167.554, 1188.6298, 1228.8164, 1241.0925, 1260.1366, 1278.5925, 1363.3752, 1394.5838, 1402.6817, 1404.4827, 1405.3334, 1426.1329, 1439.2985, 1480.1545, 1483.2597, 1490.0747, 1492.3556, 1495.3892, 1498.5639, 1507.3223, 1511.2106, 1518.4392, 1527.4549, 3000.0535, 3025.3325, 3029.7809, 3033.9887, 3041.3085, 3050.1698, 3082.1625, 3087.2705, 3096.7462, 3097.0816, 3100.0784, 3107.427, 3109.1137, 3112.4874, 3126.6405, 3147.4868

Compound: $tBuCHCMe_2 + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -539.265526918345
Reaction Coordinates: 6 -1.632890 -0.363740 -0.038094 6 -0.429763 0.310868 -0.690752 6 0.324803 1.353600 -0.291209 6 1.418373 1.871464 -1.183497 1 1.234294 2.918002 -1.444902 1 2.382368 1.837189 -0.670266	**Frequencies (cm^{-1}):** 30.9442, 37.6476, 52.1308, 54.9747, 74.6594, 101.6515, 140.0704, 162.633, 186.5701, 205.0574, 222.9856, 232.3392, 254.2087, 289.3297, 310.2149, 326.1317, 354.682, 377.6114, 427.0166, 447.4998,

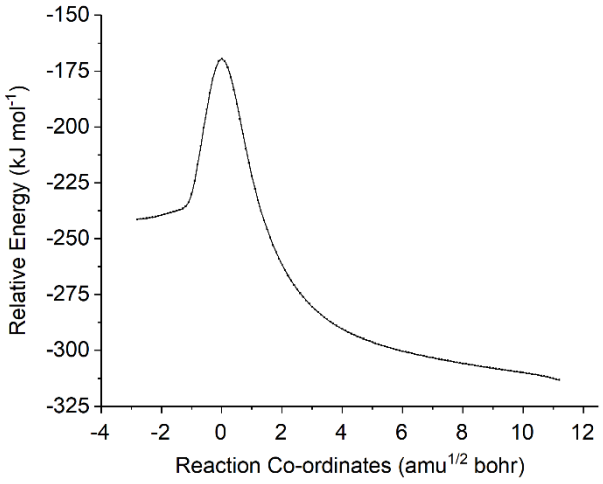
1 1.503404 1.295242 -2.102313 6 0.151483 2.147781 0.974412 1 1.106866 2.238749 1.495350 1 -0.166968 3.165965 0.730913 1 -0.571403 1.727777 1.664577 1 -0.179903 -0.090968 -1.666889 6 -2.105296 -1.488740 -0.978040 1 -2.391733 -1.090518 -1.953151 1 -2.970370 -2.004617 -0.558701 1 -1.315719 -2.225390 -1.135074 6 -1.285835 -0.998771 1.323892 1 -0.510026 -1.756657 1.214991 1 -0.936485 -0.267384 2.049706 1 -2.168488 -1.487643 1.741639 6 -2.796493 0.636579 0.131082 1 -3.064304 1.084684 -0.826758 1 -3.678208 0.123127 0.520934 1 -2.550028 1.443510 0.818775 8 2.420046 -0.407536 0.965862 8 2.162480 -1.524162 0.431266 8 1.968776 -1.533967 -0.817827	512.2073, 563.7791, 737.5549, 761.8683, 822.7831, 853.1217, 927.0167, 930.5099, 947.4473, 960.2709, 962.8428, 1007.7204, 1048.6469, 1050.061, 1099.5815, 1103.2451, 1161.5029, 1178.8357, 1181.4919, 1219.9116, 1253.0953, 1271.5368, 1390.5746, 1398.3699, 1401.8715, 1411.438, 1421.0428, 1434.0506, 1470.4054, 1480.4365, 1481.4603, 1488.3906, 1489.4895, 1490.811, 1497.8706, 1507.4661, 1509.1625, 1521.3878, 1658.9915, 3009.2608, 3017.7663, 3019.1038, 3023.7565, 3031.1639, 3053.7751, 3060.1983, 3078.6436, 3083.6565, 3083.9951, 3089.8689, 3106.6494, 3111.7127, 3112.3438, 3130.3894, 3151.8273

Compound: $tBuCHCMe_2 + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -539.256271387596
Reaction Coordinates: 6 -1.556663 0.034326 -0.034528 6 -0.181899 0.245852 -0.660636 6 0.906603 0.971816 -0.211011 6 1.977901 1.322431 -1.205159 1 1.979845 0.638888 -2.051318 1 2.964580 1.302109 -0.743414 1 1.814114 2.337744 -1.581847 6 0.963707 1.758503 1.070717 1 1.984074 1.799940 1.448299 1 0.326749 1.364436 1.854305 1 0.653123 2.789692 0.873315 1 -0.153662 0.012147 -1.717130 6 -2.373067 -0.862198 -0.983516 1 -3.380131 -1.013784 -0.592808 1 -1.899529 -1.837018 -1.097399 1 -2.463372 -0.409476 -1.972845 6 -1.537555 -0.639461 1.350960 1 -0.981308 -0.074845 2.095694 1 -1.110826 -1.638507 1.296620 1 -2.562566 -0.733551 1.713935 6 -2.266740 1.404780 0.067615 1 -2.302159 1.903691 -0.902178 1 -1.770460 2.070000 0.772433 1 -3.294344 1.262849 0.408264 8 2.210054 -0.794364 0.571826 8 1.347270 -1.755064 0.529464 8 0.767945 -1.849398 -0.622612	**Frequencies (cm^{-1}):** -182.0827, 54.5369, 66.171, 129.4737, 139.6262, 162.4678, 180.2883, 190.7544, 202.8194, 211.4033, 224.3888, 256.0198, 285.4569, 307.5131, 330.5054, 338.9148, 378.8596, 411.6041, 448.2256, 460.3677, 558.2471, 579.3681, 736.8611, 758.9415, 818.455, 882.8058, 925.2355, 927.9553, 945.6943, 953.49, 966.0294, 1012.7119, 1044.7666, 1049.0199, 1073.4436, 1075.9417, 1087.6856, 1121.045, 1182.8916, 1214.7134, 1254.4116, 1275.302, 1385.4988, 1397.3856, 1401.868, 1409.4216, 1420.8972, 1432.1767, 1469.601, 1474.791, 1482.2913, 1485.7805, 1491.0804, 1492.2271, 1498.1131, 1507.0724, 1511.5601, 1523.947, 1559.8969, 3007.648, 3014.701, 3021.6328, 3026.0458, 3040.6844, 3076.694, 3078.759, 3084.8869, 3087.0346, 3099.735, 3102.6927, 3104.9281, 3120.4962, 3126.5482, 3153.234, 3157.747
IRC:	



Compound: $tBuCHCMe_2 + O_3$ POZ 2	**Energy (kJ mol^{-1}):** -539.357832299616
Reaction Coordinates: 6 1.504174 0.113384 0.003509 6 0.090722 -0.215603 -0.548228 6 -1.223360 0.474428 -0.039085 6 -1.660360 1.624919 -0.937027 1 -2.650730 1.971474 -0.643560 1 -0.969224 2.461168 -0.846156 1 -1.696361 1.311963 -1.979307 6 -1.302538 0.852251 1.437060 1 -2.312910 1.202288 1.648654 1 -1.095210 -0.001385 2.075541 1 -0.610410 1.654406 1.685189 1 0.125559 -0.024053 -1.624825 6 1.709597 -0.295208 1.470348 1 1.383256 -1.320689 1.638618 1 2.771292 -0.237952 1.715744 1 1.182031 0.352389 2.165963 6 2.501341 -0.688205 -0.859831 1 3.524676 -0.465335 -0.554583 1 2.341580 -1.760690 -0.753545 1 2.403973 -0.434892 -1.917308 6 1.799274 1.609643 -0.185648 1 2.836406 1.817158 0.081933 1 1.662387 1.916158 -1.224720 1 1.169384 2.240928 0.440715 8 -2.165132 -0.591648 -0.301307 8 -1.486294 -1.722143 0.219553 8 -0.170923 -1.628284 -0.412613	**Frequencies (cm^{-1}):** 51.0782, 94.5258, 186.5379, 202.5518, 211.9824, 245.5409, 248.5029, 256.5475, 274.5599, 283.5052, 296.9066, 307.8899, 324.2383, 364.6322, 386.0471, 401.5335, 475.9873, 516.099, 540.6345, 615.3699, 694.9578, 748.6247, 770.9239, 821.9376, 867.4428, 919.7046, 930.1384, 940.5628, 944.9789, 949.1961, 967.5352, 992.9131, 999.1402, 1027.7963, 1055.043, 1062.4796, 1174.5989, 1200.9098, 1235.5174, 1244.0955, 1255.5219, 1271.6656, 1353.7676, 1391.5798, 1401.3038, 1403.7077, 1407.0454, 1425.0451, 1437.6446, 1481.1113, 1484.0114, 1489.3225, 1492.6268, 1496.2037, 1499.9662, 1508.8784, 1513.2251, 1518.6218, 1527.1226, 3005.9437, 3022.1232, 3026.7116, 3040.7109, 3045.393, 3051.8436, 3079.4364, 3084.6288, 3092.8585, 3096.331, 3102.6909, 3108.464, 3113.9793, 3121.0409, 3127.2425, 3143.0158

Compound: $tBuCHCMe_2 + O_3$ TS_{ANTI}	**Energy (kJ mol^{-1}):** -539.327032833075
Reaction Coordinates: 6 -1.540215 -0.155755 -0.027950 6 -0.159816 0.403136 -0.384328 6 1.525252 -0.457664 0.016289 6 1.681560 -1.452642 -1.143261	**Frequencies (cm^{-1}):** -477.3822, 73.794, 77.5295, 175.8847, 188.591, 208.3787, 216.5621, 231.0017, 241.3669, 251.2152, 269.3275, 282.4735,

1 0.892698 -2.200318 -1.172844 1 2.633042 -1.971348 -1.014008 1 1.720427 -0.922274 -2.092893 6 1.416029 -1.088217 1.406598 1 0.668738 -1.878008 1.458407 1 1.197887 -0.327696 2.152778 1 2.384414 -1.528364 1.653253 1 0.039448 0.463635 -1.451122 6 -2.554795 0.716296 -0.807657 1 -3.567010 0.352385 -0.625743 1 -2.372473 0.676507 -1.882680 1 -2.504324 1.757976 -0.492160 6 -1.859189 -0.060194 1.472517 1 -1.206651 -0.690800 2.071408 1 -1.770562 0.961750 1.837294 1 -2.885652 -0.388315 1.641117 6 -1.688448 -1.606808 -0.508263 1 -1.050222 -2.292068 0.046260 1 -2.720538 -1.927463 -0.362790 1 -1.459021 -1.706472 -1.569932 8 2.330138 0.553885 -0.052033 8 1.198006 2.118578 -0.243541 8 0.106546 1.556532 0.253073	299.1787, 341.2072, 354.7064, 381.1608, 422.5781, 440.5439, 482.9363, 509.3246, 566.091, 603.2183, 617.9604, 769.0503, 797.4205, 905.262, 913.3312, 938.4944, 948.7907, 969.7748, 991.9959, 1024.535, 1038.5257, 1054.8993, 1065.1038, 1114.9027, 1151.8488, 1188.6723, 1207.2784, 1230.0709, 1252.7153, 1283.2772, 1358.0867, 1372.0879, 1388.6172, 1400.1263, 1404.9052, 1409.1667, 1440.197, 1477.0628, 1481.1232, 1486.4694, 1493.0681, 1493.4215, 1495.0816, 1504.1499, 1508.8781, 1512.8288, 1526.4713, 3025.9577, 3033.8963, 3034.496, 3040.3172, 3044.8798, 3086.7591, 3091.9852, 3093.5652, 3100.3468, 3101.2156, 3104.6114, 3105.697, 3111.5835, 3128.8333, 3129.2424, 3133.4551
IRC:  	

Compound: $tBuCHCMe_2 + O_3$ C_{ANTI}	**Energy (kJ mol^{-1}):** -539.384267927067
Reaction Coordinates: 6 -2.100740 -0.194484 -0.001364 6 -0.835957 0.447290 -0.468939 6 2.411503 -0.574374 0.022534 6 2.897263 -0.130974 1.381323 1 2.741645 0.945695 1.464387 1 3.965502 -0.323742 1.495964 1 2.341115 -0.638723 2.165329 6 3.250292 -0.161705 -1.161940 1 3.437067 0.911270 -1.135197 1 2.751383 -0.426683 -2.090033 1 4.217892 -0.668669 -1.113713 1 -0.391178 0.206188 -1.429981	**Frequencies (cm^{-1}):** 22.8809, 32.8118, 64.0477, 66.774, 77.6082, 91.8327, 102.7135, 120.0675, 138.4211, 192.0999, 206.5667, 227.2571, 263.2604, 265.8178, 330.1897, 340.728, 353.1951, 385.0515, 460.8436, 463.2049, 485.1919, 536.2985, 554.9666, 775.4154, 788.3248, 891.6386, 898.2931, 902.1882, 922.0936, 928.9479, 958.8792, 961.6558, 974.5545, 1045.8639, 1066.9774, 1087.0046, 1117.2707, 1211.9628,

6 -3.219112 0.272603 -0.964632 1 -4.150129 -0.231860 -0.703468 1 -2.983876 0.027694 -2.001098 1 -3.380154 1.348266 -0.893066 6 -2.440473 0.193987 1.441090 1 -1.656938 -0.121958 2.128794 1 -2.568076 1.270522 1.547880 1 -3.370662 -0.291170 1.737361 6 -1.921596 -1.722839 -0.128624 1 -1.116467 -2.078582 0.510980 1 -2.850823 -2.216487 0.158269 1 -1.685308 -2.011421 -1.153201 8 1.413369 -1.259279 -0.106467 8 0.903413 1.883363 -0.289989 8 -0.260291 1.316246 0.220720	1229.2461, 1242.393, 1298.3924, 1365.166, 1380.2487, 1388.2558, 1400.1004, 1408.9062, 1435.8529, 1458.0846, 1468.3542, 1470.6594, 1478.8787, 1487.8279, 1488.6113, 1489.3635, 1501.8179, 1503.2288, 1520.0283, 1573.6085, 1750.3308, 3027.3763, 3027.8123, 3033.9305, 3035.6951, 3040.4023, 3092.4703, 3092.8327, 3096.9914, 3097.8043, 3099.6937, 3104.0914, 3109.9575, 3121.8062, 3132.5351, 3140.1558, 3150.1772

Compound: $tBuCHCMe_2 + O_3$ TS_{DMFO} 1	**Energy (kJ mol^{-1}):** -539.333201921061
Reaction Coordinates: 6 -1.559433 0.107331 -0.017397 6 -0.213417 -0.313093 -0.676451 1 -0.097493 0.114448 -1.688109 8 0.102828 -1.563541 -0.596582 6 -2.622827 -0.786473 -0.694098 1 -3.613134 -0.553192 -0.299153 1 -2.646430 -0.626178 -1.774276 1 -2.413369 -1.839339 -0.513818 6 -1.915117 1.569950 -0.318137 1 -1.781496 1.802480 -1.377875 1 -2.964176 1.751565 -0.079409 1 -1.327689 2.277601 0.261915 6 -1.576449 -0.166843 1.491022 1 -2.585834 -0.029412 1.882963 1 -1.267710 -1.190552 1.699382 1 -0.914418 0.501542 2.040314 6 1.364081 0.486269 -0.053608 6 1.286719 1.926320 0.384353 1 0.872265 2.542686 -0.409344 1 0.685205 2.045432 1.281063 1 2.295371 2.289671 0.594131 6 2.349704 0.213319 -1.168925 1 2.235664 -0.785789 -1.573389 1 3.361939 0.316192 -0.770377 1 2.217171 0.950048 -1.959443 8 1.467019 -0.321365 1.042753 8 1.588223 -1.588579 0.679438	**Frequencies (cm^{-1}):** -453.8957, 62.2583, 109.2404, 175.3298, 180.4832, 212.6275, 224.9261, 245.8047, 252.6287, 264.0732, 270.8779, 290.9924, 319.0619, 339.8559, 360.9034, 374.7008, 395.2826, 411.5103, 465.8846, 544.3341, 568.4464, 647.9159, 683.8495, 749.9751, 801.1489, 876.9394, 930.6561, 942.5147, 953.5123, 965.302, 981.02, 999.5584, 1015.5781, 1044.5512, 1051.1292, 1116.1606, 1150.9483, 1219.5385, 1236.9242, 1259.2227, 1271.9702, 1276.5786, 1298.0377, 1384.5961, 1396.347, 1401.3272, 1404.6069, 1420.7614, 1437.0048, 1470.6628, 1479.0805, 1485.2025, 1487.8637, 1491.4591, 1496.859, 1504.6547, 1508.0825, 1515.8569, 1522.0503, 2898.828, 3018.9973, 3024.332, 3033.5938, 3034.1468, 3039.3361, 3073.2651, 3079.0515, 3089.7142, 3102.4333, 3106.852, 3108.3556, 3111.5422, 3119.9597, 3146.2134, 3163.7718
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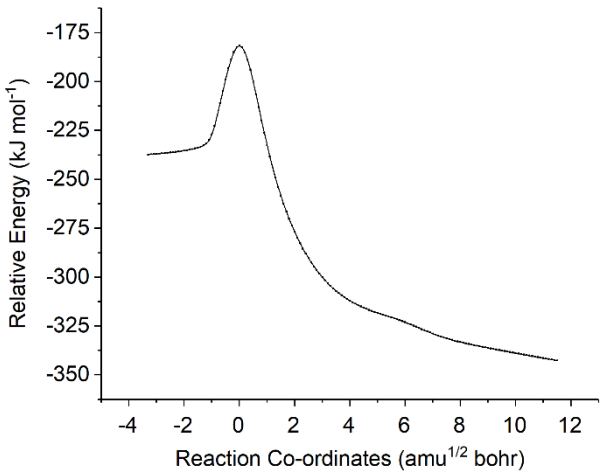
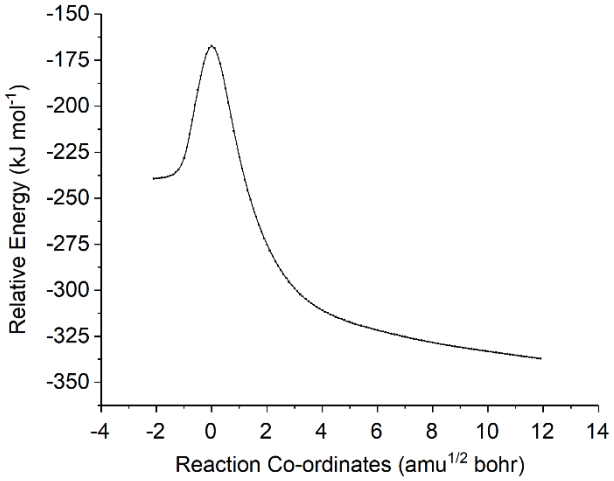
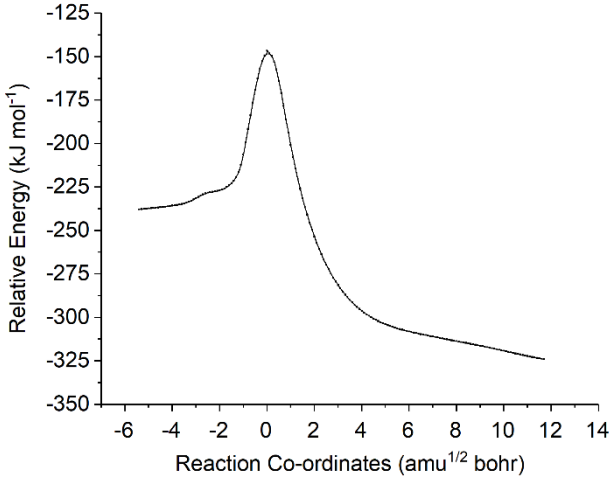


Compound: $tBuCHCMe_2 + O_3$ CPr_{DMFO} 1	**Energy (kJ mol^{-1}):** -539.386089436056
Reaction Coordinates: 6 -2.425526 -0.018182 0.014799 6 -0.918651 -0.059875 -0.164668 6 2.696933 -0.178116 0.067026 6 3.020860 -1.468331 0.723969 1 2.835381 -1.418081 1.793726 1 2.399345 -2.253206 0.285988 1 4.063793 -1.735435 0.540975 6 2.902649 0.086429 -1.366588 1 3.474324 1.010546 -1.479332 1 1.932100 0.285656 -1.826237 1 3.392019 -0.749553 -1.858712 1 -0.402135 0.904331 0.005496 6 -2.964966 1.033978 -0.974655 1 -4.037489 1.167304 -0.825370 1 -2.483183 2.002224 -0.829762 1 -2.803592 0.724679 -2.008282 6 -2.690132 0.454743 1.458337 1 -2.198744 1.407129 1.663042 1 -3.761760 0.588870 1.613408 1 -2.332046 -0.275338 2.185473 6 -3.057225 -1.385859 -0.239759 1 -4.138729 -1.332766 -0.105631 1 -2.853917 -1.731074 -1.253209 1 -2.663244 -2.135233 0.446392 8 2.207521 0.714618 0.814045 8 1.844274 1.920792 0.221456 8 -0.277516 -1.041507 -0.467843	**Frequencies (cm^{-1}):** 17.2979, 22.8032, 35.3498, 43.503, 60.9597, 73.0904, 100.0733, 153.6927, 158.7598, 196.2318, 242.7639, 247.2562, 275.5636, 284.0457, 308.689, 326.5983, 348.028, 366.9551, 388.8633, 405.2265, 481.5998, 592.7604, 594.0371, 762.8467, 812.2487, 878.8721, 909.0483, 927.2355, 929.6802, 950.91, 968.7064, 975.5163, 988.7815, 1056.1143, 1071.9655, 1088.6752, 1096.6944, 1228.0941, 1236.0747, 1294.6373, 1305.9418, 1387.4046, 1397.171, 1403.102, 1403.8518, 1422.9509, 1441.9525, 1452.9188, 1459.0625, 1470.889, 1476.7098, 1479.7185, 1486.6395, 1489.2461, 1499.6033, 1507.6607, 1520.0178, 1569.548, 1765.8735, 2917.0812, 3021.7958, 3024.2491, 3026.9097, 3033.5942, 3033.8071, 3076.4121, 3078.5359, 3086.4394, 3088.1301, 3088.8148, 3091.1404, 3095.2828, 3102.47, 3136.7388, 3139.921

Compound: $tBuCHCMe_2 + O_3$ TS_{DMFO} 2	**Energy (kJ mol^{-1}):** -539.326403788511
Reaction Coordinates: 6 -1.587253 0.071811 0.011905 6 -0.228285 -0.428369 -0.609920 6 1.341519 0.523091 -0.011397 6 1.553972 1.806890 -0.779421	**Frequencies (cm^{-1}):** -473.749, 71.1381, 88.826, 145.1644, 180.8624, 204.8006, 225.2504, 230.1856, 242.6057, 260.2243, 281.3929, 311.4431,

1 1.688276 1.602184 -1.847609 1 0.703860 2.481492 -0.649815 1 2.451939 2.320270 -0.404824 6 1.297148 0.614307 1.496702 1 2.317909 0.844234 1.841062 1 0.984291 -0.323842 1.955195 1 0.639860 1.429082 1.813475 1 -0.148853 -0.105118 -1.671080 6 -2.649124 -0.608146 -0.890191 1 -3.656867 -0.286937 -0.590832 1 -2.509239 -0.340157 -1.947094 1 -2.588288 -1.700163 -0.804669 6 -1.769175 1.591626 -0.103129 1 -1.573122 1.945083 -1.125642 1 -2.807423 1.857682 0.139533 1 -1.124402 2.146165 0.589690 6 -1.806591 -0.403112 1.455771 1 -2.870364 -0.306711 1.714175 1 -1.520615 -1.455648 1.563937 1 -1.242786 0.188414 2.184583 8 2.189289 -0.422625 -0.504291 8 2.026645 -1.581648 0.106303 8 0.076885 -1.658804 -0.374762	323.0625, 343.1809, 356.446, 388.8726, 392.508, 399.1523, 470.5705, 531.2167, 559.3571, 636.9642, 647.0485, 743.2231, 804.5353, 858.2963, 930.708, 945.5949, 947.8582, 961.2478, 979.4863, 993.5743, 1031.8814, 1033.7028, 1042.2973, 1150.4023, 1162.6698, 1211.1718, 1239.0388, 1247.7556, 1272.5574, 1281.5447, 1333.0739, 1379.2447, 1381.6098, 1386.7138, 1394.7887, 1401.9776, 1425.4645, 1452.8894, 1459.5414, 1462.2986, 1469.3594, 1473.1037, 1478.2628, 1483.6943, 1494.1374, 1498.1589, 1508.816, 2888.4072, 3023.5053, 3028.7236, 3033.835, 3041.6468, 3045.2088, 3088.5583, 3094.6876, 3105.8198, 3109.7537, 3117.2438, 3117.7991, 3128.0863, 3139.7508, 3164.5241, 3192.5219
IRC  	

Compound: $tBuCHCMe_2 + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -539.321133713651
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.438273 0.245843 -0.061044 6 0.107187 -0.209754 -0.700605 1 0.028495 0.090043 -1.744129 8 -0.234201 -1.516831 -0.643497 8 -0.326074 -1.929025 0.609983 6 2.499238 -0.745953 -0.603273 1 3.485063 -0.434468 -0.256340 1 2.516111 -0.761074 -1.694288 1 2.317849 -1.757704 -0.246415 6 1.516401 0.241011 1.473868 1 0.774206 0.886615 1.933474 1 1.373175 -0.757495 1.873929 1 2.504116 0.599455 1.770676 6 1.790507 1.645586 -0.598777	-474.0027, 73.0102, 103.0439, 163.8777, 184.0068, 193.272, 204.932, 235.8217, 248.8922, 264.6371, 265.9348, 286.8771, 307.9847, 343.4053, 368.4874, 400.7176, 415.1825, 423.4938, 461.5554, 502.4692, 558.0882, 586.722, 666.7763, 790.7271, 817.9262, 881.5021, 907.259, 932.4163, 943.6579, 974.1756, 982.3214, 989.7524, 1039.305, 1053.7853, 1064.0162, 1068.8144, 1128.4099, 1180.092, 1182.1331, 1215.1553, 1235.8341, 1263.8782,

1 1.150357 2.423779 -0.192009 1 2.816656 1.886883 -0.320285 1 1.729079 1.686433 -1.688252 6 -1.532930 0.338395 0.099715 6 -2.585056 0.049958 -0.979800 1 -2.632330 -1.014153 -1.195103 1 -2.398397 0.600598 -1.902919 1 -3.558876 0.359703 -0.595598 6 -1.382457 1.844354 0.374975 1 -0.662347 2.051009 1.158108 1 -2.357773 2.195773 0.716052 1 -1.125500 2.398958 -0.525252 8 -1.573082 -0.418018 1.143264	1362.6203, 1392.7958, 1399.2851, 1405.1011, 1406.9841, 1410.373, 1443.6096, 1474.6778, 1481.1576, 1482.4375, 1491.0594, 1492.4354, 1497.5188, 1501.7278, 1506.5224, 1514.2586, 1525.1685, 3028.6247, 3030.4703, 3032.2384, 3040.2962, 3043.6867, 3084.6765, 3085.5197, 3091.144, 3101.5521, 3104.0364, 3118.4001, 3121.9951, 3131.6211, 3134.1343, 3152.5906, 3167.0636
IRC  	

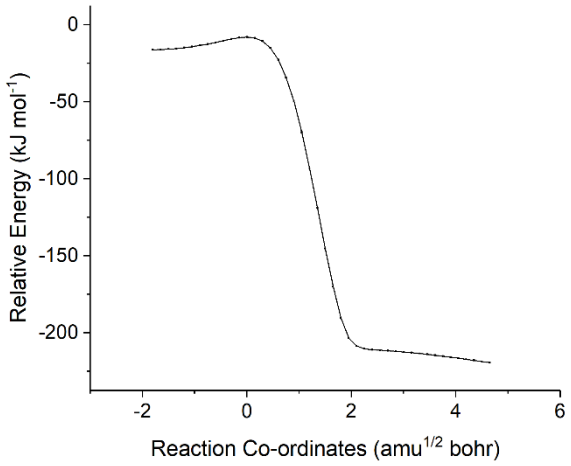
Compound: $tBuCHCMe_2 + O_3$ CPr_{SYN}	**Energy (kJ mol^{-1}):** -539.378570198983
Reaction Coordinates: 6 -1.942457 -0.487812 0.100242 6 -1.037153 0.097490 -0.936327 6 2.720780 -0.269734 0.028139 6 2.590147 1.115218 0.614385 1 1.563850 1.471436 0.576291 1 3.245567 1.815547 0.093346 1 2.926117 1.090529 1.654885 6 4.126505 -0.782489 -0.194435 1 4.105916 -1.828935 -0.486681 1 4.731748 -0.655173 0.704914 1 4.605758 -0.195881 -0.982021 1 -0.703091 -0.493177 -1.783466 6 -3.277000 0.295230 0.088581 1 -3.937660 -0.131889 0.844417 1 -3.774693 0.212321 -0.878687 1 -3.110296 1.345513 0.312187 6 -1.294135 -0.416352 1.500335 1 -0.352203 -0.962377 1.516730 1 -1.111085 0.614154 1.789372 1 -1.975286 -0.876366 2.218195 6 -2.190451 -1.956790 -0.280474 1 -1.259811 -2.525582 -0.285930 1 -2.862923 -2.416380 0.443490 1 -2.652549 -2.042971 -1.265866	**Frequencies (cm^{-1}):** 23.8496, 28.4593, 32.7835, 52.7825, 70.3128, 75.7995, 93.2174, 118.2773, 139.0582, 198.6539, 212.8402, 235.0021, 247.2438, 267.8687, 311.2885, 372.2292, 389.6111, 391.8509, 395.0511, 496.2453, 538.8213, 541.0535, 661.5679, 786.2641, 787.838, 855.2096, 863.3946, 888.3332, 898.8263, 925.0339, 940.014, 948.7482, 975.9066, 1047.9037, 1062.5769, 1086.8404, 1122.5259, 1215.1868, 1235.4501, 1239.9829, 1274.8997, 1386.0027, 1387.6143, 1392.2817, 1398.4277, 1401.5493, 1427.43, 1462.1511, 1466.0286, 1473.7763, 1474.7274, 1491.138, 1492.042, 1494.8275, 1500.3875, 1509.9896, 1529.5912, 1565.0894, 1764.5924, 3022.3243, 3024.6803, 3029.959, 3031.0956, 3036.3065, 3075.4265, 3083.9901, 3085.1599, 3088.8792, 3099.6017, 3104.1133, 3133.2902,

8 -0.589453 1.270110 -0.999584 8 -0.866653 2.180982 0.001767 8 1.754009 -0.949759 -0.251413	3136.038, 3137.0716, 3142.8817, 3152.8617

6.12 Ozonolysis of Mesityl Oxide (Alkene 10)

Compound: Mes Oxy + O_3 PRC1.1	**Energy (kJ mol^{-1}):** -534.707074071554
Reaction Coordinates: 6 0.966494 -2.493703 0.588069 6 1.395925 -1.123049 0.109650 6 0.651204 0.011125 0.705989 6 0.680758 1.306621 0.326879 6 -0.159651 2.314448 1.053846 1 -0.685289 1.884374 1.904288 1 -0.894950 2.755322 0.374448 1 0.461239 3.141332 1.408957 6 1.507790 1.857410 -0.793286 1 0.933615 2.597222 -1.354673 1 2.374045 2.382909 -0.378224 1 1.880348 1.084337 -1.454797 1 0.004118 -0.255276 1.534257 8 2.296727 -0.993578 -0.700493 1 -0.095766 -2.647066 0.388180 1 1.102066 -2.573677 1.669366 1 1.553592 -3.259734 0.089462 8 -2.773310 -0.908079 0.386682 8 -2.570487 -0.008900 -0.478998 8 -1.563949 -0.132799 -1.223209	**Frequencies (cm^{-1}):** 17.7202, 27.6305, 32.2906, 37.4581, 50.1491, 62.0042, 71.3251, 121.4824, 155.1253, 193.9083, 203.5049, 217.9875, 343.1115, 375.1574, 440.461, 470.8107, 598.5393, 628.0504, 741.758, 822.1098, 855.8543, 912.3833, 963.3576, 972.1276, 996.7554, 1044.2347, 1092.9591, 1100.98, 1168.3065, 1188.3413, 1203.1426, 1239.451, 1382.9529, 1390.648, 1410.8358, 1414.9978, 1463.6882, 1468.0146, 1471.9552, 1475.4292, 1486.8516, 1492.4833, 1642.8037, 1741.2431, 3011.129, 3017.3469, 3027.8711, 3053.6877, 3060.8839, 3081.2563, 3109.0457, 3139.8213, 3141.9805, 3162.9066

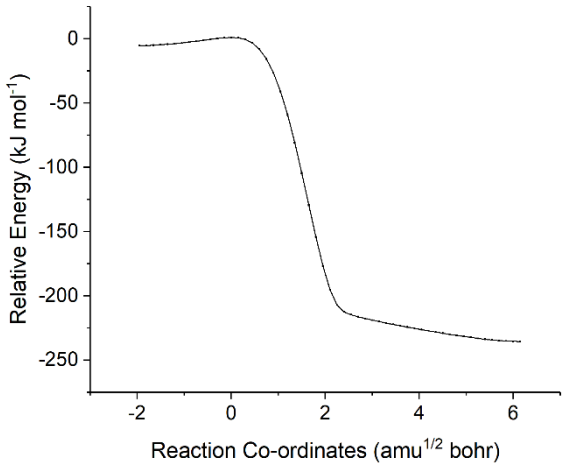
Compound: Mes Oxy + O_3 TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -534.698506360429
Reaction Coordinates: 6 -0.356106 -0.205421 0.687553 6 -1.673606 -0.382996 0.014841 8 -1.825572 -1.098076 -0.964783 6 -2.831720 0.374231 0.631521 1 -2.622464 1.453493 0.624232 1 -2.963737 0.075489 1.682738 1 -3.747576 0.165627 0.070342 6 0.844429 -0.823193 0.328464 6 1.971231 -0.816259 1.331322 1 1.907908 0.037468 2.017273 1 2.947562 -0.806521 0.833570 1 1.917902 -1.737585 1.934732 6 0.969130 -1.786601 -0.818304 1 2.025149 -1.947175 -1.066583 1 0.533343 -2.755734 -0.528710 1 0.421867 -1.442614 -1.698152 1 -0.389524 0.302867 1.651428 8 -0.140978 1.888903 -0.211357 8 1.148668 1.885866 -0.238028 8 1.621560 0.885321 -0.907489	**Frequencies (cm^{-1}):** -211.2311, 51.2459, 58.4127, 105.0959, 110.3152, 115.1166, 158.5968, 188.563, 194.8053, 217.9483, 224.6224, 342.4022, 369.3792, 442.3678, 455.5138, 481.5849, 598.9948, 625.6514, 743.3417, 815.4443, 862.849, 914.4808, 938.6592, 965.7756, 1008.7719, 1024.4916, 1059.9548, 1061.7307, 1087.9312, 1123.6406, 1184.6385, 1236.5047, 1363.2016, 1370.6699, 1391.0674, 1401.8472, 1439.95, 1445.5866, 1450.9085, 1451.9302, 1459.1158, 1475.2275, 1546.0802, 1738.6463, 3018.4462, 3031.4986, 3033.6036, 3092.356, 3096.6108, 3101.8261, 3133.6038, 3156.315, 3172.3647, 3179.2673
IRC:	



Compound: Mes Oxy + O_3 POZ1.1	**Energy (kJ mol^{-1}):** -534.792113773323
Reaction Coordinates: 6 0.232720 -0.355335 -0.559733 6 1.658427 -0.245774 -0.006791 8 2.037299 -0.911949 0.921775 6 2.547117 0.745606 -0.720267 1 2.022149 1.678499 -0.932702 1 3.435511 0.940256 -0.125901 1 2.845938 0.323490 -1.683388 6 -0.830400 0.612586 0.122171 6 -1.460493 1.533128 -0.916999 1 -2.221196 2.159163 -0.451947 1 -0.708395 2.185261 -1.364860 1 -1.924848 0.948756 -1.710033 6 -0.348919 1.363016 1.356690 1 -1.197885 1.846598 1.839016 1 0.116937 0.686620 2.069284 1 0.363453 2.141433 1.082550 8 -1.798210 -0.338550 0.610672 8 -1.693343 -1.429744 -0.307748 8 -0.266514 -1.654441 -0.316925 1 0.243775 -0.151972 -1.634635	**Frequencies (cm^{-1}):** 48.8583, 54.5844, 129.1908, 163.0119, 220.887, 230.9281, 260.6635, 277.3775, 321.9422, 350.8581, 373.9176, 393.6743, 494.1725, 569.4748, 581.4426, 629.9456, 698.5106, 761.6902, 776.7405, 858.2267, 929.0369, 934.5367, 941.4165, 950.6641, 963.3676, 1015.2591, 1040.2354, 1088.0874, 1176.7108, 1184.0756, 1205.151, 1236.8536, 1329.8222, 1374.5725, 1388.8704, 1405.7096, 1424.3902, 1463.0242, 1475.1827, 1481.9846, 1490.3103, 1498.083, 1510.9211, 1800.9056, 3014.6689, 3029.3552, 3033.7122, 3045.58, 3081.8287, 3096.3284, 3105.5248, 3116.2783, 3132.4802, 3141.9337

Compound: Mes Oxy + O_3 PRC1.2	**Energy (kJ mol^{-1}):** -534.704594960998
Reaction Coordinates: 6 0.592415 -0.482630 -0.769913 6 1.751345 0.274781 -0.233681 8 2.472283 0.843196 -1.035698 6 2.046253 0.389090 1.246537 1 1.144680 0.584256 1.825355 1 2.760637 1.196110 1.387669 1 2.495244 -0.534806 1.616422 6 -0.204199 -1.429999 -0.234418 6 -1.271759 -2.054763 -1.091568 1 -1.324592 -1.601500 -2.079119 1 -2.250046 -1.966688 -0.612531 1 -1.083256 -3.125051 -1.214213 6 -0.125072 -2.017491 1.144171	**Frequencies (cm^{-1}):** 23.6592, 37.7428, 38.5841, 44.1712, 50.0253, 54.1445, 90.0346, 145.0702, 188.3823, 209.3195, 225.7722, 238.5944, 327.4102, 370.1096, 469.3341, 521.9023, 567.2346, 596.4632, 745.1888, 780.6778, 870.7128, 884.2999, 957.086, 1009.6045, 1010.1348, 1048.5655, 1090.4114, 1102.7155, 1174.9379, 1202.3441, 1215.9022, 1278.813, 1372.5299, 1389.6694, 1409.362, 1419.3872, 1467.8418, 1471.1796, 1483.5714,

1 -1.088409 -1.917202 1.649027 1 0.071055 -3.090650 1.067075 1 0.637453 -1.579692 1.774355 1 0.439405 -0.238623 -1.815219 8 -0.918742 2.189989 -0.410519 8 -1.971961 1.619555 -0.031528 8 -1.898588 0.872251 0.982047	1484.0179, 1493.7021, 1500.8991, 1658.1629, 1717.1267, 3015.1422, 3025.3618, 3036.9242, 3056.6742, 3063.2853, 3100.4283, 3113.6883, 3135.7666, 3147.5157, 3183.3475

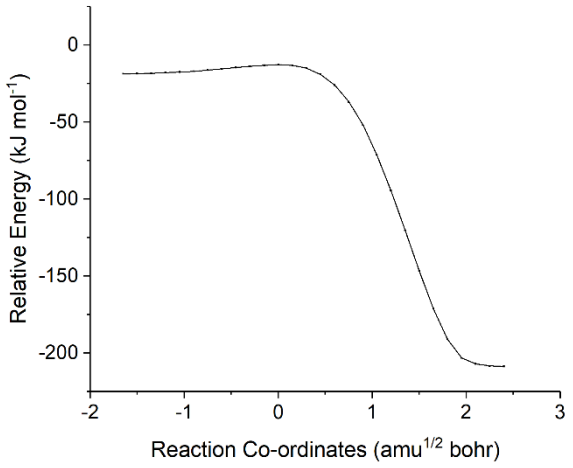
Compound: Mes Oxy + O_3 TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -534.695179931383
Reaction Coordinates: 6 0.351124 -0.266850 -0.743449 6 1.754256 -0.153625 -0.251700 8 2.641743 -0.168232 -1.082730 6 2.072313 0.016303 1.215321 1 1.272449 0.518359 1.754346 1 2.996285 0.584359 1.297493 1 2.244094 -0.962580 1.667933 6 -0.729944 -0.927984 -0.183905 6 -1.921484 -1.179204 -1.067638 1 -2.032473 -0.405584 -1.826100 1 -2.839863 -1.239969 -0.486634 1 -1.796552 -2.134332 -1.587460 6 -0.682452 -1.743079 1.075546 1 -1.659274 -1.752381 1.556452 1 -0.437331 -2.779041 0.822400 1 0.049998 -1.388979 1.790773 1 0.281399 -0.003788 -1.790919 8 -0.104847 1.918216 -0.255536 8 -1.358450 1.761751 -0.005828 8 -1.571147 0.874584 0.911177	**Frequencies (cm^{-1}):** -203.9293, 42.2512, 63.8996, 98.4315, 110.6976, 164.8593, 174.8074, 186.3833, 199.7198, 216.9075, 238.3345, 325.0365, 365.9207, 442.5551, 480.1867, 525.594, 563.4464, 609.922, 743.0238, 780.1646, 856.1936, 902.7492, 950.8256, 1007.4837, 1021.4108, 1043.6945, 1062.8886, 1073.1178, 1082.3066, 1121.8923, 1205.4466, 1267.419, 1361.3883, 1389.3699, 1406.9605, 1420.8978, 1466.976, 1468.7297, 1474.2813, 1484.4201, 1491.021, 1505.5514, 1550.462, 1731.2829, 3016.8014, 3025.6726, 3039.3612, 3081.9359, 3092.5138, 3106.4339, 3119.8271, 3140.8272, 3171.4166, 3172.7901
IRC:  	

Compound: Mes Oxy + O_3 POZ1.2	**Energy (kJ mol^{-1}):** -534.797488909827
Reaction Coordinates: 6 0.228018 -0.195930 -0.698717 6 1.648138 0.194952 -0.281026 8 2.109227 1.220308 -0.727337 6 2.396686 -0.706818 0.659727	**Frequencies (cm^{-1}):** 35.9509, 66.9584, 151.9999, 172.1197, 222.8066, 239.9914, 259.0011, 266.5828, 327.9963, 345.2904, 383.8728, 438.8488, 501.5514, 522.122, 591.1203, 621.042,

1 2.602662 -1.658416 0.165236 1 3.328728 -0.231438 0.952747 1 1.789285 -0.947559 1.532918 6 -0.922088 0.520997 0.126496 6 -1.991530 1.058920 -0.818123 1 -2.819405 1.474364 -0.244302 1 -1.575540 1.846043 -1.447565 1 -2.372040 0.266837 -1.460487 6 -0.469826 1.567199 1.132898 1 -1.333529 1.941576 1.680886 1 0.238164 1.155603 1.849928 1 0.001482 2.402002 0.617789 8 -1.427093 -0.584688 0.898988 8 -1.363804 -1.668272 -0.017766 8 0.017798 -1.584743 -0.481348 1 0.114781 0.054240 -1.754974	689.7289, 746.9947, 772.2767, 848.6953, 889.5146, 932.3283, 938.9608, 959.8788, 998.2174, 1020.8116, 1044.6947, 1056.424, 1178.6446, 1199.3972, 1232.2607, 1254.1917, 1302.32, 1341.7345, 1392.7723, 1405.2773, 1424.6052, 1457.6892, 1465.2794, 1481.1631, 1488.8698, 1498.7954, 1513.7212, 1778.6648, 3038.735, 3039.9281, 3050.3423, 3052.6879, 3091.9303, 3106.122, 3116.9338, 3120.4391, 3128.0958, 3144.1798

Compound: Mes Oxy + O_3 PRC 2.1	**Energy (kJ mol^{-1}):** -534.710263574005
Reaction Coordinates: 6 -0.160857 -0.782950 0.653593 6 -1.413577 -0.795694 -0.133820 8 -1.450943 -0.736696 -1.351368 6 -2.689168 -0.862838 0.680815 1 -2.760562 0.009924 1.333636 1 -2.686617 -1.744658 1.325020 1 -3.549297 -0.892350 0.017817 6 1.089714 -1.041238 0.214216 6 2.240212 -1.001522 1.176634 1 1.937778 -0.680472 2.171219 1 3.013577 -0.321198 0.812101 1 2.704872 -1.988415 1.253002 6 1.450814 -1.428160 -1.188196 1 2.060546 -0.642480 -1.641793 1 2.071627 -2.327689 -1.169453 1 0.582249 -1.586694 -1.816053 1 -0.288200 -0.579772 1.710348 8 -0.596128 2.239890 0.657177 8 0.030782 2.305911 -0.433165 8 1.242689 1.969423 -0.424557	**Frequencies (cm^{-1}):** 25.9802, 28.7382, 45.1804, 52.6124, 59.1388, 67.0696, 97.1328, 108.0249, 145.9557, 193.5056, 206.7742, 216.4951, 344.2889, 376.6945, 440.5134, 471.6263, 600.2664, 627.0059, 746.4433, 822.487, 853.4436, 912.877, 960.6881, 971.1167, 999.5386, 1044.0932, 1094.4783, 1104.5016, 1175.1535, 1189.3252, 1213.5919, 1242.5602, 1382.0962, 1389.2845, 1411.5415, 1415.0729, 1463.7146, 1466.6985, 1474.4187, 1475.508, 1486.1655, 1497.4367, 1640.7825, 1735.2755, 3016.2604, 3023.5835, 3028.4513, 3058.2883, 3063.6408, 3080.838, 3113.288, 3139.2433, 3148.7759, 3164.478

Compound: Mes Oxy + O_3 TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -534.699569322360
Reaction Coordinates: 6 -0.321957 -0.365462 0.682237 6 -1.598781 -0.431982 -0.070359 8 -1.654427 -0.731935 -1.248668 6 -2.842512 -0.108445 0.727034 1 -2.764908 0.891044 1.158021 1 -2.953608 -0.811242 1.556100 1 -3.715436 -0.165509 0.083047 6 0.916280 -0.812568 0.235887 6 2.001163 -1.032392 1.249202 1 1.824592 -0.474143 2.165930 1 2.972863 -0.750962 0.845531 1 2.051295 -2.097477 1.496215 6 1.132340 -1.432029 -1.114300	**Frequencies (cm^{-1}):** -215.5984, 43.7579, 80.2933, 103.4714, 113.4622, 129.8935, 171.3373, 177.563, 198.9209, 217.8028, 232.9856, 339.9431, 374.9124, 456.4203, 468.9863, 479.0592, 612.3332, 627.2522, 746.658, 815.9238, 885.6802, 914.1677, 955.2251, 969.1381, 1016.2315, 1041.9839, 1061.2929, 1073.1819, 1082.5874, 1124.3416, 1184.9313, 1236.109, 1376.3747, 1388.1064, 1409.538, 1420.8051, 1463.768, 1467.6979, 1472.172,

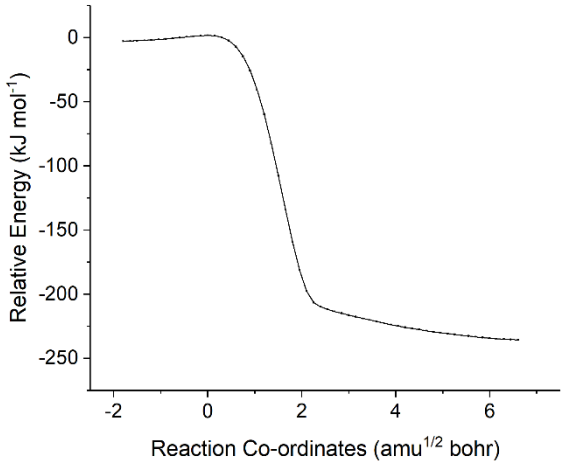
1 2.196250 -1.535724 -1.318489 1 0.680736 -2.428367 -1.131554 1 0.654391 -0.867047 -1.907232 1 -0.407337 -0.124690 1.732364 8 -0.217081 1.873240 0.333414 8 0.620090 1.816853 -0.643086 8 1.719163 1.224515 -0.308927	1474.6967, 1477.6041, 1494.5548, 1538.0649, 1736.5001, 3018.4427, 3026.688, 3031.3897, 3083.6266, 3086.5972, 3094.0378, 3124.381, 3142.592, 3153.676, 3180.5793
IRC:  	

Compound: Mes Oxy + O_3 POZ 2.1	**Energy (kJ mol^{-1}):** -534.792044532333
Reaction Coordinates: 6 0.245352 -0.212611 -0.692229 6 1.626468 -0.197985 -0.017902 8 1.972655 -1.071086 0.735192 6 2.522792 0.960365 -0.394345 1 1.979307 1.906587 -0.409822 1 3.360385 1.019970 0.295201 1 2.905137 0.797460 -1.405519 6 -0.873055 0.590442 0.090924 6 -1.306369 1.859953 -0.626350 1 -2.161654 2.303736 -0.117852 1 -0.499393 2.592520 -0.623275 1 -1.585299 1.646664 -1.657066 6 -0.544644 0.828615 1.561404 1 -1.404946 1.286463 2.048076 1 -0.309936 -0.106637 2.063565 1 0.305519 1.502338 1.674512 8 -1.974675 -0.329175 -0.024447 8 -1.342420 -1.589295 0.157176 8 -0.274068 -1.524204 -0.829469 1 0.335678 0.188313 -1.704452	**Frequencies (cm^{-1}):** 51.0298, 69.7701, 115.7249, 169.3575, 214.9059, 231.2789, 258.1257, 268.6933, 323.3572, 330.549, 371.7014, 409.714, 506.8461, 576.1476, 579.2623, 636.5966, 691.4151, 742.5116, 816.3254, 864.961, 893.071, 929.1058, 944.459, 951.0607, 965.8531, 1013.5964, 1040.7039, 1060.2442, 1173.0655, 1188.251, 1202.2852, 1238.061, 1304.1405, 1370.4463, 1386.1017, 1407.6351, 1424.896, 1463.0535, 1475.2677, 1481.08, 1489.4762, 1498.9758, 1510.2903, 1803.3439, 3027.5997, 3040.2202, 3041.6369, 3046.2436, 3081.3782, 3101.8036, 3109.1222, 3116.994, 3134.8567, 3140.4409

Compound: Mes Oxy + O_3 PRC 2.2	**Energy (kJ mol^{-1}):** -534.704122867276
Reaction Coordinates: 6 0.788178 -0.211594 0.000006 6 0.313680 1.188422 0.000007	**Frequencies (cm^{-1}):** 12.4087, 19.5325, 22.9232, 32.8742, 56.397, 62.9345, 80.6485, 142.98,

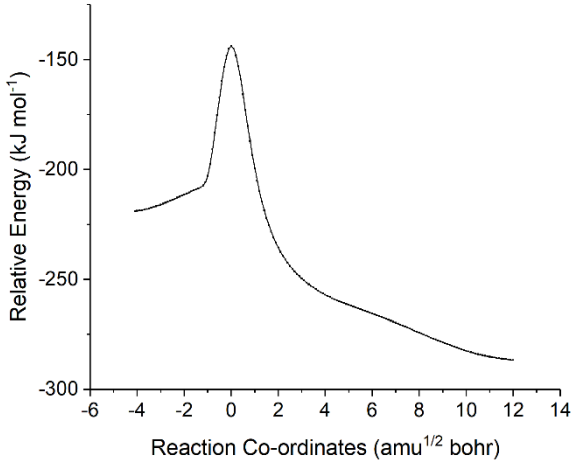
8 -0.893862 1.377709 0.000010 6 1.238808 2.387510 0.000004 1 1.881206 2.388588 0.881297 1 0.629316 3.287146 0.000009 1 1.881196 2.388592 -0.881298 6 2.014495 -0.763651 -0.000001 6 2.133767 -2.264167 0.000001 1 1.162370 -2.753106 0.000011 1 2.693863 -2.603585 0.875688 1 2.693845 -2.603588 -0.875698 6 3.343772 -0.066406 -0.000011 1 3.288809 1.013838 -0.000018 1 3.921942 -0.379361 0.873738 1 3.921935 -0.379372 -0.873761 1 -0.058716 -0.887886 0.000012 8 -2.913485 -0.644329 -1.075333 8 -3.405674 -0.225514 0.000002 8 -2.913474 -0.644361 1.075320	144.8051, 213.7758, 232.2177, 242.8921, 322.0617, 374.1857, 473.4836, 525.8892, 584.7314, 586.201, 749.4671, 782.3707, 877.5935, 889.3302, 956.4738, 1007.6729, 1015.8919, 1050.601, 1093.1779, 1104.8973, 1193.6333, 1204.6019, 1241.9039, 1288.9911, 1379.5975, 1391.3639, 1410.5514, 1420.1125, 1467.1998, 1470.9165, 1483.3021, 1483.8396, 1495.3879, 1501.5063, 1682.416, 1703.2213, 3013.0954, 3022.2276, 3037.8419, 3051.7413, 3056.7095, 3097.2822, 3117.6208, 3135.5978, 3153.4351, 3184.1817

Compound: Mes Oxy + O_3 TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -534.695849937139
Reaction Coordinates: 6 0.322965 -0.419851 -0.717441 6 1.721020 -0.290713 -0.217985 8 2.618639 -0.432035 -1.026683 6 2.036809 0.009749 1.229762 1 1.348234 0.733493 1.663668 1 3.053742 0.389999 1.282725 1 1.981422 -0.905758 1.821491 6 -0.805113 -0.918223 -0.089505 6 -1.948605 -1.369079 -0.952087 1 -1.910634 -0.919852 -1.941595 1 -2.905474 -1.127407 -0.490886 1 -1.910433 -2.457080 -1.067052 6 -0.861108 -1.374851 1.342563 1 -0.417932 -2.371798 1.428543 1 -0.330205 -0.717399 2.023002 1 -1.894014 -1.447846 1.676440 1 0.291085 -0.354977 -1.796184 8 -0.042906 1.833301 -0.678262 8 -0.765047 1.875484 0.383772 8 -1.823387 1.142804 0.299673	**Frequencies (cm^{-1}):** -186.9738, 42.8294, 76.3793, 110.6847, 129.4643, 154.841, 170.2827, 192.9062, 203.4787, 217.6898, 247.006, 323.3496, 372.5964, 451.9266, 471.0942, 527.3511, 574.1249, 606.0575, 742.909, 780.0591, 861.0281, 907.4923, 959.5767, 1005.7347, 1021.1014, 1044.8461, 1069.2749, 1079.1834, 1087.8139, 1124.5456, 1204.5939, 1270.6468, 1364.5027, 1393.826, 1408.4514, 1420.2996, 1463.1585, 1471.2756, 1472.7095, 1483.6868, 1488.9416, 1508.612, 1549.6958, 1727.147, 3016.2138, 3021.8339, 3040.8502, 3082.2535, 3098.1436, 3102.4889, 3127.6516, 3137.4874, 3149.4437, 3184.0356
IRC:	



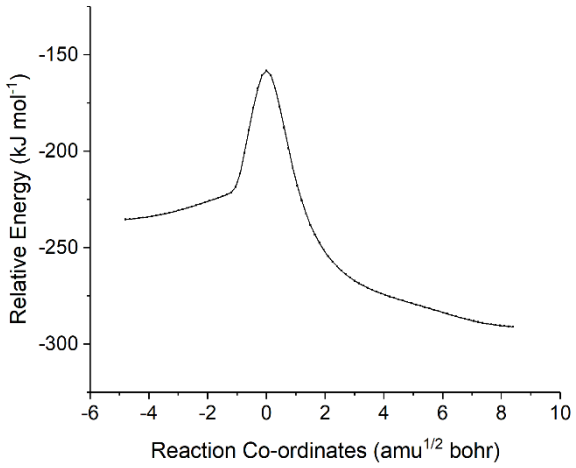
Compound: Mes Oxy + O_3 POZ 2.2	**Energy (kJ mol^{-1}):** -534.797714881535
Reaction Coordinates: 6 -0.234839 0.080930 -0.742274 6 -1.581980 -0.410372 -0.203275 8 -1.865547 -1.577340 -0.354005 6 -2.499507 0.584878 0.450439 1 -2.844321 1.304244 -0.295410 1 -3.350070 0.064779 0.882172 1 -1.971807 1.163775 1.208917 6 1.022186 -0.405318 0.086956 6 1.880214 -1.394797 -0.685313 1 2.792329 -1.616066 -0.131758 1 1.330188 -2.324437 -0.825845 1 2.151291 -0.992825 -1.660365 6 0.695563 -0.899940 1.492323 1 1.625468 -1.123955 2.013397 1 0.160628 -0.141931 2.061961 1 0.092060 -1.804988 1.457874 8 1.777584 0.823368 0.158652 8 0.766959 1.806824 0.322955 8 -0.119475 1.498731 -0.794323 1 -0.151760 -0.273550 -1.770301	**Frequencies (cm^{-1}):** 38.8592, 63.7719, 145.3558, 174.2169, 226.7094, 233.3381, 250.3973, 274.9418, 315.6352, 336.4519, 406.039, 445.9726, 508.7695, 525.2494, 587.9163, 624.5293, 688.7089, 740.3333, 791.1881, 843.1909, 887.346, 933.3965, 944.2567, 959.9606, 1000.8196, 1015.7992, 1038.3557, 1046.1565, 1182.8305, 1197.0859, 1228.5177, 1246.1747, 1297.856, 1335.5448, 1391.3942, 1406.0038, 1422.6586, 1458.1648, 1467.2145, 1484.9996, 1489.2996, 1504.0195, 1511.9606, 1775.4871, 3039.1633, 3042.701, 3050.027, 3068.1365, 3093.2995, 3110.849, 3116.3622, 3118.8149, 3126.2189, 3145.0632

Compound: Mes Oxy + O_3 TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -534.758759688438
Reaction Coordinates: 6 0.307354 0.474926 -0.494682 6 1.675085 0.186170 0.069766 8 2.008803 0.622869 1.145480 6 2.581397 -0.650739 -0.797864 1 2.889535 -0.063348 -1.666860 1 3.461995 -0.941811 -0.232189 1 2.068247 -1.533936 -1.179691 6 -1.091420 -0.683485 0.130948 6 -0.908593 -1.929350 -0.746837 1 0.053359 -2.413409 -0.584873 1 -1.030449 -1.682457 -1.799507	**Frequencies (cm^{-1}):** -486.4642, 45.5532, 83.3248, 99.3583, 148.9841, 183.3597, 205.4112, 226.6078, 247.1195, 279.102, 307.4185, 371.6308, 423.7204, 437.2622, 478.7305, 560.9162, 591.8926, 615.2779, 627.983, 777.5695, 916.3132, 925.5042, 960.8785, 979.924, 1010.6716, 1034.7561, 1062.4514, 1116.1454, 1135.8682, 1182.992, 1194.9168, 1232.4895, 1355.9078,

1 -1.687734 -2.643857 -0.477903 6 -0.834140 -0.884121 1.621060 1 -0.802089 0.072655 2.137041 1 0.090081 -1.424715 1.819516 1 -1.664285 -1.462872 2.030033 1 0.151129 0.326001 -1.557831 8 -0.224357 1.617351 -0.027883 8 -1.403029 1.806432 -0.588604 8 -2.119904 0.039265 -0.176754	1381.9894, 1394.4578, 1400.8688, 1411.346, 1464.2128, 1469.397, 1475.7154, 1485.7221, 1491.2044, 1504.7369, 1773.7117, 3031.2801, 3036.8738, 3041.0962, 3087.7763, 3097.7763, 3102.662, 3124.7053, 3131.7965, 3135.1955, 3144.967
IRC:  	

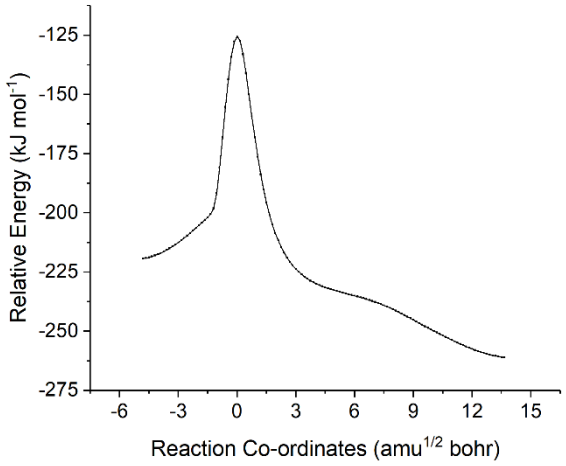
Compound: Mes Oxy + O_3 C_{ANTI} 1	**Energy (kJ mol^{-1}):** -534.806025516833
Reaction Coordinates: 6 2.015139 -1.978640 -0.627637 6 2.029624 -0.708258 0.177696 6 1.366504 0.455653 -0.486008 1 0.932497 0.418571 -1.476744 8 1.306888 1.543149 0.143938 8 0.677772 2.589573 -0.440287 8 2.522625 -0.603796 1.277522 1 2.543517 -2.758984 -0.087924 1 0.981378 -2.278671 -0.810124 1 2.484331 -1.819389 -1.601504 6 -2.199338 -0.327217 0.002243 6 -2.360041 1.142815 0.290958 1 -3.278537 1.526001 -0.156475 1 -1.500551 1.713369 -0.055357 1 -2.459343 1.276906 1.371974 6 -3.427717 -1.192744 0.156522 1 -3.166792 -2.243839 0.069255 1 -4.151007 -0.932996 -0.620291 1 -3.913952 -1.003348 1.114957 8 -1.134356 -0.809836 -0.334974	**Frequencies (cm^{-1}):** 26.0742, 30.0187, 57.5506, 68.762, 74.6665, 81.6325, 106.6702, 131.6677, 147.406, 188.1096, 194.8649, 228.9937, 374.9457, 393.9947, 462.2004, 497.2747, 544.1782, 565.0713, 617.3798, 791.5103, 888.09, 892.8297, 908.2755, 912.6079, 932.612, 1032.3061, 1048.5668, 1090.4772, 1122.7511, 1199.4668, 1245.9589, 1363.8349, 1389.0051, 1390.9899, 1399.1185, 1461.8245, 1463.4678, 1466.4785, 1473.1354, 1475.8169, 1493.8168, 1505.5236, 1753.6192, 1763.0578, 3020.6804, 3029.7557, 3032.2759, 3077.5571, 3085.7906, 3086.0933, 3122.681, 3139.6836, 3147.3204, 3189.3751

Compound: Mes Oxy + O_3 TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -534.764679805393
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 0.291126 0.364665 -0.620373 6 1.639607 -0.202418 -0.283078 8 1.982729 -1.223240 -0.839049 6 2.496939 0.516970 0.723535 1 3.394669 -0.066141 0.908016 1 2.769224 1.502251 0.339437 1 1.953801 0.682710 1.653876 6 -1.155893 -0.544763 0.217021 6 -1.308131 -1.769418 -0.692541 1 -0.374764 -2.320245 -0.793734 1 -1.665490 -1.466612 -1.674408 1 -2.055063 -2.428092 -0.246517 6 -0.707262 -0.849318 1.646547 1 -0.496469 0.071843 2.186463 1 0.160078 -1.508483 1.680282 1 -1.528929 -1.351736 2.159599 1 -0.038205 0.228243 -1.643959 8 0.051384 1.585025 -0.109595 8 -1.159766 1.979274 -0.466944 8 -2.081493 0.354185 0.101123	-490.0647, 61.7722, 86.9588, 110.0727, 144.9355, 198.8362, 217.9317, 236.7446, 250.3079, 292.1201, 307.0353, 390.5085, 425.3732, 473.3876, 484.485, 539.1787, 573.0902, 610.4145, 619.6787, 773.0316, 843.5264, 917.7925, 981.8813, 1007.4702, 1014.2731, 1041.5659, 1067.8061, 1115.61, 1139.4584, 1189.152, 1222.533, 1251.804, 1348.5371, 1361.7125, 1392.768, 1395.2136, 1407.4258, 1461.6891, 1470.3874, 1480.2014, 1486.6685, 1496.8677, 1503.6097, 1759.4355, 3034.1803, 3039.0026, 3040.9695, 3094.068, 3098.2812, 3104.7718, 3120.4132, 3131.1522, 3147.4591, 3151.0265
IRC:  	

Compound: Mes Oxy + O_3 C_{ANTI} 2	**Energy (kJ mol^{-1}):** -534.809649087298
Reaction Coordinates: 6 2.391909 -1.027762 1.192280 6 2.046755 -0.710723 -0.234146 6 1.327980 0.554056 -0.528402 1 0.939043 0.763382 -1.516997 8 1.210547 1.417504 0.379347 8 0.547705 2.570205 0.101639 8 2.307917 -1.428212 -1.177187 1 3.005653 -1.923397 1.220973 1 2.912574 -0.194555 1.664890 1 1.470564 -1.192981 1.754056 6 -2.186800 -0.391089 -0.006413 6 -2.536636 1.056956 -0.239885 1 -2.982327 1.153368 -1.234209 1 -1.651504 1.687629 -0.180042 1 -3.290199 1.393488 0.473860 6 -3.333448 -1.339506 0.255430 1 -2.982588 -2.367795 0.258391	**Frequencies (cm^{-1}):** 25.409, 34.8438, 40.4654, 59.4227, 78.0114, 87.9757, 105.9357, 108.8285, 139.8925, 166.5056, 193.5539, 246.2413, 391.7459, 395.1423, 494.9224, 495.7167, 544.2258, 558.989, 569.8111, 790.1655, 833.6049, 889.9159, 908.067, 919.8319, 979.2988, 1024.8148, 1050.7451, 1091.2863, 1122.9055, 1244.8312, 1245.4119, 1341.1692, 1388.5361, 1396.3568, 1399.0772, 1462.1583, 1464.1392, 1464.7127, 1470.8219, 1475.8703, 1493.0306, 1510.513, 1748.8812, 1757.3464, 3018.6245, 3031.3335, 3041.8106, 3077.0785,

1 -4.118518 -1.211035 -0.491736 1 -3.780136 -1.105511 1.224905 8 -1.038811 -0.791270 -0.029709	3084.9171, 3099.1432, 3119.7206, 3139.8553, 3148.141, 3192.3128

Compound: Mes Oxy + O_3 TS_{DMFO} 1.1	**Energy (kJ mol^{-1}):** -534.766832706485
Reaction Coordinates: 6 0.382137 -0.443930 0.750952 6 1.659912 -0.213869 -0.071683 8 1.782719 -0.656753 -1.184598 6 2.748631 0.565164 0.633002 1 3.126566 -0.022931 1.473042 1 3.561490 0.774706 -0.056816 1 2.361268 1.496211 1.051509 6 -0.957766 0.654717 -0.074835 6 -0.419856 1.871967 -0.776075 1 -1.247903 2.501323 -1.109271 1 0.185107 2.465299 -0.092261 1 0.179661 1.593471 -1.639210 6 -1.913181 0.885944 1.071052 1 -2.856265 1.256271 0.659954 1 -2.111176 -0.026051 1.622936 1 -1.510996 1.643632 1.740628 1 0.375785 0.064947 1.727684 8 -0.126237 -1.618778 0.715600 8 -1.735628 -1.390999 -0.377930 8 -1.303705 -0.291825 -0.974657	**Frequencies (cm^{-1}):** -423.199, 58.1878, 75.3686, 112.4049, 147.1989, 185.0204, 214.8614, 238.1603, 246.9126, 289.1586, 334.0638, 351.6465, 371.6548, 399.697, 524.1063, 543.7577, 625.3093, 646.4945, 673.2083, 790.4517, 832.4498, 945.6563, 956.3447, 989.534, 1006.1283, 1016.5101, 1032.8363, 1114.1777, 1144.73, 1175.0422, 1281.9692, 1294.8162, 1330.9133, 1380.671, 1404.0493, 1413.8666, 1419.9495, 1462.4207, 1470.8338, 1471.6616, 1484.8058, 1495.472, 1505.7601, 1794.5339, 2931.3097, 3028.6794, 3031.2055, 3039.0142, 3079.81, 3099.0411, 3107.0033, 3138.2118, 3140.5717, 3162.9852
IRC:  	

Compound: Mes Oxy + O_3 CPr_{DMFO} 1.1	**Energy (kJ mol^{-1}):** -534.815354982453
Reaction Coordinates: 6 2.442611 1.409196 0.015735 6 1.595120 0.267945 -0.478472 6 1.767799 -1.067195 0.276889 1 2.328831 -1.005160 1.226341 8 1.352224 -2.109283 -0.152429	**Frequencies (cm^{-1}):** 33.324, 54.8279, 71.7283, 92.7006, 98.0452, 127.6262, 132.0077, 151.8264, 161.643, 205.0216, 276.4828, 310.0763, 315.2038, 372.2681, 402.9845, 481.0672, 487.7678, 592.7621, 643.9583, 811.7403,

8 0.869250 0.333087 -1.445268 1 3.497048 1.180161 -0.166244 1 2.183997 2.326047 -0.506978 1 2.316973 1.539135 1.090232 6 -1.861276 0.079257 0.085087 6 -2.788474 -0.870504 -0.576735 1 -3.823084 -0.598092 -0.357043 1 -2.656840 -0.794836 -1.658769 1 -2.593140 -1.891193 -0.260469 6 -1.896824 1.537543 -0.131214 1 -1.865644 2.041762 0.836284 1 -0.990280 1.835411 -0.661197 1 -2.773611 1.825336 -0.704896 8 -1.030274 -0.443805 0.877188 8 -0.088448 0.395500 1.472384	825.0493, 891.4262, 912.0428, 929.1655, 976.5939, 988.1836, 1058.8944, 1076.6211, 1100.8795, 1187.3553, 1306.5343, 1384.0861, 1387.4657, 1403.1761, 1404.8894, 1448.2479, 1456.3786, 1461.1197, 1468.5441, 1473.5069, 1481.7586, 1578.8017, 1762.2916, 1800.6774, 2927.2434, 3024.061, 3029.6445, 3039.6222, 3078.6609, 3091.3265, 3091.9224, 3140.3127, 3141.1911, 3146.268

Compound: Mes Oxy + O_3 TS_{DMFO} 1.2	**Energy (kJ mol^{-1}):** -534.777037370371
Reaction Coordinates: 6 -0.342941 -0.225277 -0.887784 6 -1.667639 0.184987 -0.241120 8 -2.167247 1.248774 -0.562697 6 -2.295182 -0.777458 0.731622 1 -1.574704 -1.058092 1.512193 1 -3.193730 -0.330831 1.168017 1 -2.547198 -1.707643 0.202594 6 1.018377 0.543753 0.156498 6 0.611357 1.834643 0.818868 1 1.503850 2.360151 1.186673 1 0.102795 2.480046 0.093810 1 -0.068326 1.654380 1.658674 6 2.183018 0.606023 -0.808737 1 3.105957 0.729078 -0.222147 1 2.268033 -0.301871 -1.409384 1 2.065970 1.478949 -1.461097 1 -0.125827 0.377413 -1.791219 8 -0.045410 -1.480907 -0.922724 8 1.351845 -1.625638 0.478897 8 1.038467 -0.477430 1.062249	**Frequencies (cm^{-1}):** -414.7799, 67.8122, 95.123, 119.4608, 152.9746, 199.2026, 207.4744, 245.6865, 257.4259, 276.9652, 331.1384, 371.2906, 395.0585, 436.46, 518.7693, 538.3302, 594.8471, 643.8782, 665.9342, 775.9286, 818.6798, 953.35, 973.5207, 988.5287, 994.1375, 1007.9702, 1026.0946, 1113.6375, 1144.1686, 1235.435, 1269.3768, 1278.0736, 1294.1246, 1369.3055, 1390.301, 1393.5927, 1406.7836, 1433.3335, 1441.0118, 1450.8911, 1456.8379, 1471.0281, 1483.4895, 1762.878, 2964.9345, 3040.6314, 3044.2257, 3046.1238, 3107.3246, 3120.0513, 3122.5491, 3146.8091, 3161.0402, 3175.8067

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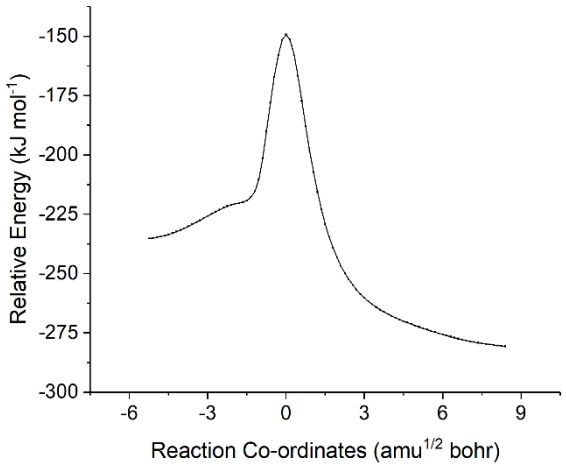
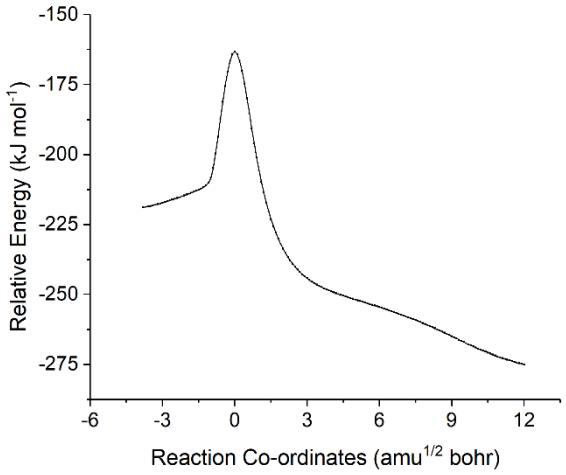


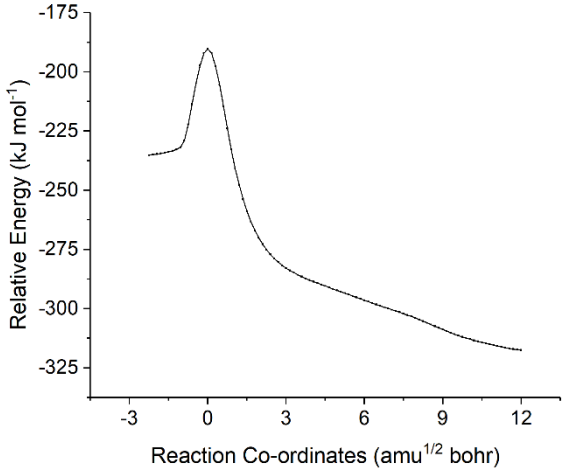
Compound: Mes Oxy + O_3 CPr_{DMFO} 1.2	**Energy (kJ mol^{-1}):** -534.819148971057
Reaction Coordinates: 6 1.877572 1.658149 -0.395539 6 1.373668 0.576861 0.509975 6 2.021231 -0.802848 0.377948 1 1.501443 -1.589108 0.953037 8 3.041412 -0.999308 -0.227513 8 0.535269 0.738014 1.375468 1 1.700092 1.366349 -1.431040 1 1.379699 2.597581 -0.171469 1 2.957453 1.761915 -0.278701 6 -2.000084 -0.121331 -0.120688 6 -3.043319 0.921817 0.040489 1 -4.034186 0.479403 -0.084835 1 -2.996084 1.322888 1.055466 1 -2.906011 1.727650 -0.675305 6 -1.936339 -1.341925 0.700508 1 -1.778954 -2.203018 0.048553 1 -1.054300 -1.279232 1.342662 1 -2.829792 -1.453203 1.308866 8 -1.156499 0.090595 -1.037430 8 -0.132149 -0.838746 -1.203448	**Frequencies (cm^{-1}):** 39.4941, 51.369, 72.8599, 82.9, 91.1104, 97.365, 135.5356, 162.3678, 173.1807, 198.0153, 256.5841, 307.963, 312.7899, 370.0074, 468.6213, 482.9884, 491.7759, 584.4694, 591.5706, 786.0934, 812.1789, 907.4165, 917.5145, 928.9838, 987.5831, 1013.742, 1064.8698, 1073.7737, 1098.723, 1250.4509, 1306.3545, 1366.908, 1385.6182, 1388.2229, 1405.5694, 1445.3441, 1456.6532, 1457.7634, 1466.9281, 1469.5568, 1482.1726, 1569.4418, 1750.0017, 1789.7738, 2939.7544, 3028.4894, 3033.7141, 3043.6484, 3077.8838, 3082.955, 3101.6395, 3140.0222, 3141.97, 3143.2545

Compound: Mes Oxy + O_3 TS_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -534.766584568438
Reaction Coordinates: 6 0.357100 -0.518082 -0.701274 6 1.665042 -0.269723 0.096919 8 1.866119 -0.749428 1.179034 6 2.695952 0.546791 -0.650479 1 2.254787 1.430717 -1.111694 1 3.499118 0.828697 0.024900 1 3.105884 -0.060726 -1.461043 6 -0.890346 0.669712 0.124729 6 -0.701293 2.088016 -0.339709 1 -1.443585 2.734620 0.132945 1 0.281303 2.453402 -0.048232 1 -0.809074 2.168091 -1.419751 6 -0.844503 0.397505 1.604254 1 -1.832017 0.631716 2.010637 1 -0.616980 -0.638463 1.827230 1 -0.106602 1.035358 2.083432 1 0.396623 -0.082021 -1.712495 8 -0.181593 -1.665483 -0.571427 8 -2.073398 -1.174371 -0.192914 8 -1.913774 0.090944 -0.556264	**Frequencies (cm^{-1}):** -415.4877, 62.9614, 92.5795, 126.0664, 166.2667, 172.9802, 190.637, 241.2498, 256.1407, 287.3618, 333.6769, 361.8137, 371.8115, 390.6598, 532.578, 538.8522, 607.0818, 641.2281, 652.9859, 788.2777, 827.8611, 948.3359, 961.133, 983.4487, 999.2857, 1023.0105, 1044.3651, 1125.0069, 1135.3224, 1168.8388, 1273.4584, 1287.3457, 1363.0214, 1381.2592, 1403.9143, 1411.1983, 1422.1879, 1464.4898, 1466.9975, 1470.4454, 1478.9342, 1492.1068, 1496.1282, 1801.1189, 2925.6171, 3034.0219, 3034.4714, 3039.1016, 3090.0016, 3100.604, 3119.0698, 3130.2733, 3142.1014, 3168.0626
IRC:	



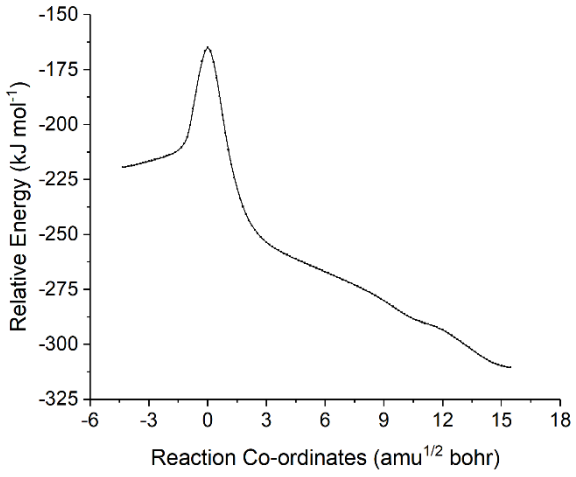
Compound: Mes Oxy + O_3 CPr_{DMFO} 2.1	**Energy (kJ mol^{-1}):** -534.815991219137
Reaction Coordinates: 6 1.892839 0.850304 0.209507 6 1.489821 -0.477774 -0.461408 8 0.719705 -0.480679 -1.396314 6 2.160484 -1.712267 0.076491 1 1.977013 -1.795422 1.147665 1 1.790640 -2.594822 -0.438256 1 3.242102 -1.635797 -0.067656 6 -1.844394 0.016633 0.090456 6 -2.913015 -0.749857 -0.597268 1 -3.884297 -0.291748 -0.398504 1 -2.746679 -0.697632 -1.675623 1 -2.920023 -1.788825 -0.279807 6 -1.608681 1.451198 -0.136683 1 -1.426337 1.941400 0.820771 1 -0.689709 1.570807 -0.717126 1 -2.440721 1.900816 -0.672219 1 2.390227 0.750476 1.190673 8 1.733523 1.919318 -0.318544 8 -0.096648 0.006704 1.554299 8 -1.150898 -0.648928 0.910998	**Frequencies (cm^{-1}):** 55.2014, 58.9985, 85.6964, 87.0779, 109.4312, 113.6025, 139.6153, 165.1225, 185.6452, 209.8405, 276.9853, 312.7902, 317.8043, 374.2839, 400.2894, 483.3275, 494.8155, 590.387, 646.0556, 811.9878, 829.2425, 897.067, 905.6429, 924.4675, 981.1784, 988.4061, 1061.9845, 1075.3485, 1099.2239, 1189.7704, 1306.9756, 1381.0137, 1383.0929, 1400.9374, 1404.3508, 1446.7048, 1457.7563, 1461.3306, 1469.5896, 1475.7308, 1484.7034, 1571.5732, 1759.6992, 1793.3069, 2927.6127, 3025.8224, 3027.7778, 3033.0489, 3080.6817, 3083.3703, 3091.6944, 3139.0643, 3141.2045, 3143.487

Compound: Mes Oxy + O_3 TS_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -534.773958861196
Reaction Coordinates: 6 0.340222 -0.347517 -0.839418 6 1.658856 0.147793 -0.210856 8 2.084147 1.232958 -0.528948 6 2.401329 -0.806590 0.682335 1 2.940717 -1.507796 0.040356 1 3.118515 -0.261020 1.290170 1 1.726679 -1.402868 1.290767 6 -0.968934 0.568084 0.177703 6 -1.105954 1.976062 -0.323899 1 -1.723041 2.563035 0.358904 1 -0.121862 2.439372 -0.380414	**Frequencies (cm^{-1}):** -416.8877, 75.8852, 97.5141, 120.5624, 167.026, 194.7282, 219.8246, 235.3631, 266.1258, 271.6497, 332.9154, 372.7159, 393.7847, 449.5794, 526.4177, 538.9167, 577.664, 629.4933, 642.7996, 772.3633, 805.8098, 956.234, 984.7878, 992.5555, 1005.0136, 1022.3623, 1039.3268, 1127.7345, 1156.8232, 1195.065, 1278.1147, 1285.6328, 1332.9809,

1 -1.558136 1.990729 -1.313552 6 -0.635731 0.380313 1.635931 1 -1.506864 0.689794 2.219410 1 -0.417468 -0.654258 1.873117 1 0.200081 1.016884 1.917505 1 0.167160 0.141075 -1.808958 8 0.051811 -1.588242 -0.719435 8 -1.794838 -1.488970 0.034070 8 -1.961685 -0.221223 -0.312947	1383.2269, 1401.4295, 1403.8934, 1421.3189, 1460.3512, 1462.564, 1476.2653, 1481.992, 1495.6464, 1504.8607, 1769.5191, 2963.1101, 3033.6092, 3038.428, 3040.6494, 3102.4461, 3107.6683, 3110.7951, 3128.2779, 3154.5482, 3169.4089
IRC:  	

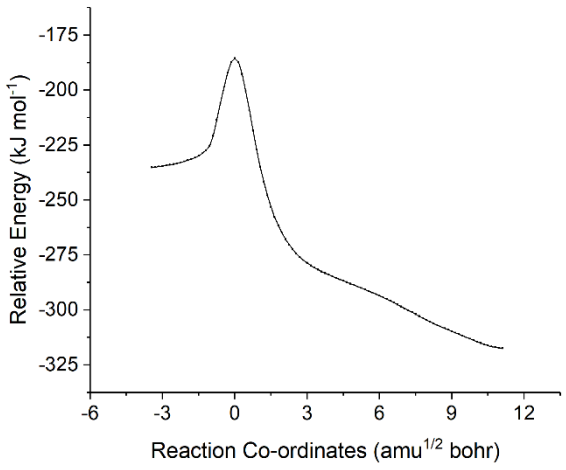
Compound: Mes Oxy + O_3 CPr_{DMFO} 2.2	**Energy (kJ mol^{-1}):** -534.818525930480
Reaction Coordinates: 6 -1.919020 -0.959574 0.280125 6 -1.400974 0.450901 0.570323 8 -0.549689 0.590814 1.427175 6 -2.066037 1.581354 -0.157660 1 -3.135864 1.571388 0.057800 1 -1.633310 2.530865 0.146770 1 -1.960973 1.437735 -1.232908 6 2.017805 -0.110141 -0.115496 6 3.011888 -0.627706 0.856267 1 4.020577 -0.525475 0.450003 1 2.967908 -0.024689 1.766328 1 2.814640 -1.667474 1.101880 6 2.050460 1.256403 -0.667204 1 1.978893 1.200222 -1.755590 1 1.160829 1.794329 -0.336461 1 2.945990 1.785484 -0.353380 1 -1.269987 -1.759236 0.675812 8 -2.979225 -1.171720 -0.248181 8 0.143589 -0.473723 -1.344512 8 1.128646 -0.931691 -0.474281	**Frequencies (cm^{-1}):** 36.6001, 54.7023, 63.415, 82.5663, 94.5904, 108.6572, 138.1355, 149.9398, 162.3128, 204.9669, 258.5808, 309.3476, 314.3382, 370.6683, 464.5625, 483.0074, 490.5077, 585.972, 594.72, 784.0162, 812.2534, 914.3613, 922.3675, 927.8266, 987.777, 1012.3435, 1063.811, 1074.3558, 1097.8847, 1248.8111, 1306.751, 1367.8396, 1387.0755, 1388.9487, 1405.5525, 1446.5177, 1457.2004, 1458.1362, 1466.7473, 1469.0909, 1480.0455, 1573.2151, 1748.0797, 1786.387, 2951.1199, 3029.286, 3039.1847, 3043.0613, 3077.8234, 3091.3687, 3101.9214, 3138.9607, 3142.2627, 3143.6408

Compound: Mes Oxy + O_3 TS_{SYN} 1	**Energy (kJ mol^{-1}):** -534.750836106521

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.309641 -0.239607 0.785086 6 1.592586 0.028284 0.021253 8 2.000735 -0.693349 -0.850369 6 2.376612 1.222177 0.524408 1 1.730194 2.035003 0.852211 1 3.051012 1.565889 -0.255289 1 2.972965 0.907869 1.384984 6 -1.212399 0.489005 -0.214384 6 -0.658570 1.684803 -0.996458 1 -0.221323 2.445329 -0.351044 1 0.065893 1.359119 -1.739204 1 -1.495538 2.143125 -1.525869 6 -2.164748 0.850300 0.930598 1 -1.753251 1.613229 1.592009 1 -3.085831 1.242911 0.495589 1 -2.419659 -0.036246 1.507711 1 0.295087 0.188091 1.783369 8 -0.157310 -1.496385 0.861355 8 -0.369825 -1.994973 -0.335552 8 -1.548384 -0.524556 -0.931369	-464.5031, 39.7641, 65.4695, 100.4754, 154.7862, 203.2515, 223.4725, 247.8715, 252.2338, 278.8153, 287.6317, 351.952, 409.8556, 442.8117, 478.5336, 548.153, 561.1297, 618.1822, 694.5184, 801.9295, 880.3942, 909.729, 958.274, 991.3133, 994.3453, 1031.2095, 1061.4952, 1072.0162, 1123.2957, 1162.3909, 1187.5601, 1195.951, 1369.0131, 1385.5481, 1388.9193, 1403.3874, 1429.734, 1465.8359, 1475.4142, 1478.9255, 1488.0494, 1495.7885, 1507.0638, 1786.7108, 3029.8372, 3033.3644, 3038.8842, 3088.3017, 3094.3861, 3099.0109, 3121.0407, 3131.3353, 3132.7259, 3144.0328
IRC  	

Compound: Mes Oxy + O_3 CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -534.799290258670
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.559092 -0.093942 -0.887184 6 -1.610145 0.761615 0.332125 8 -1.654514 0.313010 1.453835 6 -1.628502 2.240313 0.022247 1 -0.720617 2.514116 -0.517760 1 -1.690304 2.799960 0.950990 1 -2.481077 2.491876 -0.612860 6 2.103605 0.076950 -0.072309 6 1.850463 -1.131336 0.791457 1 2.041288 -0.865464 1.834819 1 0.826328 -1.484256 0.697463 1 2.550242 -1.930805 0.540596 6 3.536854 0.543088 -0.189302 1 3.989005 0.647914 0.798416 1 4.119845 -0.210539 -0.724058 1 3.587340 1.486201 -0.726549	25.756, 32.466, 59.6795, 68.9403, 74.3434, 76.5639, 82.5302, 96.1902, 119.1334, 133.2616, 213.6681, 315.1372, 343.2935, 393.8668, 467.8377, 497.8666, 543.9537, 595.6251, 691.5942, 791.3941, 820.1253, 863.3732, 889.4761, 902.7117, 970.9562, 995.0567, 1042.5735, 1090.5236, 1123.6725, 1183.9596, 1245.0277, 1385.702, 1388.2064, 1388.6345, 1401.152, 1461.8246, 1464.0065, 1465.6522, 1474.9298, 1476.5967, 1489.2045, 1498.3617, 1753.8295, 1758.4496, 3022.472, 3030.7998, 3032.7043, 3076.4512,

1 -1.594148 0.359613 -1.869446 8 -1.501938 -1.357900 -0.964798 8 -1.401135 -2.142174 0.118938 8 1.209212 0.663471 -0.652202	3086.1686, 3088.6814, 3131.0123, 3138.5276, 3145.5435, 3184.5613

Compound: Mes Oxy + O_3 TS_{SYN} 2	**Energy (kJ mol^{-1}):** -534.761576102987
Reaction Coordinates: 6 0.235237 0.128753 -0.876663 6 1.525533 -0.410075 -0.286315 8 1.919402 -1.455627 -0.756029 6 2.258804 0.332526 0.790390 1 3.186877 -0.192158 1.001412 1 2.462271 1.358363 0.481554 1 1.639695 0.405388 1.684318 6 -1.209307 -0.355636 0.274581 6 -2.410721 -0.349245 -0.673904 1 -2.546355 0.635305 -1.116134 1 -2.318239 -1.095650 -1.462750 1 -3.303753 -0.580620 -0.090681 6 -0.825000 -1.746674 0.799407 1 -0.554332 -2.431005 -0.001767 1 -0.008977 -1.684777 1.514471 1 -1.697723 -2.147133 1.317303 1 0.035487 -0.300547 -1.852806 8 -0.043428 1.445356 -0.904818 8 -0.001699 1.968334 0.308731 8 -1.167053 0.596304 1.147129	**Frequencies (cm^{-1}):** -473.9806, 64.3865, 80.3371, 149.8119, 207.4112, 208.8863, 234.3095, 243.6465, 260.406, 282.2636, 303.2425, 353.1323, 408.7603, 466.2164, 491.2692, 547.1306, 561.5524, 607.6317, 690.6367, 802.5275, 826.8206, 916.0209, 971.5595, 996.9674, 1024.3189, 1040.1003, 1058.6034, 1065.1741, 1128.1852, 1183.1503, 1191.2676, 1239.4622, 1354.7154, 1389.29, 1397.3085, 1398.8233, 1411.8265, 1454.9541, 1464.198, 1475.5414, 1485.0414, 1494.2323, 1503.292, 1750.8556, 3034.5701, 3043.8728, 3046.3842, 3094.9725, 3103.7546, 3109.8154, 3125.5191, 3140.3013, 3143.7237, 3153.7004
IRC  	

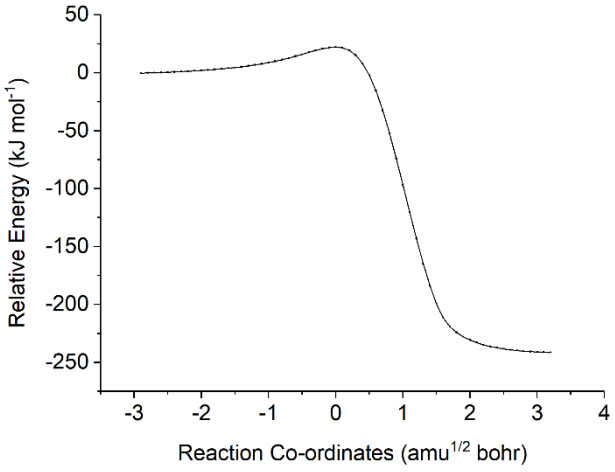
Compound: Mes Oxy + O_3 CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -534.806174822771
Reaction Coordinates: 6 1.857919 -0.465199 1.511062 6 1.916930 -0.777898 0.051499 6 1.482819 0.205575 -0.989070 1 1.478603 -0.144055 -2.014165 8 1.171926 1.422453 -0.878352 8 1.104754 2.031304 0.333187	**Frequencies (cm^{-1}):** 24.2836, 35.5953, 43.8971, 60.4944, 66.0332, 74.8258, 91.9163, 95.5158, 148.8765, 184.1353, 242.686, 323.1557, 352.3544, 389.5705, 496.1505, 498.5493, 541.2358, 583.8794, 667.1188, 789.2391, 817.1219, 863.4568, 888.5761, 901.1413,

8 2.332920 -1.826500 -0.400871 1 2.175896 -1.341995 2.069688 1 2.492736 0.393396 1.732850 1 0.847798 -0.165359 1.785750 6 -2.195995 -0.245545 -0.018333 6 -3.479765 -1.042178 -0.061004 1 -3.293334 -2.039476 -0.449737 1 -3.894578 -1.117196 0.947091 1 -4.228155 -0.534002 -0.671796 6 -2.309012 1.213760 0.347726 1 -2.926861 1.338290 1.239070 1 -1.326214 1.653521 0.501686 1 -2.818322 1.745840 -0.460396 8 -1.127719 -0.767264 -0.270380	904.0688, 1040.6037, 1050.8463, 1090.6546, 1123.6791, 1243.4168, 1259.3988, 1360.9666, 1388.8475, 1396.3479, 1398.3708, 1441.1237, 1455.758, 1461.2233, 1466.3962, 1473.9967, 1493.8767, 1510.1376, 1735.9384, 1760.7047, 3021.7191, 3031.7938, 3047.234, 3075.6494, 3084.5583, 3107.7516, 3128.1691, 3139.7368, 3144.563, 3189.0573

6.13 Ozonolysis of HFO-1234yf (Alkene 11)

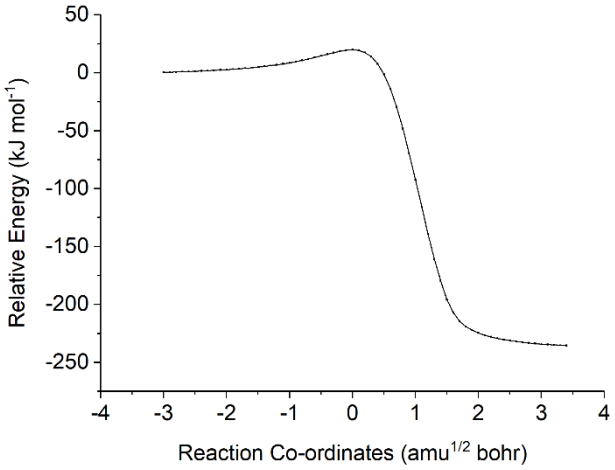
Compound: $CF_3CFCH_2 + O_3$ PRC1	**Energy (kJ mol^{-1}):** -739.704017975154
Reaction Coordinates: 6 2.366534 0.192348 0.000014 6 0.923971 -0.246650 -0.000202 6 -0.132815 0.538171 -0.001543 1 -0.008047 1.608388 -0.002625 1 -1.128809 0.121555 -0.001567 9 0.831934 -1.587107 0.001197 9 3.016742 -0.273685 -1.082685 9 2.468925 1.530510 -0.001349 9 3.015716 -0.271400 1.084312 8 -4.650726 -0.099369 0.000307 8 -4.369788 1.122942 0.001566 8 -3.705628 -0.925825 -0.001709	**Frequencies (cm^{-1}):** 2.8018, 9.7622, 13.5268, 16.7997, 36.1499, 59.3702, 71.5957, 235.0321, 239.2738, 366.5013, 415.5494, 494.267, 570.7015, 611.3137, 680.5606, 748.0155, 762.6568, 786.9689, 945.1032, 956.0301, 1139.1849, 1151.2571, 1177.1701, 1189.6372, 1249.9106, 1352.2013, 1426.4206, 1747.0728, 3178.2036, 3275.138

Compound: $CF_3CFCH_2 + O_3$ TS_{OZO} 1	**Energy (kJ mol^{-1}):** -739.686579729444
Reaction Coordinates: 6 -1.301722 -0.168739 0.139210 6 -0.069540 0.670016 -0.137723 6 0.716401 1.242251 0.813683 1 0.568747 0.983442 1.847529 1 1.293952 2.119082 0.569552 9 -2.391949 0.630610 0.158584 9 -1.511202 -1.098758 -0.793832 9 -1.208691 -0.763671 1.334270 9 -0.036038 1.134116 -1.388193 8 2.318546 -0.502838 -0.419425 8 2.518359 0.080807 0.715867 8 1.212769 -1.163515 -0.434638	**Frequencies (cm^{-1}):** -284.5197, 59.9672, 81.6435, 126.8502, 181.0213, 216.8594, 242.4476, 291.8462, 359.0811, 417.05, 477.8938, 504.9689, 573.9183, 609.601, 660.6419, 751.9521, 788.7854, 825.8995, 954.5578, 968.1963, 1067.5536, 1098.2635, 1125.741, 1168.7243, 1202.602, 1352.8469, 1412.0436, 1577.7424, 3190.092, 3293.9674
IRC:	



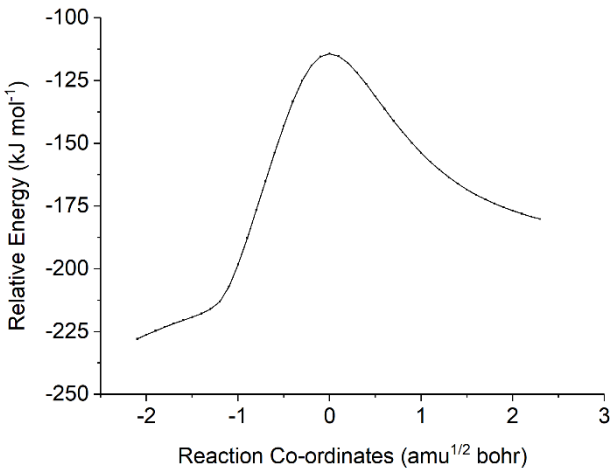
Compound: $CF_3CFCH_2 + O_3$ POZ1	**Energy (kJ mol^{-1}):** -739.797128378695
Reaction Coordinates: 6 -1.215887 0.208797 -0.082906 6 0.184908 -0.408426 0.129831 6 1.109475 0.363563 1.108437 1 1.506422 -0.350926 1.829824 1 0.630982 1.206286 1.599374 8 2.117299 0.878910 0.256960 8 2.252487 -0.170115 -0.691708 8 0.850401 -0.395257 -1.078096 9 -0.010116 -1.687709 0.596196 9 -1.107461 1.489756 -0.456922 9 -1.905318 -0.452814 -1.013462 9 -1.907090 0.167738 1.067673	**Frequencies (cm^{-1}):** 63.8141, 102.5079, 182.3465, 227.1793, 312.4554, 332.8409, 368.5427, 399.5693, 461.5239, 536.5317, 571.1624, 599.0191, 675.8711, 737.0759, 745.3646, 813.8926, 933.0012, 941.2868, 1022.1221, 1095.7224, 1116.7061, 1137.5328, 1185.3372, 1207.3091, 1233.585, 1346.0986, 1353.9955, 1489.0164, 3066.8896, 3150.1913

Compound: $CF_3CFCH_2 + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -739.688008555115
Reaction Coordinates: 6 1.242497 -0.239984 -0.128900 6 0.109980 0.759838 0.013940 6 -0.714783 1.137281 -0.997235 1 -0.668214 0.629372 -1.945531 1 -1.233867 2.079277 -0.934307 9 0.234426 1.514799 1.100668 9 1.539689 -0.846241 1.020200 9 0.937827 -1.167825 -1.048997 9 2.360425 0.396151 -0.545689 8 -2.088697 -0.921790 0.030786 8 -2.584580 0.173438 -0.433429 8 -1.273645 -0.717075 1.004812	**Frequencies (cm^{-1}):** -260.716, 60.9396, 84.7628, 121.9684, 186.6972, 210.3566, 254.1304, 288.8069, 361.1063, 423.453, 473.2666, 497.0548, 573.9981, 610.2223, 649.4718, 748.4911, 785.8867, 813.4827, 953.2475, 969.0414, 1075.8996, 1103.8236, 1123.6842, 1167.4126, 1202.5834, 1357.1061, 1411.8363, 1584.3306, 3190.0946, 3291.253
IRC:	



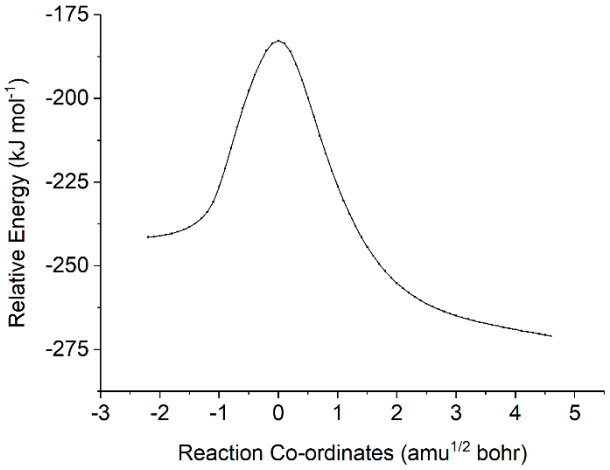
Compound: $CF_3CFCH_2 + O_3$ POZ 2	**Energy (kJ mol^{-1}):** -739.794322813255
Reaction Coordinates: 6 1.246372 -0.168078 0.099672 6 -0.191001 0.316956 -0.195205 6 -1.091184 0.461244 1.044530 1 -1.072476 1.470358 1.444145 1 -0.852362 -0.287911 1.799581 9 1.217957 -1.364820 0.701651 9 1.966941 -0.268658 -1.016693 9 1.858619 0.698366 0.926048 9 -0.074108 1.524332 -0.844404 8 -2.114253 -0.916744 -0.309054 8 -2.365350 0.234524 0.468494 8 -0.843518 -0.586051 -1.014082	**Frequencies (cm^{-1}):** 62.5132, 89.2922, 177.374, 225.3333, 306.5514, 327.7609, 370.1787, 383.4959, 464.4149, 484.5684, 569.2694, 578.7513, 689.2232, 735.1249, 745.9715, 833.2725, 937.4981, 947.591, 1017.9447, 1056.6006, 1137.732, 1156.8917, 1178.7283, 1214.4183, 1256.9172, 1313.7162, 1367.0753, 1480.8355, 3068.2629, 3161.6058

Compound: $CF_3CFCH_2 + O_3$ TS_{ANTI}	**Energy (kJ mol^{-1}):** -739.744889303011
Reaction Coordinates: 6 -1.323211 0.055491 -0.108681 6 0.151087 -0.199734 0.226234 6 1.308963 1.373380 -0.100397 1 0.941219 1.851850 0.820259 1 0.886258 1.748740 -1.042349 9 -1.478730 0.247354 -1.418125 9 -2.082051 -0.980191 0.269919 9 -1.743647 1.144465 0.544898 9 0.355723 -0.424299 1.511677 8 2.020397 -1.221720 -0.283984 8 2.449244 0.844360 -0.089699 8 0.766589 -0.980312 -0.633337	**Frequencies (cm^{-1}):** -424.4518, 50.0441, 116.1709, 141.132, 193.3669, 239.6595, 281.1479, 296.9608, 366.0627, 412.4421, 441.5573, 519.6081, 539.6682, 575.7821, 629.0636, 735.7756, 810.945, 840.983, 1080.5561, 1101.4987, 1155.0155, 1180.401, 1206.7092, 1226.2239, 1330.9602, 1346.3726, 1420.7761, 1557.0537, 2927.3856, 3005.0632
IRC:	



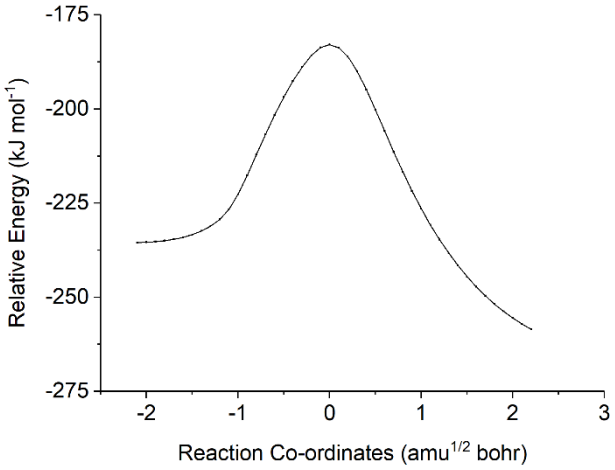
Compound: $CF_3CFCH_2 + O_3$ C_{ANTI}	**Energy (kJ mol^{-1}):** -739.776841541082
Reaction Coordinates: 6 1.373556 -0.259006 -0.115945 6 0.138511 0.563762 0.231956 9 -0.185019 0.625415 1.477947 8 -0.451523 1.207739 -0.646878 8 -1.552393 1.965126 -0.283631 9 1.470007 -0.428445 -1.428662 9 2.468239 0.389625 0.320747 9 1.324429 -1.443151 0.489424 6 -2.930388 -1.078249 -0.123109 1 -3.244913 -0.024337 -0.090866 1 -3.712585 -1.838846 -0.293104 8 -1.775018 -1.396223 0.016940	**Frequencies (cm^{-1}):** 23.739, 47.6668, 51.7628, 81.1309, 98.966, 128.1685, 131.7745, 173.6461, 189.4533, 296.5251, 347.524, 369.5338, 406.7679, 514.3385, 576.5233, 664.3793, 728.5641, 857.9193, 881.2041, 1137.7419, 1178.2712, 1216.7635, 1232.8472, 1273.0752, 1403.8184, 1527.2196, 1623.8384, 1786.6602, 2911.3223, 3007.0573

Compound: $CF_3CFCH_2 + O_3$ TS_{FO} 1	**Energy (kJ mol^{-1}):** -739.771495440171
Reaction Coordinates: 6 -1.216967 -0.270321 -0.078312 6 0.074082 0.598053 -0.115209 6 1.217915 -0.219836 1.107939 1 1.610849 0.712920 1.495511 1 0.712108 -0.895826 1.784744 9 -1.719544 -0.359412 1.164229 9 -2.153379 0.262938 -0.866089 9 -0.944412 -1.505786 -0.508257 9 -0.200364 1.781515 0.560040 8 2.576216 -0.042854 -0.576251 8 2.010908 -0.873164 0.259414 8 0.711145 0.656297 -1.172673	**Frequencies (cm^{-1}):** -384.5764, 64.7709, 100.7807, 170.0438, 226.311, 288.4162, 306.4745, 333.9714, 370.0746, 450.9903, 483.2011, 539.9964, 582.2279, 600.527, 653.3495, 685.0321, 782.1583, 918.4408, 1020.1608, 1062.9688, 1105.8913, 1171.6779, 1193.3069, 1222.7526, 1246.8546, 1258.9605, 1484.2703, 1511.4265, 3112.1632, 3236.1854
IRC:	



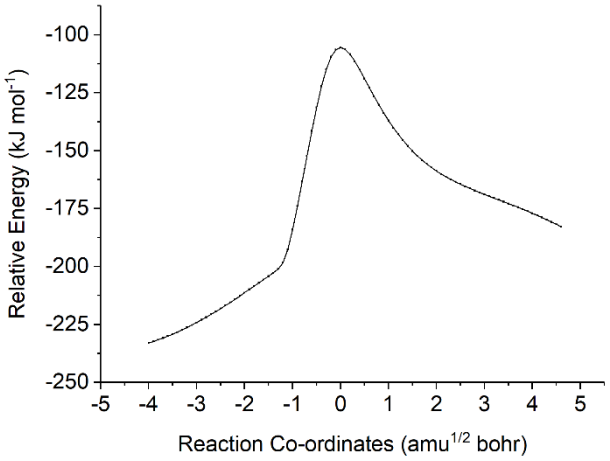
Compound: $CF_3CFCH_2 + O_3$ CPr_{FO} 1	**Energy (kJ mol^{-1}):** -739.812611750193
Reaction Coordinates: 6 1.276276 -0.317441 0.042768 6 0.199237 0.765686 0.278781 9 0.332320 1.754487 -0.609756 8 -0.466774 0.863601 1.257424 9 1.452943 -0.610239 -1.240654 9 2.442962 0.159259 0.528183 9 0.975427 -1.429876 0.713343 6 -2.711550 -0.451865 0.655072 1 -2.030034 -1.117147 1.167434 1 -3.638928 -0.080588 1.070988 8 -2.468023 -0.081048 -0.512669 8 -1.283662 -0.487955 -1.072029	**Frequencies (cm^{-1}):** 42.1251, 63.9575, 88.0625, 113.404, 161.9039, 192.8444, 220.1104, 240.5009, 279.5027, 379.8265, 428.5047, 513.3363, 528.5897, 586.6354, 680.5969, 693.1995, 716.2171, 802.101, 885.1881, 1024.7157, 1084.4537, 1147.2233, 1223.5333, 1243.7926, 1311.4472, 1417.8105, 1571.3513, 1851.8505, 3127.1564, 3272.4481

Compound: $CF_3CFCH_2 + O_3$ TS_{FO} 2	**Energy (kJ mol^{-1}):** -739.771113693420
Reaction Coordinates: 6 -1.298987 -0.198865 -0.033111 6 0.107368 0.452863 -0.197846 6 1.144499 -0.545739 0.973930 1 0.897596 -1.545399 0.634602 1 0.934082 -0.257871 1.995443 9 -1.285531 -1.449663 -0.505100 9 -1.674536 -0.244058 1.256359 9 -2.207933 0.505557 -0.707130 9 0.059625 1.695737 0.417969 8 2.550828 -0.405976 -0.680190 8 2.322631 -0.077164 0.562263 8 0.679844 0.356336 -1.287918	**Frequencies (cm^{-1}):** -378.0235, 64.8244, 111.6296, 175.0858, 229.2574, 273.908, 292.0458, 320.4111, 371.2873, 436.9077, 489.869, 537.3613, 580.4607, 591.9972, 651.465, 713.9643, 792.452, 906.042, 1012.2988, 1073.6458, 1110.1415, 1172.2038, 1190.0287, 1227.6708, 1240.8853, 1266.5903, 1481.885, 1515.8434, 3109.1164, 3237.8153
IRC	



Compound: $CF_3CFCH_2 + O_3$ CPr_{FO} 2	**Energy (kJ mol^{-1}):** -739.813259682201
Reaction Coordinates: 6 1.260836 -0.292596 -0.100143 6 0.149504 0.780864 -0.149444 9 0.297955 1.652770 0.857863 8 -0.528324 1.011186 -1.101148 9 0.919770 -1.358554 -0.820669 9 2.367461 0.250369 -0.655394 9 1.568501 -0.670948 1.136250 6 -2.843813 0.077420 -0.381769 1 -2.757537 1.070839 0.035688 1 -3.523078 -0.196672 -1.178448 8 -2.165570 -0.862809 0.084248 8 -1.243822 -0.539755 1.050455	**Frequencies (cm^{-1}):** 47.5136, 65.2631, 85.3942, 118.6927, 174.3963, 200.9237, 245.3677, 260.8967, 295.8934, 379.0472, 431.0075, 513.1768, 531.8408, 586.9013, 683.8108, 689.5254, 708.551, 800.1059, 888.7153, 1029.3867, 1075.4919, 1142.7536, 1227.7508, 1241.4539, 1305.2938, 1418.1905, 1572.9376, 1830.5607, 3129.4158, 3274.4357

Compound: $CF_3CFCH_2 + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -739.741532989524
Reaction Coordinates: 6 -1.060471 -0.333333 -0.070663 6 0.091876 0.684665 0.125441 6 1.482220 0.198652 -1.254549 1 1.873204 1.221182 -1.359152 1 0.725701 -0.102745 -1.996675 9 -0.649258 -1.568473 -0.293643 9 -1.827339 -0.320315 1.030200 9 -1.804937 0.069271 -1.108354 9 -0.322645 1.926767 -0.065492 8 1.414098 -0.600232 1.332427 8 2.158210 -0.681905 -0.678618 8 0.897312 0.609188 1.157449	**Frequencies (cm^{-1}):** -375.3467, 39.9264, 123.0034, 166.8233, 201.7191, 225.6332, 259.4709, 308.2617, 366.9875, 434.446, 474.8721, 485.108, 534.9566, 581.6948, 615.5931, 663.9282, 779.1994, 812.9961, 1093.5939, 1103.6017, 1154.7925, 1177.0012, 1215.7391, 1232.0429, 1316.4748, 1328.6756, 1437.0707, 1572.1713, 2918.396, 2990.8998
IRC	



Compound: $CF_3CFCH_2 + O_3$ CPr_{SYN}	**Energy (kJ mol^{-1}):** -739.762725474063
Reaction Coordinates: 6 1.111331 -0.309681 0.025383 6 -0.152560 0.583121 -0.030935 6 -1.146402 0.408203 1.121136 1 -1.615137 1.379800 1.293864 1 -0.683400 0.030882 2.031464 9 1.874009 -0.126592 -1.053416 9 1.838891 -0.010053 1.116237 9 0.766359 -1.600393 0.095233 9 0.282139 1.868780 -0.116658 8 -1.934787 -0.617224 -0.797867 8 -2.068196 -0.555599 0.671125 8 -0.925549 0.337047 -1.172182	**Frequencies (cm^{-1}):** 15.633, 16.7936, 37.3743, 39.162, 59.8455, 67.599, 72.3947, 183.6602, 221.2273, 270.1777, 293.4127, 363.8324, 483.1669, 493.255, 581.7978, 630.3575, 657.9854, 778.8575, 924.4956, 1154.9874, 1197.3309, 1202.6062, 1204.5994, 1265.2001, 1396.8657, 1531.6116, 1582.1827, 1810.1959, 2892.081, 2950.9964

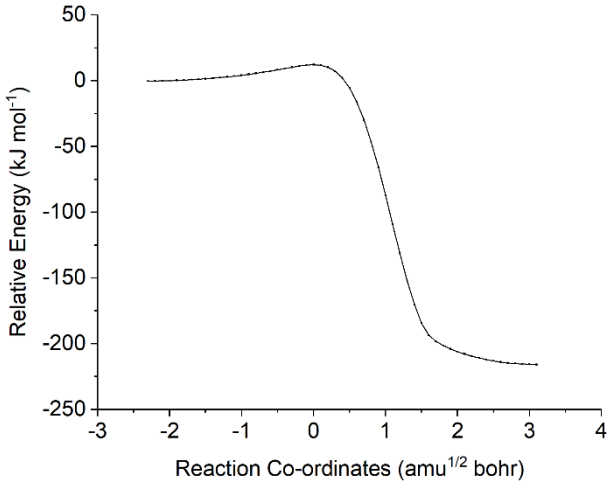
Compound: $CF_3CFCH_2 + O_3$ TS_{POZ} 1	**Energy (kJ mol^{-1}):** -739.781901277090
Reaction Coordinates: 6 1.111331 -0.309681 0.025383 6 -0.152560 0.583121 -0.030935 6 -1.146402 0.408203 1.121136 1 -1.615137 1.379800 1.293864 1 -0.683400 0.030882 2.031464 9 1.874009 -0.126592 -1.053416 9 1.838891 -0.010053 1.116237 9 0.766359 -1.600393 0.095233 9 0.282139 1.868780 -0.116658 8 -1.934787 -0.617224 -0.797867 8 -2.068196 -0.555599 0.671125 8 -0.925549 0.337047 -1.172182	**Frequencies (cm^{-1}):** -217.8941, 59.6792, 100.7244, 192.2746, 214.1565, 313.9204, 327.2066, 371.7674, 450.4214, 527.938, 571.46, 589.2847, 695.92, 711.685, 780.3448, 811.3369, 928.2147, 969.3171, 1062.8998, 1108.0534, 1115.6848, 1174.7636, 1195.1615, 1210.9755, 1223.6617, 1337.0756, 1371.2487, 1507.5895, 3038.0034, 3114.2192
IRC TS energy too close to POZ to perform IRC	

6.14 Ozonolysis of HFO-1345fz (Alkene 12)

Compound: $CF_3CF_2CHCH_2 + O_3$ PRC1.1	**Energy (kJ mol^{-1}):** -878.141781427975
Reaction Coordinates: 6 -1.236517 0.531170 0.437861 6 0.202710 0.727240 0.080330 6 0.658224 1.800873 -0.544424 1 1.711003 1.898340 -0.767660 1 0.003235 2.606036 -0.845739 1 0.856328 -0.081124 0.379248 6 -1.919744 -0.637050 -0.328049 9 -1.243216 -1.779050 -0.126061 9 -1.938175 -0.385778 -1.643467 9 -3.177157 -0.813609 0.085559 9 -1.982329 1.642636 0.201584 9 -1.350227 0.237035 1.769143 8 4.321719 0.562966 -0.489544 8 4.492690 -0.549671 0.065234 8 3.488258 -1.146765 0.521689	**Frequencies (cm^{-1}):** 9.8792, 11.2729, 14.8647, 33.4046, 37.649, 62.9296, 70.5328, 82.022, 203.2553, 220.9725, 277.2121, 316.6621, 354.7651, 378.8707, 460.3974, 523.1339, 566.9711, 580.3836, 646.9792, 731.0786, 747.3116, 768.7346, 1008.8436, 1024.0496, 1029.8492, 1037.5318, 1125.1706, 1181.8648, 1189.7479, 1191.9055, 1245.9206, 1250.1604, 1312.9506, 1327.9285, 1454.5802, 1713.1957, 3155.2576, 3188.6359, 3242.7309

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -878.131328640169
Reaction Coordinates: 6 -1.215445 1.487943 -0.230475 6 -0.592664 0.355700 -0.670308 6 0.437703 -0.357712 0.159101 6 1.884717 0.166613 -0.094155 1 -1.748700 2.121105 -0.921460 1 -1.005703 1.889757 0.748310 1 -0.612028 0.068625 -1.710977 9 0.460313 -1.684160 -0.131280 9 0.197680 -0.215237 1.486418 9 1.984001 1.456663 0.256261 9 2.773610 -0.532483 0.611367 9 2.191326 0.058631 -1.396079 8 -3.088362 0.690958 0.506913 8 -3.205106 -0.288126 -0.326652 8 -2.229257 -1.121016 -0.247890	**Frequencies (cm^{-1}):** -251.8685, 46.5152, 60.8627, 84.0151, 107.6669, 170.0386, 219.795, 241.4667, 259.808, 289.5022, 354.2552, 387.4531, 420.641, 469.5385, 487.4296, 530.0538, 581.2424, 610.3762, 664.4918, 736.683, 761.5447, 771.5974, 969.6046, 993.9601, 1025.0917, 1043.3897, 1076.9138, 1119.2093, 1156.7359, 1183.8756, 1195.8595, 1240.1666, 1292.5511, 1298.9294, 1449.086, 1580.0551, 3174.0227, 3207.193, 3268.0812

IRC:



Compound: $CF_3CF_2CHCH_2$+ O_3 POZ1.1	**Energy (kJ mol^{-1}):** -878.225644669177
Reaction Coordinates: 6 -1.481142 -1.258772 0.092572 6 -0.813024 0.055616 0.589835 6 0.414269 0.508220 -0.211423 6 1.706948 -0.287090 0.128412 1 -1.710763 -1.906849 0.938344 1 -0.908212 -1.790948 -0.660352 1 -0.539142 -0.016498 1.643623 9 0.680623 1.810549 0.057554 9 0.201061 0.391283 -1.543453 9 1.531422 -1.598446 -0.114146 9 2.731416 0.143987 -0.602293 9 2.011509 -0.143554 1.425892 8 -2.665692 -0.799630 -0.537350 8 -3.043034 0.274244 0.323027 8 -1.817332 1.046898 0.398075	**Frequencies (cm^{-1}):** 45.3202, 62.661, 76.497, 139.4397, 217.0306, 235.8331, 262.1586, 299.416, 340.963, 369.662, 398.6802, 450.879, 525.4452, 575.0189, 603.5812, 689.4584, 720.7625, 747.7636, 769.9985, 783.6651, 928.9611, 948.9021, 1005.6814, 1017.245, 1042.937, 1071.5994, 1151.6993, 1173.7314, 1197.4637, 1234.0993, 1255.292, 1299.8876, 1324.2562, 1363.7984, 1404.4211, 1501.4561, 3055.1724, 3067.1804, 3152.2089

Compound: $CF_3CF_2CHCH_2$ + O_3 PRC1.2	**Energy (kJ mol^{-1}):** -878.139007095758
Reaction Coordinates: 6 1.026704 -0.582157 -0.000016 6 -0.308571 0.090153 -0.000049 6 -0.548452 1.391691 -0.000051 1 -1.568249 1.749543 -0.000077 1 0.232632 2.137417 -0.000029 1 -1.121418 -0.626289 -0.000072 6 2.295996 0.310947 0.000018 9 2.327172 1.095912 1.087324 9 2.327223 1.095921 -1.087281 9 3.395923 -0.445893 0.000040 9 1.127188 -1.395616 -1.095594 9 1.127133 -1.395619 1.095565 8 -4.387692 1.051769 -0.000005 8 -4.798327 -0.134183 0.000049 8 -3.948828 -1.057189 -0.000010	**Frequencies (cm^{-1}):** 11.5615, 14, 15.0554, 32.165, 36.956, 63.6659, 78.7207, 97.8705, 177.8762, 218.1651, 288.791, 316.0225, 347.0276, 417.7337, 426.8409, 498.3885, 573.8987, 587.3896, 651.5009, 714.8363, 747.3627, 760.936, 982.578, 1004.3847, 1030.9237, 1088.8833, 1132.288, 1182.0928, 1182.1315, 1190.001, 1197.9348, 1250.1782, 1317.758, 1376.3304, 1472.2865, 1717.7914, 3159.1586, 3169.1975, 3243.7808

Compound: $CF_3CF_2CHCH_2$ + O_3 TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -878.127589524666
Reaction Coordinates: 6 -1.207443 -0.095965 1.565864 6 -0.633273 0.860812 0.777927 6 0.723366 0.766955 0.131258 6 1.305936 -0.642863 -0.174476 1 -2.023955 0.169511 2.218308 1 -0.740789 -1.051840 1.737809 1 -0.988212 1.881658 0.807867 9 1.626286 1.380164 0.961616 9 0.735223 1.461421 -1.033988 9 0.494998 -1.342867 -0.967933 9 1.486422 -1.334397 0.965189 9 2.491463 -0.520400 -0.775486 8 -2.602987 -1.007411 0.190110 8 -2.893329 0.053987 -0.486595 8 -1.864694 0.562394 -1.067515	**Frequencies (cm^{-1}):** -263.9454, 35.5308, 65.3488, 85.1656, 128.665, 174.9015, 218.794, 234.5999, 283.2629, 292.5673, 350.9422, 384.1623, 428.5588, 458.7717, 507.2156, 515.5332, 587.8166, 594.341, 648.2225, 733.7161, 759.2155, 770.3966, 962.6699, 981.9849, 1018.1307, 1073.5411, 1083.3322, 1115.134, 1142.1393, 1178.1561, 1184.22, 1210.6587, 1289.3436, 1359.9333, 1460.7652, 1583.6638, 3179.8362, 3190.2156, 3271.9818

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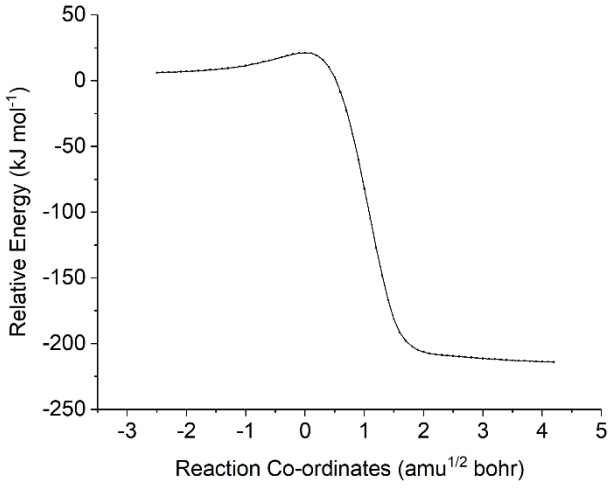

Compound: $CF_3CF_2CHCH_2 + O_3$ POZ1.2	**Energy (kJ mol^{-1}):** -878.224904510059
Reaction Coordinates: 6 -1.675355 0.258240 1.164365 6 -0.897747 0.918648 -0.005243 6 0.628553 0.775343 0.019747 6 1.259161 -0.647392 -0.034735 1 -2.436017 0.943672 1.537411 1 -1.047100 -0.100261 1.973722 1 -1.083474 1.995728 -0.027619 9 1.066763 1.361383 1.171008 9 1.151077 1.472718 -1.020439 9 0.996262 -1.256011 -1.187670 9 2.586085 -0.546389 0.100446 9 0.794296 -1.405487 0.971202 8 -2.269915 -0.872448 0.549965 8 -2.650671 -0.329787 -0.711883 8 -1.413343 0.289224 -1.170487	**Frequencies (cm^{-1}):** 26.4184, 66.3457, 91.8999, 160.5666, 195.1393, 223.7344, 272.0259, 322.562, 355.1185, 365.7783, 402.6798, 482.9657, 508.3151, 575.7327, 590.4381, 635.2202, 718.037, 740.6714, 761.8933, 773.9347, 930.0483, 956.3489, 996.6716, 1024.6946, 1053.4317, 1109.6471, 1140.6767, 1176.715, 1191.3975, 1215.8685, 1241.7288, 1293.7557, 1318.6713, 1361.7077, 1420.7409, 1502.8601, 3038.5984, 3064.8928, 3153.0076

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -878.128995844190
Reaction Coordinates: 6 1.713899 1.434917 0.492549 6 0.646173 0.633062 0.769726 6 -0.589737 0.693833 -0.088715 6 -1.575408 -0.502993 0.045653 1 2.461077 1.629378 1.245130 1 1.721460 2.062809 -0.385028 1 0.524902 0.172874 1.738139 9 -0.285844 0.840267 -1.399610 9 -1.310264 1.802431 0.283000 9 -1.842192 -0.722884 1.345064 9 -1.072823 -1.620161 -0.478035 9 -2.722502 -0.224051 -0.578787 8 3.094709 0.067249 -0.474847 8 2.768086 -0.999907 0.171619	**Frequencies (cm^{-1}):** -237.1764, 22.8776, 67.1404, 82.2527, 114.1043, 172.085, 217.9739, 233.1311, 275.5604, 298.005, 343.4735, 375.1809, 401.3593, 447.7179, 497.2209, 524.5576, 583.3496, 595.9025, 697.0222, 733.321, 758.2642, 774.5082, 970.0289, 1008.4917, 1026.4475, 1048.5436, 1081.1016, 1081.8754, 1133.2057, 1175.6821, 1206.2228, 1240.9817, 1299.8893, 1322.7218, 1450.303, 1581.572, 3172.0816, 3213.9879, 3265.9439

8 1.540409 -1.329640 -0.004049	

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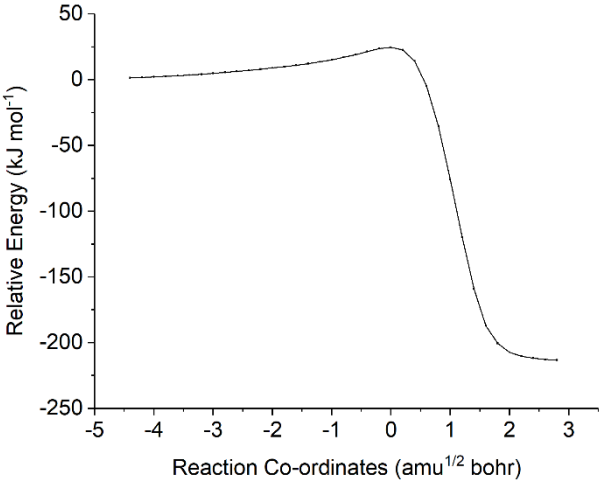
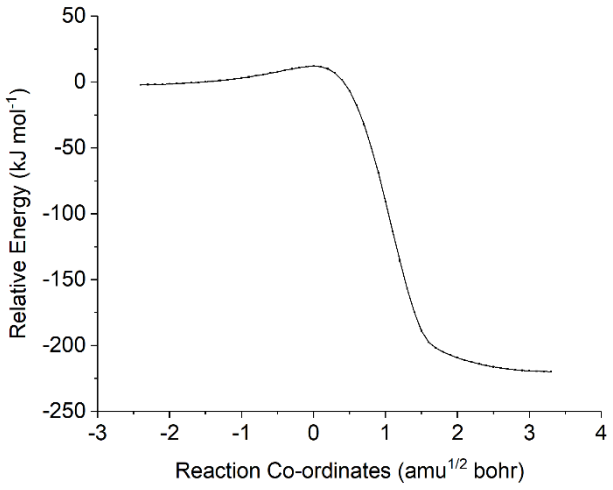


Compound: $CF_3CF_2CHCH_2 + O_3$ POZ1.3	**Energy (kJ mol^{-1}):** -878.226966377122
Reaction Coordinates: 6 2.068577 0.956273 0.424907 6 0.830250 0.038793 0.635869 6 -0.419734 0.566420 -0.075509 6 -1.679276 -0.338480 0.024652 1 2.573939 1.130579 1.374537 1 1.840008 1.895323 -0.072026 1 0.601343 -0.069467 1.697103 9 -0.181922 0.802326 -1.384024 9 -0.742677 1.755322 0.513216 9 -1.938033 -0.610743 1.314334 9 -2.737815 0.286561 -0.496450 9 -1.498474 -1.487922 -0.624951 8 2.880817 0.200138 -0.457263 8 2.665696 -1.123562 0.026564 8 1.212999 -1.202123 0.060917	**Frequencies (cm^{-1}):** 44.2044, 64.7431, 77.5873, 131.1057, 216.0336, 233.5827, 262.9289, 299.1599, 341.9378, 372.3824, 402.0765, 444.6021, 524.669, 577.8985, 615.9997, 669.3166, 727.9152, 739.3241, 769.659, 783.0207, 928.344, 937.8548, 1001.7575, 1036.7278, 1050.0949, 1078.9292, 1124.0817, 1186.0785, 1205.7748, 1229.4852, 1255.8886, 1294.9825, 1329.8955, 1359.9716, 1400.7825, 1501.3593, 3057.0616, 3068.8621, 3140.3132

Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.1	**Energy (kJ mol^{-1}):** -878.143298472086
Reaction Coordinates: 6 -0.932594 1.582928 -0.620343 6 -0.276634 0.434742 -0.692503 6 0.709504 -0.015349 0.339389 6 2.169642 -0.109118 -0.187234 1 -1.646993 1.858606 -1.381981 1 -0.779070 2.275501 0.195008 1 -0.419017 -0.258931 -1.510064 9 0.377873 -1.266019 0.784273 9 0.733396 0.807454 1.420355 9 2.608689 1.099555 -0.560559 9 2.223289 -0.925636 -1.251327 9 2.989423 -0.585559 0.752404 8 -3.902428 0.685743 0.363717	**Frequencies (cm^{-1}):** 10.6521, 15.0289, 16.4412, 37.9615, 50.9073, 66.3684, 88.0201, 125.0772, 202.1667, 220.2032, 277.0756, 315.1452, 354.5689, 378.6379, 459.194, 522.9282, 565.7729, 580.2998, 646.2519, 729.5036, 746.9122, 768.7139, 1009.0499, 1019.8311, 1023.9611, 1037.6217, 1123.4635, 1182.9974, 1187.5537, 1193.1183, 1243.088, 1246.301, 1312.7889, 1325.6119, 1456.6463, 1707.3894, 3158.5205, 3187.7715, 3246.4749

8 -3.710008 -0.554485 0.321410 8 -3.333620 -1.056577 -0.765770	

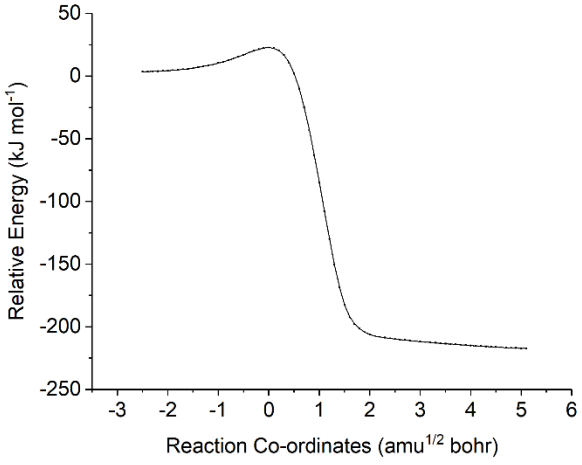
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -878.131034335178
Reaction Coordinates: 6 1.190001 1.519627 0.276042 6 0.573981 0.403234 0.766992 6 -0.407965 -0.389329 -0.047815 6 -1.857677 0.183660 0.011077 1 1.671205 2.209364 0.949683 1 1.016742 1.853253 -0.735412 1 0.556887 0.195474 1.825899 9 -0.491412 -1.668799 0.396252 9 -0.051533 -0.415465 -1.360783 9 -1.896602 1.418739 -0.508256 9 -2.273020 0.248110 1.284941 9 -2.701627 -0.588439 -0.673609 8 3.155990 0.777111 -0.221302 8 2.850818 -0.461094 -0.424204 8 2.304799 -1.004587 0.604898	**Frequencies (cm^{-1}):** -262.9292, 45.7288, 60.2135, 84.718, 105.674, 172.9141, 217.8631, 228.6404, 263.5263, 291.2651, 353.8901, 388.8815, 420.9498, 476.7102, 494.8223, 533.874, 580.3525, 613.8902, 662.1593, 745.9821, 754.3414, 771.9327, 974.8388, 985.1461, 1028.2646, 1042.8705, 1074.8484, 1118.3319, 1159.8399, 1184.8255, 1195.3548, 1233.094, 1289.5409, 1296.3925, 1443.9672, 1576.2241, 3175.3436, 3211.3284, 3270.31
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.1	**Energy (kJ mol^{-1}):** -878.226983332881
Reaction Coordinates: 6 1.442878 1.258271 0.004513 6 0.815219 -0.016401 0.635149 6 -0.418509 -0.561476 -0.102512 6 -1.684920 0.326398 0.045814 1 1.317565 2.145026 0.619956 1 1.072681 1.428004 -1.004726 1 0.549928 0.124433 1.682234 9 -0.735713 -1.778585 0.404737 9 -0.175417 -0.712927 -1.426737 9 -1.461515 1.551013 -0.463407 9 -2.723299 -0.211492 -0.587946 9 -1.997125 0.468975 1.342970 8 2.828251 0.949663 -0.010380 8 2.800007 -0.428163 -0.373580	**Frequencies (cm^{-1}):** 44.5308, 73.425, 86.788, 139.2935, 214.8697, 232.1562, 267.8255, 298.4755, 340.417, 367.7882, 413.0171, 458.0614, 527.6602, 571.7052, 607.1067, 672.1154, 716.83, 732.2008, 755.3072, 801.1359, 925.7964, 941.4223, 998.7884, 1005.8708, 1057.7656, 1078.5876, 1156.0363, 1172.5531, 1191.4808, 1236.9797, 1251.9412, 1294.8535, 1323.589, 1360.9366, 1397.9815, 1499.9499, 3077.0529, 3089.9436, 3144.4833

8 1.867923 -0.970384 0.606232	

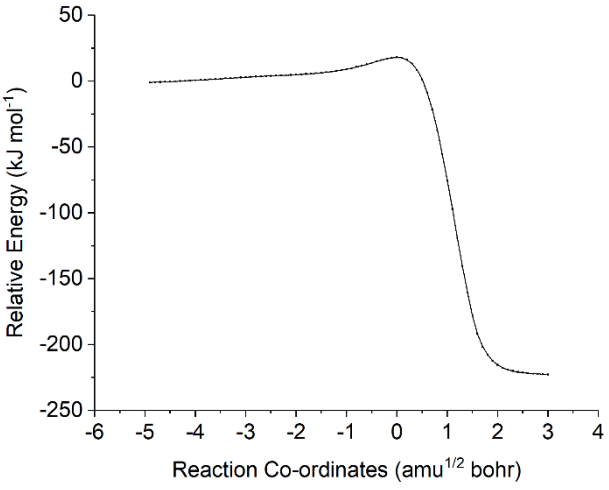
Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.2	**Energy (kJ mol^{-1}):** -878.143726505406
Reaction Coordinates: 6 -0.929864 0.742644 0.098633 6 0.228025 0.637060 1.039694 6 0.676909 -0.457605 1.635306 1 1.529898 -0.403150 2.295838 1 0.229543 -1.430783 1.497574 1 0.699445 1.598494 1.204854 6 -1.733109 -0.546646 -0.219955 9 -2.262288 -1.066880 0.896801 9 -0.941649 -1.472717 -0.782822 9 -2.727442 -0.275928 -1.067864 9 -0.495419 1.233600 -1.102796 9 -1.829220 1.649448 0.585606 8 3.429338 -1.168130 -0.004697 8 3.444299 -0.139455 -0.724516 8 3.425551 0.979461 -0.155871	**Frequencies (cm^{-1}):** 9.6204, 15.4637, 17.084, 39.1426, 48.6847, 81.7188, 94.1674, 120.5956, 176.2415, 218.0713, 288.2365, 312.2791, 347.0333, 416.5943, 426.5513, 498.0488, 573.5807, 587.0454, 651.3666, 711.0839, 747.0108, 760.9173, 981.2825, 1003.6475, 1022.1198, 1090.1209, 1132.2266, 1181.1905, 1181.5656, 1188.0612, 1199.5517, 1244.4236, 1315.5223, 1375.9186, 1473.6869, 1712.4531, 3161.4402, 3169.43, 3246.7236

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -878.128280531763
Reaction Coordinates: 6 -1.239465 0.391379 1.531729 6 -0.612711 1.089450 0.534709 6 0.744869 0.779476 -0.038223 6 1.240564 -0.693990 -0.008422 1 -2.006132 0.876879 2.112421 1 -0.841804 -0.530619 1.924335 1 -0.904376 2.109091 0.326670 9 1.672032 1.506501 0.665503 9 0.824073 1.199890 -1.325225 9 0.370853 -1.502122 -0.625510 9 1.384553 -1.120446 1.257471 9 2.421313 -0.793948 -0.618137 8 -2.853832 -0.561701 0.487473 8 -2.318223 -0.637420 -0.686826 8 -1.965776 0.516355 -1.134284	**Frequencies (cm^{-1}):** -285.7393, 36.5395, 73.0945, 81.7421, 127.9564, 176.7332, 219.3405, 230.0436, 278.0444, 296.7981, 352.9024, 382.7606, 437.3771, 470.0553, 505.9447, 528.7509, 590.0696, 592.2243, 648.3149, 747.2529, 759.8374, 764.0507, 970.0373, 977.428, 1021.7369, 1071.0593, 1080.4107, 1111.436, 1143.0665, 1177.0123, 1185.0736, 1207.1537, 1287.3031, 1359.5582, 1454.0313, 1576.4673, 3182.0756, 3193.3038, 3273.4742
IRC:	

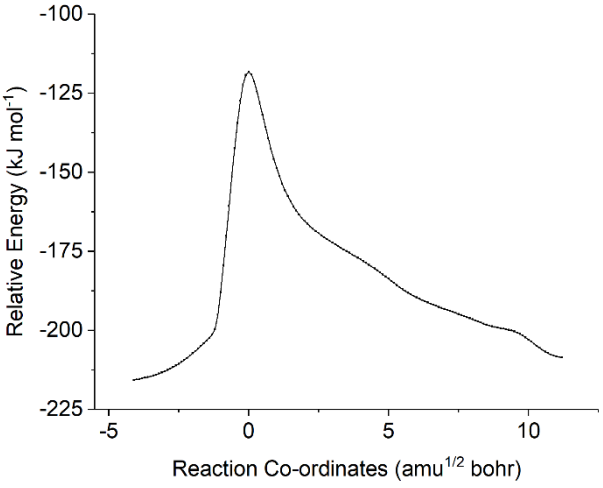


Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.2	**Energy (kJ mol^{-1}):** -878.228055342350
Reaction Coordinates: 6 -1.753991 0.622009 0.966387 6 -0.912193 0.887997 -0.314087 6 0.610684 0.771106 -0.133699 6 1.245930 -0.622362 0.145544 1 -2.296559 1.503284 1.298331 1 -1.150431 0.216446 1.775079 1 -1.072631 1.893045 -0.705907 9 0.961260 1.588028 0.902481 9 1.212799 1.247254 -1.253329 9 1.041703 -1.457757 -0.870925 9 2.563962 -0.479374 0.321006 9 0.735032 -1.165963 1.261269 8 -2.726450 -0.316842 0.521322 8 -1.993310 -1.068752 -0.447439 8 -1.437208 -0.008778 -1.273494	**Frequencies (cm^{-1}):** 47.9223, 70.352, 92.1224, 167.7802, 197.2627, 223.1259, 275.2895, 321.7806, 352.356, 362.1329, 403.2616, 497.256, 518.8909, 571.3127, 593.0343, 649.075, 699.6232, 731.5869, 761.9929, 782.781, 922.4345, 945.9983, 1000.4315, 1042.0624, 1049.2011, 1104.4041, 1143.1138, 1173.4643, 1191.6124, 1214.3423, 1234.035, 1286.8625, 1299.3839, 1359.9943, 1414.8875, 1513.0213, 3077.9226, 3084.3567, 3141.7154

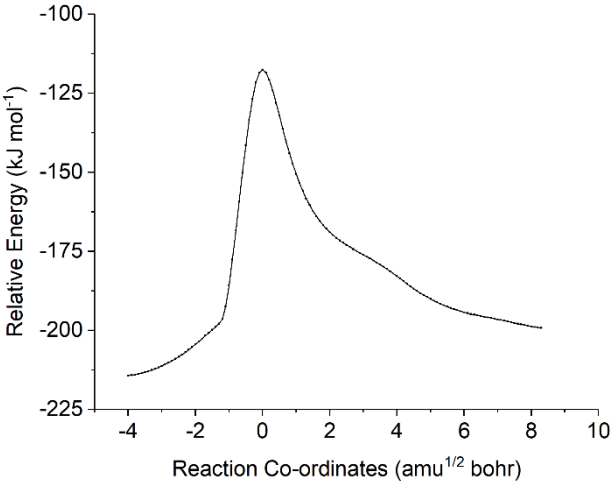
Compound: $CF_3CF_2CHCH_2 + O_3$ PRC 2.3	**Energy (kJ mol^{-1}):** -878.140337910834
Reaction Coordinates: 6 0.795004 2.075660 0.108036 6 -0.040931 1.257416 0.728737 6 -1.261503 0.682219 0.081013 6 -1.208668 -0.862164 -0.092577 1 1.657037 2.476491 0.620558 1 0.643944 2.370312 -0.920690 1 0.103575 0.959425 1.758476 9 -1.484364 1.207540 -1.151944 9 -2.363713 0.946406 0.845648 9 -2.339578 -1.326949 -0.626094 9 -1.023752 -1.454740 1.096548 9 -0.189596 -1.204499 -0.895707 8 3.367671 0.318026 -0.828464 8 3.065269 -0.722233 -0.193697 8 2.879692 -0.625148 1.043955	**Frequencies (cm^{-1}):** 13.9294, 17.4663, 21.143, 36.2041, 47.8907, 67.9227, 90.8125, 122.6484, 200.0749, 220.2201, 278.3247, 314.4285, 354.3369, 378.6923, 458.762, 522.8694, 566.1051, 580.0621, 647.0074, 729.5473, 747.2036, 768.623, 1009.6519, 1020.0518, 1024.0725, 1036.5779, 1126.4821, 1179.1538, 1186.1086, 1193.9366, 1243.7111, 1246.7655, 1313.2581, 1325.3967, 1456.6071, 1707.6325, 3158.9084, 3186.796, 3246.8065

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -878.126204877084
Reaction Coordinates: 6 1.725996 1.406097 0.608681 6 0.625259 0.628467 0.826305 6 -0.502386 0.622687 -0.171026 6 -1.629617 -0.413389 0.099380 1 2.396558 1.631522 1.421347 1 1.825206 1.992884 -0.292200 1 0.408208 0.234515 1.806443 9 -0.044261 0.428631 -1.435438 9 -1.118405 1.848215 -0.160925 9 -2.637246 -0.232219 -0.757251 9 -2.097729 -0.247820 1.349036 9 -1.189988 -1.665712 -0.022331 8 3.205691 -0.014517 -0.087376 8 2.410578 -0.931317 -0.526751 8 1.614127 -1.366910 0.379946	**Frequencies (cm^{-1}):** -253.9467, 27.6194, 64.3472, 80.5302, 113.2473, 173.37, 213.4668, 220.4703, 280.9776, 289.7567, 346.3492, 374.4681, 411.7751, 455.2236, 502.1917, 530.3331, 582.8332, 594.3762, 701.1745, 738.0915, 752.4013, 770.3841, 967.9284, 1002.9547, 1020.8741, 1053.7359, 1078.6464, 1084.8731, 1131.3627, 1176.2823, 1204.3163, 1234.519, 1297.3635, 1324.4983, 1447.4626, 1578.5854, 3171.7828, 3218.6068, 3267.756
IRC:  	

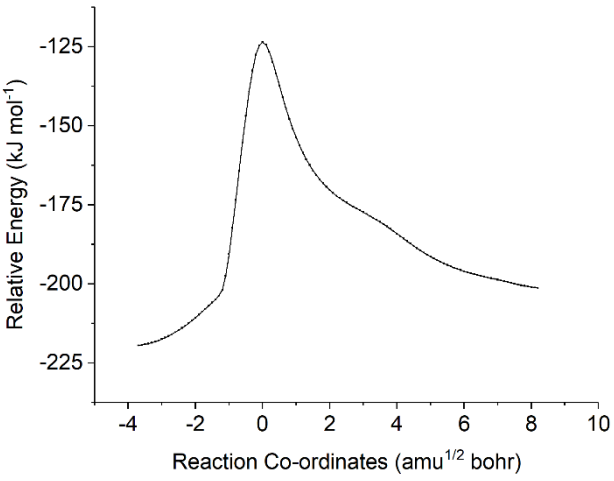
Compound: $CF_3CF_2CHCH_2 + O_3$ POZ 2.3	**Energy (kJ mol^{-1}):** -878.225983904001
Reaction Coordinates: 6 2.056416 0.986667 0.368416 6 0.824289 0.076107 0.641117 6 -0.398124 0.514901 -0.176605 6 -1.698059 -0.290814 0.095034 1 2.340342 1.586491 1.228686 1 1.900558 1.613565 -0.508659 1 0.548207 0.061794 1.694332 9 -0.151821 0.461339 -1.504464 9 -0.665231 1.814676 0.150593 9 -1.981543 -0.262259 1.408580 9 -2.723271 0.247131 -0.569630 9 -1.563316 -1.562480 -0.281660 8 3.098750 0.048031 0.150622 8 2.413600 -0.979693 -0.561864 8 1.271449 -1.226923 0.309629	**Frequencies (cm^{-1}):** 40.2086, 64.8579, 92.6896, 130.8291, 215.699, 233.8287, 263.8061, 298.2783, 338.1326, 366.5094, 416.226, 449.4973, 527.6184, 576.3057, 621.4072, 673.0262, 711.5844, 729.5339, 761.9613, 791.1097, 920.7236, 935.2848, 1000.7288, 1023.8434, 1042.6045, 1102.1431, 1120.645, 1184.4084, 1204.4831, 1235.6017, 1246.8055, 1286.151, 1330.6358, 1356.0678, 1395.4919, 1503.4997, 3069.5139, 3095.9757, 3141.8284

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -878.185149537149
Reaction Coordinates: 6 1.612496 1.405798 0.314271 6 0.837940 -0.264420 -0.380427 6 -0.528258 -0.644643 0.157072 6 -1.633877 0.409704 -0.138454 1 1.015795 2.046698 -0.350830 1 1.267541 1.351895 1.354912 1 0.902242 -0.009853 -1.430866 9 -0.926553 -1.805578 -0.434267 9 -0.489535 -0.849859 1.490720 9 -1.639719 0.707904 -1.446555 9 -2.826838 -0.068308 0.200560 9 -1.410288 1.534514 0.551429 8 2.838403 1.251797 0.055367 8 2.956864 -0.761507 -0.457306 8 1.794858 -1.052218 0.083816	**Frequencies (cm^{-1}):** -410.7211, 35.4565, 64.4701, 115.9392, 125.4556, 173.8612, 218.8248, 245.5775, 253.8434, 315.9323, 358.4816, 372.6244, 430.4355, 473.984, 513.1193, 535.4215, 549.7502, 596.4287, 636.982, 737.5812, 828.4935, 880.1703, 973.5688, 1016.4138, 1104.2432, 1134.2492, 1154.4767, 1186.1443, 1200.9677, 1222.2792, 1233.9885, 1271.9367, 1322.1525, 1401.7932, 1409.8475, 1552.8677, 2934.544, 3011.2965, 3171.3174
IRC:  	

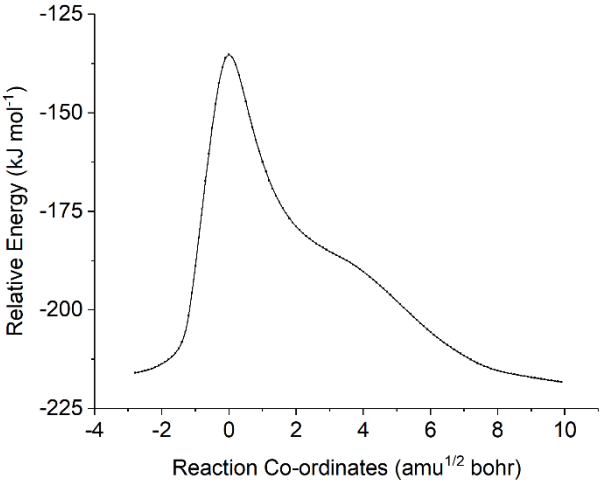
Compound: $CF_3CF_2CHCH_2 + O_3$ C_{ANTI} 1	**Energy (kJ mol^{-1}):** -878.217442305939
Reaction Coordinates: 6 3.048840 1.215818 0.049682 6 0.661739 -0.731100 -0.475519 6 -0.808800 -0.758565 -0.128847 6 -1.434687 0.651626 0.103462 1 3.348346 1.146331 1.105979 1 3.841941 1.042215 -0.692375 1 1.011076 -0.371252 -1.432560 9 -1.459947 -1.321298 -1.183655 9 -1.035188 -1.503236 0.967504 9 -1.217617 1.424994 -0.963443 9 -2.751119 0.528514 0.286276 9 -0.900279 1.220540 1.181478 8 1.926148 1.543153 -0.275686 8 2.778940 -1.223478 0.057381 8 1.454092 -1.223375 0.359910	**Frequencies (cm^{-1}):** 21.7524, 60.3706, 63.2349, 75.8706, 95.2498, 154.9196, 184.6019, 220.5153, 241.4755, 261.6599, 286.006, 330.7034, 356.1271, 379.0355, 406.0506, 425.2923, 482.7281, 531.3688, 590.3276, 624.549, 730.5959, 831.2543, 886.1366, 958.6118, 1056.2563, 1132.043, 1175.7641, 1198.7188, 1216.4605, 1237.2984, 1258.4791, 1297.208, 1348.1177, 1524.3012, 1551.6116, 1743.374, 2940.2776, 3007.3874, 3218.2102

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -878.187251466993
Reaction Coordinates: 6 1.966336 -1.004623 -0.793336 6 0.877978 -0.227355 0.626175 6 -0.607672 -0.519929 0.538832 6 -1.458151 0.363697 -0.422064 1 1.922495 -2.016733 -0.365983 1 1.318987 -0.831328 -1.661459 1 1.384914 -0.717993 1.449605 9 -1.150771 -0.397179 1.779967 9 -0.761142 -1.813031 0.156231 9 -0.953889 0.324898 -1.661447 9 -2.707778 -0.101050 -0.456291 9 -1.482514 1.628950 -0.002941 8 3.042357 -0.349928 -0.681955 8 2.512040 1.207831 0.594122 8 1.221540 1.031100 0.405397	**Frequencies (cm^{-1}):** -418.4449, 42.1802, 67.3174, 96.8445, 140.51, 157.2943, 218.5922, 244.9642, 265.3093, 338.641, 354.149, 383.3285, 415.4344, 484.7322, 516.8936, 525.7433, 550.6504, 599.7717, 643.4242, 710.69, 790.3154, 857.6712, 987.1169, 1100.2156, 1105.816, 1121.6389, 1153.3489, 1183.3814, 1199.6355, 1213.1668, 1223.1965, 1270.6172, 1328.4843, 1399.8279, 1411.3928, 1555.0234, 2939.2028, 3020.7832, 3153.4617
IRC:  	

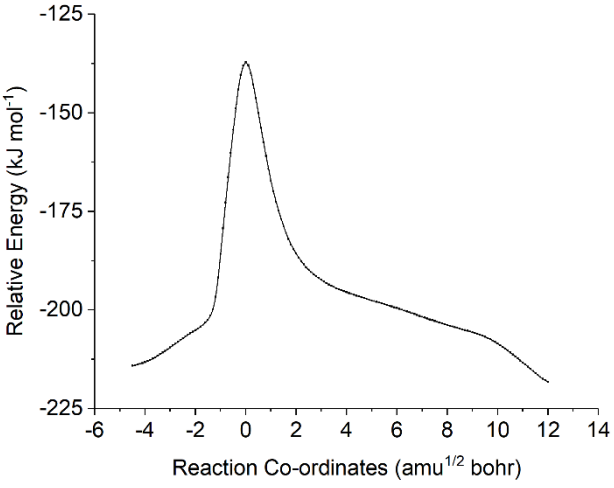
Compound: $CF_3CF_2CHCH_2 + O_3$ C_{ANTI} 2	**Energy (kJ mol^{-1}):** -878.217388987709
Reaction Coordinates: 6 4.394194 -0.177693 -0.000004 6 0.672116 0.052462 0.000003 6 -0.649639 -0.666423 0.000002 6 -1.934170 0.211555 -0.000002 1 4.049553 0.868288 -0.000004 1 5.482420 -0.360222 -0.000009 1 1.612244 -0.503398 0.000004 9 -0.694170 -1.469284 1.095482 9 -0.694167 -1.469289 -1.095474 9 -1.971869 0.984001 -1.088518 9 -3.007717 -0.580834 -0.000003 9 -1.971873 0.984004 1.088510 8 3.610859 -1.095812 0.000000 8 1.847087 1.969757 0.000003 8 0.669423 1.305873 0.000002	**Frequencies (cm^{-1}):** 16.9931, 55.0188, 55.4791, 72.1958, 100.2692, 107.152, 130.0457, 158.8648, 178.3775, 213.4398, 233.9815, 259.0309, 337.4695, 368.9536, 379.8365, 393.6261, 481.6903, 529.9689, 591.7952, 643.7123, 693.9922, 788.9396, 961.106, 973.3076, 1112.7973, 1113.4334, 1183.9023, 1207.3913, 1212.1435, 1222.0298, 1276.1492, 1339.8434, 1379.57, 1524.0824, 1554.2167, 1784.9011, 2914.7637, 3003.6302, 3062.3179

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{ANTI} 3	**Energy (kJ mol^{-1}):** -878.184687501881
Reaction Coordinates: 6 -2.345072 1.105757 0.145356 6 -0.815259 -0.086648 0.334580 6 0.468832 0.548060 -0.156328 6 1.746941 -0.296727 0.132539 1 -2.082227 1.699453 1.033050 1 -2.107105 1.570289 -0.820617 1 -0.906889 -0.255542 1.400399 9 0.621035 1.734336 0.487215 9 0.420827 0.778813 -1.485030 9 1.683176 -1.464660 -0.510783 9 2.836379 0.358316 -0.263067 9 1.839245 -0.535555 1.448681 8 -3.315588 0.300361 0.224814 8 -2.385323 -1.563523 0.043574 8 -1.279388 -1.046600 -0.448745	**Frequencies (cm^{-1}):** -412.4762, 41.8326, 58.7804, 90.3238, 128.5461, 185.4369, 192.8816, 226.1049, 275.034, 345.0588, 361.8574, 383.1289, 414.4096, 463.164, 507.0612, 531.4281, 550.6522, 592.2678, 639.2766, 736.1057, 826.1605, 873.4859, 983.9466, 1028.1781, 1104.0411, 1145.7766, 1167.3253, 1193.4624, 1204.8899, 1220.4882, 1237.2047, 1268.1015, 1300.6037, 1400.8299, 1406.6919, 1555.1306, 2932.9204, 3006.928, 3169.3833
IRC:  	

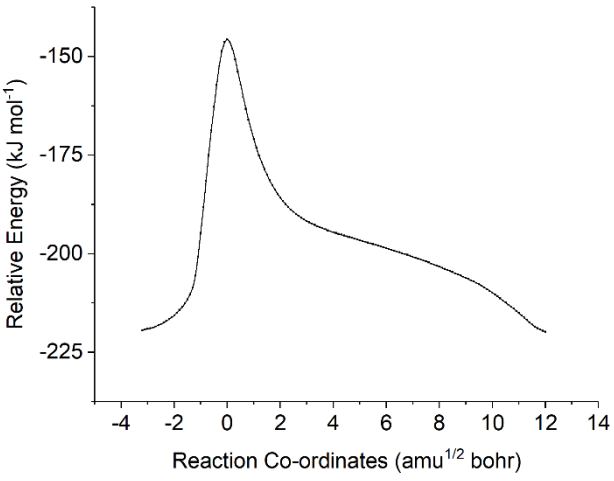
Compound: $EtCHCMe_2 + O_3$ C_{ANTI} 3	**Energy (kJ mol^{-1}):** -878.213470266616
Reaction Coordinates: 6 -3.660603 -0.402862 -0.146371 6 -0.660991 0.224629 -0.324135 6 0.552941 -0.483533 0.232565 6 1.888943 0.208297 -0.183610 1 -4.060109 -0.146242 0.845585 1 -4.171068 0.050592 -1.008480 1 -0.981266 0.078276 -1.345589 9 0.574684 -1.740085 -0.265991 9 0.515122 -0.536276 1.576324 9 1.940055 1.444020 0.320478 9 2.931416 -0.487519 0.260144 9 1.953980 0.286935 -1.520578 8 -2.760262 -1.207459 -0.283687 8 -2.350940 1.660708 -0.051902 8 -1.232124 1.051066 0.423637	**Frequencies (cm^{-1}):** 24.6187, 52.1716, 58.6166, 67.0842, 89.6055, 144.1909, 188.1244, 220.5349, 254.9541, 263.2544, 292.0326, 345.4654, 356.6234, 391.333, 411.4932, 417.8418, 479.632, 533.8024, 588.296, 632.7926, 724.4713, 815.479, 893.2168, 963.0413, 1051.1914, 1161.8621, 1172.1598, 1193.9585, 1205.8268, 1238.8724, 1257.4394, 1293.2058, 1347.1651, 1522.9163, 1551.0644, 1734.9883, 2942.7355, 3010.641, 3218.3356

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.1	**Energy (kJ mol^{-1}):** -878.191870642997
Reaction Coordinates: 6 -1.666865 -1.289336 0.341985 6 -0.725088 0.370932 0.804177 6 0.435314 0.536746 -0.220010 6 1.690657 -0.317508 0.099447 1 -2.123190 -1.414883 1.314952 1 -0.992406 -2.038994 -0.047244 1 -0.393642 -0.005060 1.782973 9 0.044080 0.239665 -1.483050 9 0.837415 1.830946 -0.208199 9 1.384855 -1.631341 0.082254 9 2.152205 -0.020608 1.322503 9 2.659491 -0.104727 -0.787252 8 -2.434965 -0.765991 -0.593506 8 -3.235791 0.153951 -0.106023 8 -1.653905 1.215606 0.756957	**Frequencies (cm^{-1}):** -393.1971, 31.1371, 62.7836, 100.741, 150.7392, 184.3902, 217.74, 260.0773, 288.8735, 313.8745, 352.3384, 380.4285, 442.412, 492.131, 525.0755, 570.4812, 580.6364, 589.256, 643.7908, 735.0275, 783.2452, 894.111, 938.5579, 1007.4483, 1059.3028, 1118.3931, 1152.071, 1161.248, 1179.2866, 1221.0667, 1238.6421, 1275.1796, 1322.0673, 1365.0007, 1483.7941, 1491.8188, 2959.746, 3125.0961, 3254.9611
IRC:  	

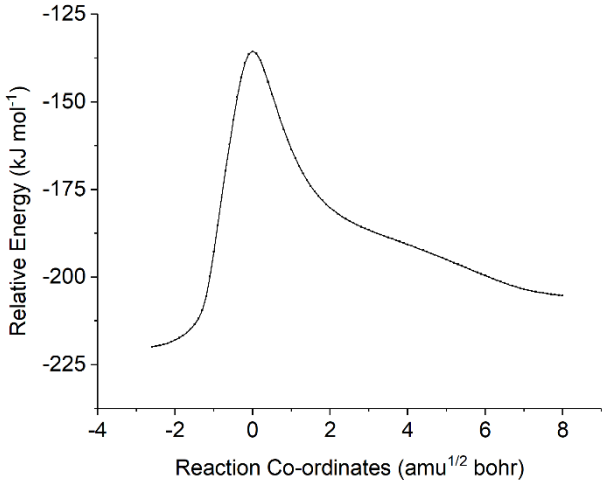
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.1	**Energy (kJ mol^{-1}):** -878.221138678696
Reaction Coordinates: 6 -1.127851 0.398599 0.511237 6 -0.321163 1.497445 -0.235536 1 0.761698 1.297807 -0.305131 8 -0.863444 2.473644 -0.663389 6 -1.343320 -0.883951 -0.331068 9 -0.156999 -1.383201 -0.713432 9 -2.055717 -0.601205 -1.426859 9 -1.989036 -1.818183 0.371020 9 -0.423100 0.046817 1.623969 9 -2.333109 0.857322 0.892356 6 4.420411 -0.678201 0.171644 1 5.164636 -0.104241 -0.367507 1 4.610808 -1.595150 0.711612 8 3.234814 -0.279768 0.193807 8 2.918136 0.866660 -0.462933	**Frequencies (cm^{-1}):** 9.9051, 12.4069, 18.7233, 31.9423, 44.5688, 63.7407, 84.3027, 93.5374, 203.5268, 212.684, 260.1576, 310.3685, 357.3105, 378.0548, 446.7042, 530.4741, 535.3708, 576.4928, 599.5383, 676.9456, 721.7579, 788.3761, 899.9906, 936.3491, 979.9024, 1087.8306, 1136.1265, 1183.1457, 1192.8531, 1228.1979, 1241.8796, 1317.3742, 1408.8512, 1433.6968, 1555.5953, 1822.9888, 2964.0595, 3115.8508, 3265.9796

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.2	**Energy (kJ mol^{-1}):** -878.196099775528
Reaction Coordinates: 6 2.094798 0.846546 -0.674941 6 0.761663 0.841902 0.715865 6 -0.646809 0.767107 0.069133 6 -1.274914 -0.642008 -0.106711 1 2.869109 1.319642 -0.084878 1 1.727584 1.323564 -1.573077 1 0.967892 1.888075 0.999725 9 -1.481216 1.482063 0.872790 9 -0.658715 1.380310 -1.149786 9 -1.466579 -1.232198 1.070607 9 -0.486798 -1.413664 -0.863510 9 -2.461421 -0.526940 -0.720049 8 2.194662 -0.466016 -0.804158 8 2.624129 -1.026037 0.303730 8 1.158653 -0.085285 1.468887	**Frequencies (cm^{-1}):** -396.6204, 26.3368, 70.6211, 94.7554, 158.1296, 191.2392, 221.2302, 266.7036, 294.3232, 308.1402, 351.6752, 395.1605, 456.6452, 500.3507, 515.6803, 570.5036, 585.725, 596.2072, 638.9174, 687.5652, 761.9465, 893.7987, 942.6459, 1060.1255, 1090.7246, 1105.47, 1141.5147, 1160.4382, 1192.1456, 1212.507, 1234.6097, 1273.4461, 1292.0787, 1363.3247, 1484.599, 1495.7038, 2922.8539, 3121.0855, 3249.1406
IRC:  	

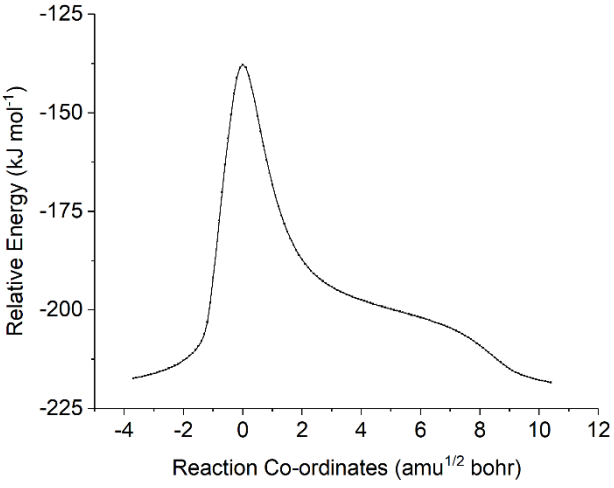
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.2	**Energy (kJ mol^{-1}):** -878.220855101528
Reaction Coordinates: 6 -4.464489 -0.674308 0.169090 6 0.302588 1.484384 -0.232614 6 1.129161 0.400057 0.513572 6 1.373472 -0.875042 -0.332094 1 -5.180345 -0.132666 -0.437669 1 -4.684375 -1.555110 0.755998 1 -0.776307 1.264761 -0.303658 9 2.323374 0.882420 0.900374 9 0.427911 0.030446 1.622686 9 2.087756 -0.575269 -1.422030 9 0.198785 -1.393801 -0.724002 9 2.031359 -1.800253 0.370620 8 -3.278646 -0.279146 0.219613 8 -2.926252 0.822947 -0.492361 8 0.826644 2.471273 -0.658655	**Frequencies (cm^{-1}):** 10.0669, 15.4785, 23.4823, 30.9468, 46.1634, 64.8526, 84.1569, 93.8584, 204.104, 213.1544, 260.1363, 310.4732, 357.4415, 378.2179, 447.023, 530.8074, 535.4789, 576.5496, 599.6859, 676.978, 721.7174, 788.3689, 900.2447, 936.4886, 979.7705, 1088.1542, 1135.9008, 1183.2657, 1193.3651, 1228.4107, 1241.8521, 1317.5969, 1408.674, 1434.5642, 1555.3283, 1823.2457, 2964.8668, 3116.4954, 3266.5907

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 1.3	**Energy (kJ mol^{-1}):** -878.192619327385
Reaction Coordinates: 6 2.245427 0.876409 0.628119 6 0.684157 -0.268750 0.775865 6 -0.386278 0.443243 -0.082249 6 -1.780395 -0.238774 -0.002071 1 2.720228 0.526629 1.535419 1 1.963406 1.915704 0.525608 1 0.543607 -0.070562 1.849480 9 -0.550064 1.721333 0.374541 9 -0.027498 0.501447 -1.380634 9 -2.169157 -0.317951 1.282191 9 -1.738315 -1.468742 -0.510966 9 -2.689406 0.473600 -0.674380 8 2.705230 0.362347 -0.498633 8 3.017779 -0.905128 -0.358939 8 1.122649 -1.386185 0.401916	**Frequencies (cm^{-1}):** -387.224, 40.8521, 60.8481, 102.0519, 125.633, 205.2782, 221.084, 243.5904, 287.5039, 295.9966, 354.0148, 396.8541, 442.87, 501.4165, 521.9906, 572.1916, 586.5832, 597.2737, 646.4937, 725.0205, 777.0694, 893.3888, 950.9197, 1013.5516, 1063.7946, 1116.749, 1148.5615, 1178.8286, 1204.3342, 1221.6653, 1234.3162, 1272.5252, 1306.4089, 1341.2321, 1483.7214, 1493.8895, 2952.7844, 3120.4829, 3247.478
IRC:  	

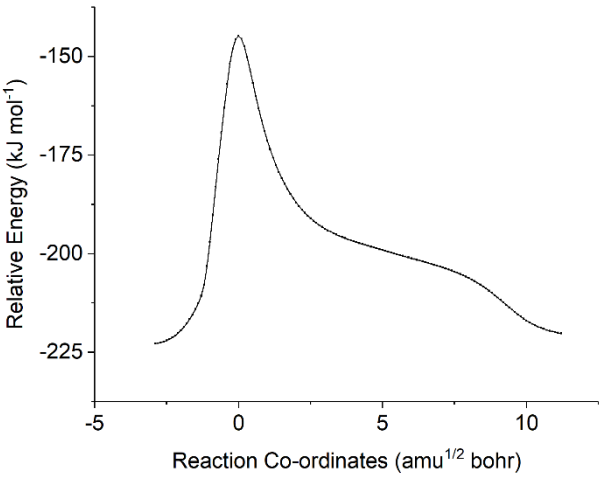
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 1.3	**Energy (kJ mol^{-1}):** -878.221083896414
Reaction Coordinates: 6 4.818140 -0.713634 -0.000040 6 0.002613 1.242162 -0.000030 6 -0.622367 -0.173889 0.000059 6 -2.168191 -0.250615 -0.000021 1 5.585452 0.051365 0.000374 1 4.999893 -1.779274 -0.000352 1 1.107161 1.209102 0.000026 9 -0.165549 -0.832889 -1.098182 9 -0.165671 -0.832701 1.098461 9 -2.665880 0.340964 -1.088860 9 -2.666002 0.341147 1.088663 9 -2.561854 -1.532495 0.000065 8 3.613734 -0.375618 -0.000184 8 3.305790 0.947831 0.000184 8 -0.650658 2.245092 -0.000146	**Frequencies (cm^{-1}):** 8.1377, 9.3044, 20.1166, 33.9614, 46.0446, 77.4805, 89.4291, 107.201, 156.0501, 213.7851, 274.0906, 313.6535, 345.7037, 417.0359, 426.8573, 511.0041, 530.4766, 582.0183, 586.7174, 676.9538, 686.0654, 766.2192, 899.5497, 980.1265, 1004.8218, 1096.4291, 1139.3452, 1169.4056, 1201.4159, 1207.1122, 1241.8379, 1318.4059, 1409.1012, 1449.7151, 1555.6054, 1823.6133, 2948.414, 3115.8774, 3265.981

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.1	**Energy (kJ mol^{-1}):** -878.192105449945
Reaction Coordinates: 6 1.559851 -1.210906 -0.131505 6 0.768319 0.401727 0.688087 6 -0.535512 0.640661 -0.123841 6 -1.648189 -0.423435 0.068139 1 1.197574 -2.114130 0.339566 1 1.270897 -0.969169 -1.145767 1 0.586566 -0.015092 1.687784 9 -1.065397 1.820991 0.288692 9 -0.281316 0.741784 -1.450002 9 -1.246344 -1.619571 -0.406319 9 -1.926557 -0.570775 1.371575 9 -2.762172 -0.076883 -0.571436 8 2.805804 -0.938795 0.198755 8 3.216005 0.182329 -0.354400 8 1.679970 1.255240 0.533212	**Frequencies (cm^{-1}):** -401.2565, 36.8365, 72.6064, 95.2189, 142.1401, 199.2199, 220.0017, 278.125, 284.5553, 313.1287, 349.9672, 388.187, 438.3785, 472.703, 525.2997, 561.361, 589.528, 601.9336, 607.2616, 732.9412, 800.9593, 891.0291, 940.4118, 1013.355, 1061.0385, 1109.6247, 1143.8764, 1165.1707, 1175.4003, 1218.8912, 1241.8796, 1277.953, 1323.3761, 1367.9756, 1477.5558, 1488.5312, 2979.7272, 3123.4258, 3253.5784
IRC:  	

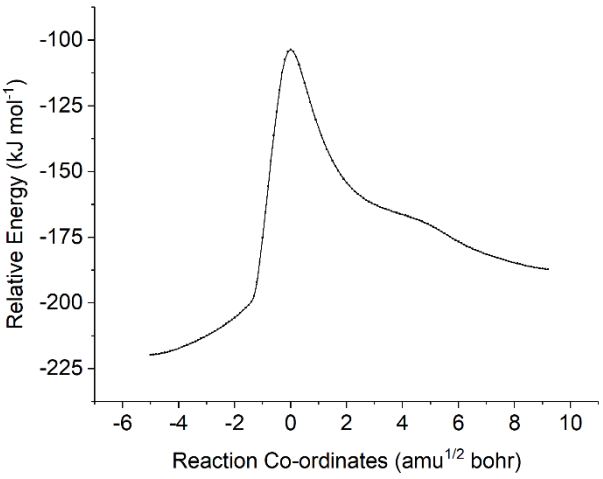
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.1	**Energy (kJ mol^{-1}):** -878.219669309907
Reaction Coordinates: 6 -3.956913 0.587962 0.726644 6 -0.335898 0.448274 -0.199479 6 1.190537 0.520499 -0.453858 6 1.980699 -0.567731 0.322353 1 -3.179069 1.240779 1.100199 1 -5.005860 0.628525 0.995080 1 -0.853032 -0.362041 -0.738463 9 1.395031 0.311367 -1.781136 9 1.674332 1.728212 -0.116751 9 1.833382 -0.386876 1.636183 9 1.500242 -1.779805 0.002799 9 3.275433 -0.524009 0.017009 8 -3.566597 -0.285081 -0.086142 8 -4.461933 -1.156933 -0.611095 8 -0.888766 1.244354 0.503022	**Frequencies (cm^{-1}):** 5.951, 26.3097, 35.9769, 41.4905, 66.8022, 84.5972, 92.6116, 121.1413, 201.9541, 211.8061, 268.7564, 308.9315, 357.0317, 382.4642, 450.5368, 530.4239, 537.3527, 577.227, 598.6507, 697.2893, 724.1617, 792.4988, 908.2894, 927.0687, 982.6487, 1079.1366, 1144.2595, 1187.5628, 1203.0546, 1237.1323, 1248.7182, 1314.3492, 1395.561, 1398.7189, 1536.9809, 1822.9769, 2983.3175, 3111.8514, 3263.0469

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.2	**Energy (kJ mol^{-1}):** -878.192918747499
Reaction Coordinates: 6 -1.877602 0.656085 -0.883716 6 -0.775433 0.656732 0.720181 6 0.673246 0.738934 0.179340 6 1.371336 -0.600619 -0.182707 1 -1.253273 0.000541 -1.474788 1 -2.067428 1.666195 -1.220418 1 -1.080160 1.644797 1.099699 9 0.729549 1.545783 -0.921751 9 1.424186 1.336973 1.140673 9 2.577906 -0.350413 -0.706212 9 0.650960 -1.266506 -1.102127 9 1.526521 -1.371968 0.887317 8 -2.941209 0.101973 -0.331651 8 -2.672450 -1.105864 0.114773 8 -1.152654 -0.379002 1.331354	**Frequencies (cm^{-1}):** -404.7679, 52.4352, 69.6298, 86.2313, 164.8344, 178.1855, 220.0956, 273.4951, 300.5241, 310.6259, 352.2768, 394.094, 462.5867, 483.6803, 513.296, 547.7329, 590.2925, 596.7691, 636.4384, 674.401, 767.3964, 893.1762, 957.956, 1060.4836, 1085.0359, 1101.403, 1140.7811, 1152.2147, 1185.7532, 1214.7865, 1235.5117, 1274.3196, 1301.7635, 1371.3658, 1482.6163, 1494.3566, 2946.8638, 3128.8965, 3253.5307
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.2	**Energy (kJ mol^{-1}):** -878.221532816887
Reaction Coordinates: 6 -0.688421 0.358814 0.639415 6 -0.108828 1.653597 0.016278 1 0.589393 2.170566 0.691742 8 -0.449135 2.064190 -1.052393 6 -1.350142 -0.639479 -0.343206 9 -1.750600 -1.733706 0.320799 9 -0.462850 -1.022178 -1.275018 9 -2.407295 -0.101001 -0.943556 9 0.289018 -0.306073 1.308977 9 -1.624074 0.735126 1.552939 6 2.974235 -1.293367 -0.138181 1 3.575685 -2.047910 0.349617 1 2.199101 -1.490973 -0.868579 8 3.223969 -0.113744 0.194079 8 2.509789 0.892231 -0.378673	**Frequencies (cm^{-1}):** 24.8851, 29.2079, 47.5469, 59.3746, 63.7761, 80.287, 109.3165, 140.38, 165.112, 214.5639, 274.9771, 322.8784, 347.1834, 410.0588, 437.9375, 511.9743, 525.583, 581.7893, 586.5209, 677.597, 684.7822, 765.6862, 893.9743, 949.9735, 988.5189, 1093.7273, 1128.1754, 1162.8397, 1193.117, 1213.1953, 1243.7259, 1311.9298, 1410.9521, 1419.1031, 1557.7245, 1831.4776, 2992.5806, 3117.9217, 3266.2286

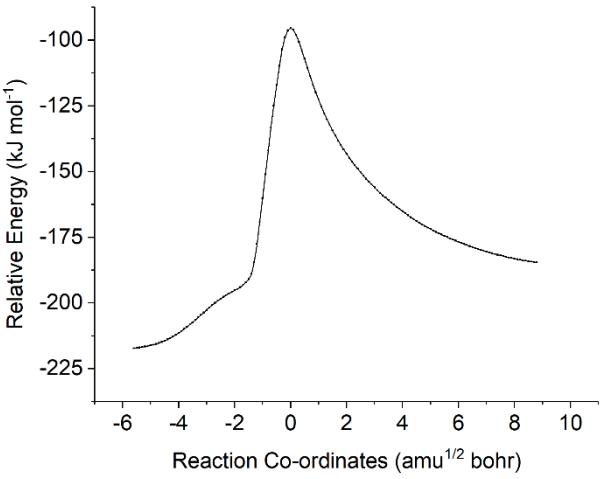
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{FO} 2.3	**Energy (kJ mol^{-1}):** -878.195879308203
Reaction Coordinates: 6 2.158658 1.013020 -0.205478 6 0.716879 -0.241519 -0.589277 6 -0.449267 0.438904 0.163132 6 -1.817840 -0.253680 -0.086841 1 2.177110 1.816480 -0.929235 1 1.875872 1.212358 0.820308 1 0.658676 -0.076407 -1.674515 9 -0.235195 0.460586 1.496295 9 -0.576501 1.729447 -0.268255 9 -2.799941 0.424062 0.514533 9 -1.809735 -1.501259 0.378973 9 -2.070985 -0.287748 -1.405364 8 3.146926 0.156142 -0.378230 8 3.077463 -0.835582 0.483332 8 1.159233 -1.335382 -0.149029	**Frequencies (cm^{-1}):** -395.2815, 51.339, 61.1772, 89.5926, 125.2833, 210.8998, 218.8086, 252.3359, 293.2252, 300.2598, 354.7231, 395.296, 448.318, 482.756, 524.7101, 562.0803, 590.0082, 598.2503, 639.6327, 714.7967, 785.4388, 896.3058, 959.4529, 1015.0878, 1064.3098, 1119.0588, 1143.6651, 1180.3723, 1201.9183, 1216.6423, 1236.9696, 1271.4747, 1308.5925, 1355.8902, 1481.1959, 1489.7891, 2971.4078, 3119.0066, 3246.9931
IRC:  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{FO} 2.3	**Energy (kJ mol^{-1}):** -878.222926627158
Reaction Coordinates: 6 -3.265638 -1.116654 0.497317 6 -0.031599 1.413095 -0.344367 6 0.351418 -0.040440 0.044893 6 1.875420 -0.310286 -0.072264 1 -3.833526 -2.024945 0.349665 1 -2.661106 -0.894765 1.368378 1 -0.403797 1.517538 -1.373373 9 -0.022910 -0.315016 1.315644 9 -0.274732 -0.916869 -0.784863 9 2.147679 -1.597657 0.163182 9 2.557612 0.436751 0.795193 9 2.286088 -0.008880 -1.315472 8 -3.337374 -0.285209 -0.433609 8 -2.651781 0.886047 -0.319114 8 0.123805 2.317028 0.420060	**Frequencies (cm^{-1}):** 17.3195, 37.0939, 51.8558, 56.7679, 64.4067, 73.9557, 108.1933, 122.6172, 215.2052, 228.5097, 252.6861, 322.591, 357.5067, 387.6918, 452.6098, 524.1586, 533.7999, 578.3556, 610.4902, 677.3269, 701.7983, 777.084, 886.7439, 905.8324, 993.9249, 1070.5734, 1142.3353, 1176.748, 1201.2961, 1219.5467, 1244.5254, 1301.8579, 1396.0704, 1412.6124, 1559.6935, 1829.0401, 3002.4913, 3117.6933, 3265.8612

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 1	**Energy (kJ mol^{-1}):** -878.181094934155
Reaction Coordinates: 6 1.797687 1.498506 0.241899 6 0.722848 -0.070484 0.839767 6 -0.297987 -0.358454 -0.271755 6 -1.699415 0.202713 0.115024 1 2.115655 1.835324 1.238634 1 0.930136 2.023650 -0.182623 1 0.297137 0.150725 1.811141 9 0.017406 0.148970 -1.475352 9 -0.430444 -1.701679 -0.401443 9 -1.625936 1.531047 0.304279 9 -2.584029 -0.046239 -0.843503 9 -2.126845 -0.357068 1.255865 8 2.635373 0.981501 -0.539035 8 2.378417 -1.093300 -0.174758 8 1.769572 -0.865535 0.966873	**Frequencies (cm^{-1}):** -404.1259, 45.6791, 59.839, 127.1398, 144.2152, 201.8457, 213.6418, 225.984, 270.7525, 308.7399, 362.624, 368.9365, 433.3007, 470.2606, 517.3366, 543.0944, 576.491, 600.5164, 616.2938, 751.1182, 822.5543, 878.1264, 916.6022, 1001.2136, 1079.6858, 1135.9659, 1153.5907, 1175.7646, 1195.7349, 1217.7335, 1227.9447, 1261.9339, 1318.296, 1414.7836, 1452.0161, 1559.0014, 2933.9114, 2999.7079, 3173.543
IRC  	

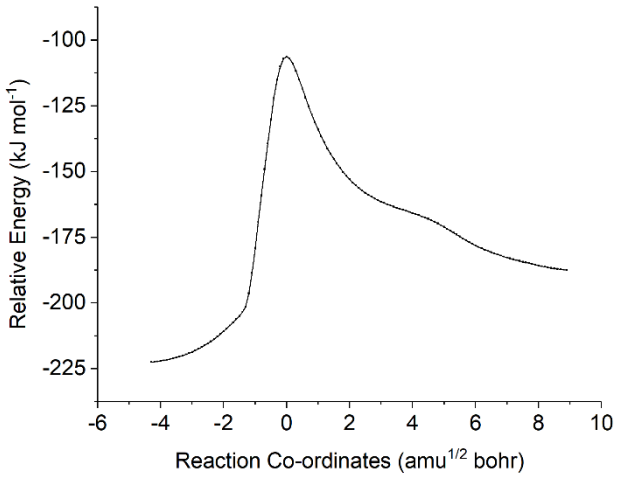
Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -878.211755328963
Reaction Coordinates: 6 3.135416 -1.099536 0.421642 6 0.439861 0.540113 -0.960801 6 -0.443957 0.385466 0.262270 6 -1.758863 -0.360454 -0.106780 1 4.115153 -0.684297 0.132724 1 2.880263 -1.048373 1.492513 1 0.114345 0.214990 -1.938491 9 0.150545 -0.299207 1.255777 9 -0.788143 1.612196 0.724547 9 -1.479035 -1.583905 -0.568898 9 -2.549050 -0.465208 0.956183 9 -2.408921 0.315485 -1.067985 8 2.390782 -1.593561 -0.388446 8 2.097986 1.534593 0.206214	**Frequencies (cm^{-1}):** 28.3497, 48.9568, 61.6998, 78.6241, 97.9848, 105.1398, 141.1293, 159.1722, 201.0592, 213.3859, 224.3797, 262.0911, 299.2154, 361.2793, 404.0391, 468.624, 535.6438, 555.9826, 595.5279, 599.7374, 751.5107, 795.6352, 871.0264, 938.4116, 1028.5517, 1139.4955, 1185.864, 1192.4755, 1194.5388, 1237.7107, 1263.2013, 1326.5309, 1383.3995, 1530.3836, 1551.9963, 1785.8155, 2919.7671, 2984.6482, 3215.6869

8 1.552099 1.122705 -0.952935	

Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 2	**Energy (kJ mol^{-1}):** -878.181994650982
Reaction Coordinates: 6 -2.005620 0.116757 1.240885 6 -0.930295 1.089730 -0.165924 6 0.552583 0.789781 0.065060 6 1.172051 -0.643679 0.015629 1 -2.782908 0.887986 1.337417 1 -1.201829 0.153156 1.989624 1 -1.112831 2.152755 -0.044443 9 1.225665 1.522262 -0.868704 9 0.855639 1.312375 1.282079 9 1.133711 -1.149888 -1.212178 9 2.458863 -0.534447 0.380528 9 0.566134 -1.466048 0.867340 8 -2.280497 -0.975598 0.687967 8 -1.570242 -0.695841 -1.293338 8 -1.623618 0.612974 -1.176889	**Frequencies (cm^{-1}):** -401.3096, 34.4455, 83.3088, 125.4053, 149.1583, 176.5452, 210.2508, 223.1739, 271.5724, 319.8813, 356.2181, 377.3091, 434.0127, 467.7121, 503.5742, 535.0893, 576.1544, 594.5496, 624.271, 750.0336, 787.0845, 834.482, 912.9544, 1054.9176, 1088.4526, 1118.131, 1134.6094, 1154.8704, 1189.6926, 1222.0719, 1230.8719, 1273.8772, 1319.3351, 1420.4009, 1451.9934, 1567.2684, 2934.1054, 3002.0453, 3155.0511
IRC  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -878.210817367452
Reaction Coordinates: 6 -4.870455 -0.256001 -0.391966 6 -0.717972 0.410241 0.230416 6 0.533714 -0.364712 0.579447 6 1.712802 -0.311091 -0.465699 1 -5.051321 0.787731 -0.701845 1 -5.747817 -0.924900 -0.375844 1 -1.674412 -0.095381 0.161421 9 1.006876 0.002545 1.791149 9 0.133953 -1.661466 0.665018 9 2.588605 0.641768 -0.195783 9 2.358419 -1.483891 -0.460522 9 1.203846 -0.120188 -1.693924 8 -3.774478 -0.647490 -0.086810 8 0.387385 2.366803 0.085204	**Frequencies (cm^{-1}):** 11.5958, 14.2006, 21.6377, 40.9262, 46.7572, 78.2062, 92.801, 108.9059, 154.5018, 202.5036, 241.153, 272.951, 333.6686, 355.876, 413.9532, 479.2006, 507.4484, 558.1199, 584.09, 652.8856, 749.0842, 803.0369, 857.0297, 936.5627, 1077.8155, 1132.3484, 1169.017, 1201.3243, 1207.3993, 1220.9303, 1265.0306, 1282.0354, 1380.0753, 1531.445, 1551.808, 1804.8891, 2908.2906, 2976.1534, 3175.4144

8 -0.750442 1.649814 0.032811	

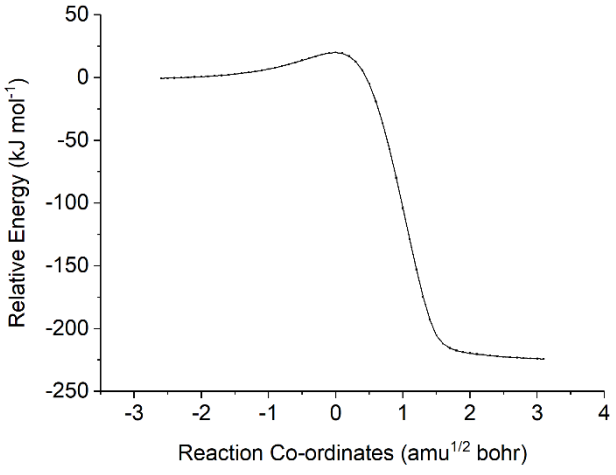
Compound: $CF_3CF_2CHCH_2 + O_3$ TS_{SYN} 3	**Energy (kJ mol^{-1}):** -878.177394077252
Reaction Coordinates: 6 2.456567 0.903285 0.342526 6 0.762685 -0.003337 0.894245 6 -0.291294 0.578495 -0.046482 6 -1.630169 -0.228685 -0.019825 1 2.940177 0.885672 1.329379 1 1.954793 1.845288 0.075588 1 0.563728 0.216914 1.936412 9 -0.578551 1.822490 0.433323 9 0.089472 0.701428 -1.323771 9 -2.070651 -0.329250 1.244731 9 -2.554848 0.398364 -0.744436 9 -1.452661 -1.455851 -0.507744 8 2.888532 0.161566 -0.575318 8 1.605480 -1.519988 -0.469479 8 1.238453 -1.226706 0.759411	**Frequencies (cm^{-1}):** -400.299, 45.1944, 62.7737, 118.9086, 131.0253, 200.681, 212.6134, 219.9965, 271.6798, 313.8946, 351.2265, 370.8021, 432.3038, 457.9481, 512.5468, 518.9986, 581.0936, 581.847, 665.371, 751.2784, 815.2217, 866.1749, 919.023, 1016.6171, 1075.3657, 1114.8106, 1157.0195, 1187.733, 1210.4942, 1218.8302, 1240.2853, 1261.1394, 1293.3918, 1410.7845, 1442.8013, 1562.312, 2928.4341, 2994.5322, 3173.8819
IRC  	

Compound: $CF_3CF_2CHCH_2 + O_3$ CPr_{SYN} 3	**Energy (kJ mol^{-1}):** -878.209591261981
Reaction Coordinates: 6 -3.558334 -0.531686 -0.596428 6 -0.515222 0.449472 1.025459 6 0.255459 -0.459777 0.090087 6 1.753656 -0.056604 -0.107968 1 -4.658335 -0.588164 -0.668946 1 -3.014319 -0.244833 -1.510502 1 -0.700424 0.115114 2.035909 9 0.269058 -1.681743 0.687101 9 -0.318950 -0.588251 -1.119612 9 2.331570 0.068568 1.099567 9 2.387426 -1.015487 -0.785781 9 1.878515 1.090379 -0.762254 8 -2.985219 -0.771435 0.435439 8 -0.822581 2.114577 -0.485019	**Frequencies (cm^{-1}):** 16.3641, 31.6549, 45.8556, 56.5894, 63.1381, 98.9647, 113.51, 120.5207, 168.4692, 197.1066, 214.4432, 278.6076, 312.0045, 354.8284, 426.7119, 462.6521, 489.5737, 558.6296, 582.2516, 649.8693, 749.3077, 786.8985, 831.316, 916.018, 1057.9379, 1133.3465, 1180.8173, 1207.2246, 1217.0806, 1226.8656, 1267.1246, 1286.047, 1372.9276, 1530.5975, 1550.5376, 1796.5979, 2913.5603, 2989.0976, 3218.3092

8 -0.963306 1.587891 0.750261	

6.15 Ozonolysis of HFO-1233zd(E) (Alkene 13)

Compound: *E*-$CF_3CHCHCl$ + O_3 PRC1	**Energy (kJ mol^{-1}):** -1099.697139477880
Reaction Coordinates: 6 -1.863849 -0.209081 -0.033137 6 -0.652192 0.546740 -0.477226 6 0.092994 1.239108 0.367874 1 -0.103462 1.300789 1.426488 17 1.486868 2.136911 -0.131944 1 -0.442201 0.499406 -1.535919 9 -2.976032 0.272045 -0.634674 9 -1.776962 -1.512552 -0.366433 9 -2.069073 -0.143878 1.295820 8 2.532664 -1.303180 -0.003452 8 1.900555 -1.637289 -1.035601 8 1.967506 -1.450634 1.108425	**Frequencies (cm^{-1}):** 12.7356, 19.492, 22.3207, 32.3352, 47.1761, 89.0705, 108.3222, 160.5259, 168.2442, 298.9084, 393.3984, 401.3337, 547.7035, 563.1713, 660.3183, 745.7689, 831.5793, 850.4282, 872.1853, 966.3596, 1117.6021, 1130.4312, 1185.1453, 1240.7191, 1260.6004, 1283.1824, 1321.6576, 1691.0746, 3205.319

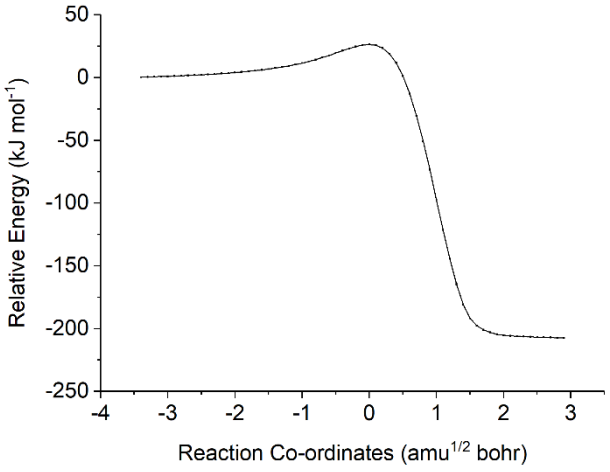
Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{OZO} 1	**Energy (kJ mol^{-1}):** -1099.684080713040
Reaction Coordinates: 6 -1.607718 -0.285980 0.003325 6 -0.184938 -0.394378 -0.477443 6 0.816781 -0.726041 0.393684 1 0.663592 -0.887361 1.446933 17 2.335520 -1.260177 -0.217291 9 -2.338579 0.518575 -0.778938 9 -2.189738 -1.510670 -0.037396 9 -1.696918 0.154589 1.265821 1 -0.073473 -0.567087 -1.536772 8 1.290940 1.806390 -0.208083 8 1.275670 1.373949 1.008528 8 0.131941 1.676335 -0.772820	**Frequencies (cm^{-1}):** -297.3646, 47.3597, 86.2763, 120.7455, 145.9362, 175.9493, 234.4353, 289.8255, 334.1032, 398.7629, 461.8145, 514.9512, 555.8573, 571.8834, 669.6838, 753.5779, 839.4216, 854.8088, 885.254, 931.2785, 1053.8401, 1097.7758, 1111.1226, 1157.7569, 1260.4159, 1275.7591, 1277.9832, 1536.378, 3217.1266, 3242.5287
IRC:  	

Compound: *E*-$CF_3CHCHCl$ + O_3 POZ1	**Energy (kJ mol^{-1}):** -1099.783475506850
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.560379 -0.284706 0.009022 6 -0.179828 0.140370 -0.491240 6 0.965680 -0.183558 0.513436 17 2.214200 -1.245278 -0.262073 1 0.650068 -0.690549 1.418657 9 -1.829990 0.196215 1.230197 9 -2.521344 0.130543 -0.825857 9 -1.612006 -1.629126 0.072200 1 0.006546 -0.333497 -1.454164 8 1.210686 1.868158 -0.296682 8 1.451192 1.061521 0.881175 8 -0.159477 1.555628 -0.582670	53.5193, 58.7984, 146.4808, 197.743, 242.6995, 293.9954, 343.8689, 391.9754, 449.4155, 525.0808, 554.4552, 648.7714, 694.4097, 745.4883, 761.0446, 801.3107, 892.1098, 936.5363, 994.8701, 1030.4386, 1062.3442, 1149.5034, 1175.3986, 1248.7726, 1270.4621, 1298.0152, 1316.0913, 1398.5159, 3090.6429, 3147.8929

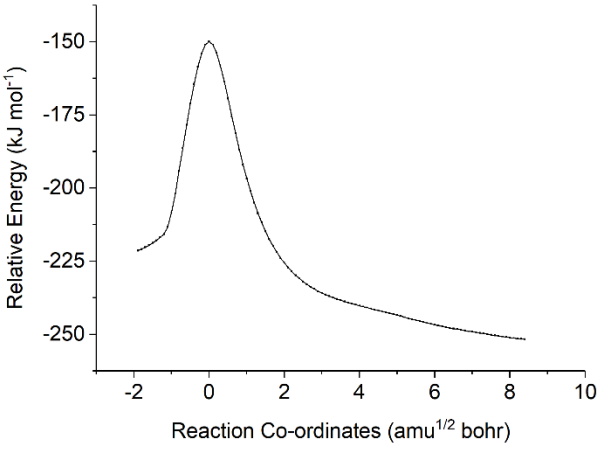
Compound: *E*-$CF_3CHCHCl + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -1099.697151869550
Reaction Coordinates: 6 -1.748565 -0.112589 -0.036399 6 -0.566987 0.690590 -0.474869 6 0.221613 1.315996 0.384093 1 0.084708 1.302253 1.453821 17 1.586352 2.247547 -0.118475 1 -0.400179 0.725426 -1.541557 9 -2.882852 0.325162 -0.622971 9 -1.611876 -1.413327 -0.388526 9 -1.946018 -0.080801 1.294737 8 1.709162 -2.124423 0.040362 8 1.904368 -1.437789 1.074172 8 1.871199 -1.572698 -1.075071	**Frequencies (cm^{-1}):** 14.5947, 23.3402, 27.7962, 31.9741, 49.5163, 92.9431, 103.0491, 159.8478, 167.4873, 299.4901, 394.3785, 401.3599, 547.4544, 564.032, 660.9847, 745.1349, 835.7105, 848.9702, 873.8801, 966.781, 1112.4101, 1127.2687, 1186.2971, 1242.2777, 1261.2837, 1282.7331, 1320.192, 1689.2485, 3206.0904, 3221.5627

Compound: *E*-$CF_3CHCHCl + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -1099.683067598280
Reaction Coordinates: 6 1.539643 -0.404169 0.016015 6 0.126567 -0.452425 -0.497235 6 -0.915656 -0.626404 0.372668 1 -0.786841 -0.662154 1.441922 17 -2.441874 -1.183125 -0.185608 9 1.991445 -1.658650 0.259283 9 2.379170 0.145938 -0.869817 9 1.634728 0.280578 1.171011 1 0.021586 -0.704577 -1.540721 8 -0.422586 2.059598 0.191443 8 -1.495664 1.508194 0.649940 8 -0.116038 1.615589 -0.983739	**Frequencies (cm^{-1}):** -284.5431, 50.0707, 85.7975, 123.4802, 143.1393, 167.6327, 245.0318, 289.7436, 327.87, 397.4713, 428.4715, 509.6353, 552.0916, 575.0795, 669.2979, 748.9252, 845.3186, 858.1306, 883.6247, 936.0313, 1057.7236, 1102.3502, 1110.3566, 1155.3844, 1250.1135, 1278.9477, 1288.0714, 1533.2182, 3220.1951, 3229.9288
IRC:	



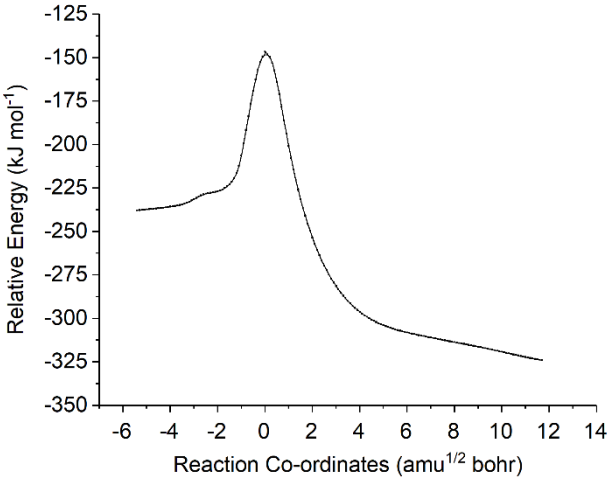
Compound: *E*-$CF_3CHCHCl$ + O_3 POZ 2	**Energy (kJ mol^{-1}):** -1099.781041505120
Reaction Coordinates: 6 1.484125 -0.394957 -0.037682 6 0.159554 0.061082 0.585019 6 -1.041350 -0.064217 -0.398648 17 -2.332923 -1.147328 0.176342 1 -0.742379 -0.414109 -1.382991 9 1.801139 0.288468 -1.145688 9 2.489058 -0.257794 0.837105 9 1.394416 -1.701056 -0.368183 1 0.000061 -0.513360 1.494885 8 -0.404144 2.055769 -0.231222 8 -1.569495 1.248798 -0.447126 8 0.176953 1.427186 0.939480	**Frequencies (cm^{-1}):** 50.8946, 53.1878, 155.6462, 184.3678, 235.3709, 296.1415, 370.4406, 374.7677, 413.6619, 521.8744, 559.8255, 646.2795, 699.8993, 732.8479, 743.1348, 864.0995, 885.9077, 928.2605, 985.5578, 1031.6728, 1049.7556, 1139.8366, 1167.4606, 1264.4395, 1274.98, 1302.3205, 1318.2613, 1393.687, 3109.9909, 3116.4402

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -1099.751193570360
Reaction Coordinates: 6 1.538842 -0.342961 0.019241 6 0.260604 0.351844 -0.418168 6 -1.265844 -0.042003 0.637764 17 -2.090925 -1.385640 -0.321628 1 -0.784228 -0.502246 1.504133 9 1.915760 0.040738 1.245419 9 2.543116 -0.069440 -0.830584 9 1.348122 -1.667684 0.026715 1 -0.154763 0.026884 -1.364517 8 -0.834313 2.220907 -0.549892 8 -1.845180 1.049668 0.750843 8 0.307008 1.666604 -0.210815	**Frequencies (cm^{-1}):** -448.8569, 37.3453, 73.39, 130.0882, 184.7786, 211.4026, 271.04, 378.9562, 391.5565, 418.7483, 469.8872, 510.0042, 571.535, 582.6383, 596.4865, 678.6213, 714.891, 892.2412, 950.9424, 1090.3448, 1118.9694, 1156.2221, 1187.9595, 1234.784, 1246.8758, 1266.7048, 1409.3547, 1445.3992, 3038.4737, 3163.5184
IRC:	



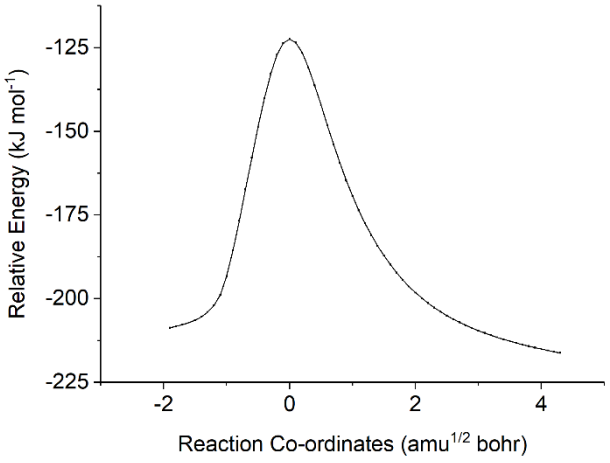
Compound: *E*-$CF_3CHCHCl$ + O_3 C_{ANTI} 1	**Energy (kJ mol^{-1}):** -1099.789970143740
Reaction Coordinates: 6 -2.190343 -0.244864 0.106547 6 -0.825583 0.326960 0.412350 1 -0.206915 -0.084867 1.199054 8 -0.453628 1.321976 -0.247091 8 0.763520 1.856247 0.016554 9 -2.745602 0.310266 -0.967092 9 -3.001262 -0.042391 1.163810 9 -2.092367 -1.567255 -0.083839 6 2.253467 -0.241237 -0.750965 1 2.490800 0.543998 -1.469179 17 3.510709 -0.312795 0.517560 8 1.335344 -0.989767 -0.788451	**Frequencies (cm^{-1}):** 21.3535, 24.1484, 46.7831, 51.4304, 121.0836, 144.0041, 194.2213, 216.1558, 238.8818, 387.6089, 404.8863, 417.3378, 451.5101, 552.5758, 562.0901, 700.5596, 718.3626, 887.2558, 900.3009, 920.9395, 966.4096, 1137.8093, 1181.2451, 1269.9661, 1327.8637, 1359.3784, 1561.4702, 1800.6882, 3096.8505, 3200.5397

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{SYN} 1	**Energy (kJ mol^{-1}):** -1099.746713532770
Reaction Coordinates: 6 -1.538839 -0.270084 0.044095 6 -0.406497 0.428232 -0.735674 6 1.187315 -0.051829 0.324106 1 0.702937 -0.061053 1.293043 17 1.961101 -1.519044 -0.145473 9 -1.673092 0.213123 1.287663 9 -2.706132 -0.100026 -0.596255 9 -1.319913 -1.599255 0.136218 1 -0.127099 -0.112793 -1.648897 8 1.236020 2.119666 0.395210 8 1.891956 1.033285 0.024875 8 -0.387251 1.688937 -0.721947	**Frequencies (cm^{-1}):** -422.0769, 42.0386, 71.0916, 135.1528, 194.1276, 238.99, 305.5824, 334.4469, 358.3122, 424.6465, 463.8262, 499.7043, 548.0362, 562.8606, 608.7027, 691.1087, 834.4284, 867.3042, 963.3811, 1085.8598, 1104.6049, 1144.2205, 1161.0135, 1224.0376, 1245.0984, 1298.7728, 1347.3492, 1483.1006, 2994.8802, 3161.7102
IRC:	



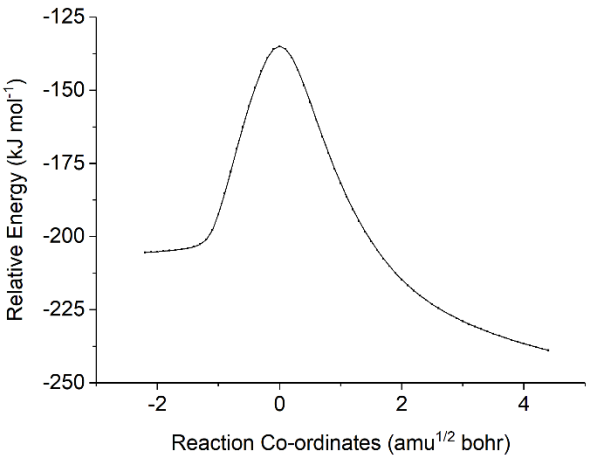
Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{SYN} 1	**Energy (kJ mol^{-1}):** -1099.784656778720
Reaction Coordinates: 6 2.737884 -0.093614 -0.000000 6 1.195520 -0.043340 0.000001 1 0.755736 0.966206 0.000001 8 0.531456 -1.042521 0.000001 9 3.200621 0.548397 1.088968 9 3.215427 -1.334284 -0.000000 9 3.200620 0.548397 -1.088968 6 -2.510733 -0.005119 0.000000 1 -1.574320 -0.559140 0.000001 17 -3.991815 -0.831924 -0.000000 8 -2.529942 1.242124 -0.000000 8 -1.302337 1.891083 0.000000	**Frequencies (cm^{-1}):** 19.0001, 27.7642, 56.3453, 63.4069, 95.6472, 104.4206, 129.2095, 233.5138, 266.1, 312.6967, 324.0951, 427.3231, 455.8691, 522.6357, 527.3453, 701.6504, 833.2318, 882.6348, 910.2688, 945.1757, 1008.1981, 1160.0357, 1178.9442, 1282.8255, 1336.4483, 1401.6061, 1485.6251, 1816.3094, 2996.9364, 3116.6598

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -1099.747027569040
Reaction Coordinates: 6 -1.513654 -0.395797 0.002887 6 -0.180442 -0.085281 -0.691779 6 1.150811 -0.233446 0.649301 1 0.774389 -1.149586 1.116263 17 2.665505 -0.691861 -0.308341 9 -2.516169 0.130737 -0.717608 9 -1.628237 0.025521 1.255627 9 -1.654045 -1.737168 0.000802 1 0.040525 -0.772293 -1.499392 8 -0.054856 2.013445 -0.065093 8 1.110879 0.848991 1.238294 8 0.108635 1.162421 -1.046566	**Frequencies (cm^{-1}):** -426.4395, 35.9052, 87.9176, 150.8103, 181.5555, 193.9187, 251.5827, 333.2695, 371.5811, 426.1663, 471.173, 528.9422, 548.4286, 577.3496, 646.1894, 668.3358, 768.6369, 890.338, 934.0581, 1042.068, 1098.7351, 1158.9891, 1171.5359, 1231.5024, 1245.3718, 1262.8063, 1425.0351, 1483.2258, 3013.7415, 3182.2486
IRC	



Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{ANTI} 2	**Energy (kJ mol^{-1}):** -1099.778251541460
Reaction Coordinates: 6 1.784448 -0.163867 -0.088304 6 0.970105 0.899690 0.683757 1 1.180187 1.929445 0.362396 8 0.288185 0.611290 1.629001 9 3.008080 -0.242656 0.488970 9 1.229794 -1.375761 -0.041775 9 1.967605 0.183589 -1.367538 6 -2.431934 0.409889 0.306630 1 -3.194061 0.704161 1.014448 17 -2.203411 -1.213467 -0.040980 8 -1.794637 1.341877 -0.236865 8 -0.782695 1.051146 -1.118333	**Frequencies (cm^{-1}):** 35.0067, 44.0839, 55.2409, 75.4857, 97.7973, 157.539, 199.4033, 246.2139, 257.0091, 362.8354, 428.4584, 465.3674, 520.9204, 531.9623, 655.7536, 701.3066, 809.6883, 832.0823, 860.9037, 895.4745, 952.3568, 1129.3181, 1188.2706, 1273.5248, 1336.8619, 1403.719, 1482.1805, 1802.1236, 3002.5106, 3211.2375

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{SYN} 2	**Energy (kJ mol^{-1}):** -1099.748405220490
Reaction Coordinates: 6 -1.513708 -0.394861 0.002619 6 -0.180853 -0.084458 -0.692416 6 1.150165 -0.235490 0.648404 17 2.665453 -0.691671 -0.308063 1 0.773805 -1.151710 1.115037 9 -1.633812 0.036755 1.251090 9 -2.517170 0.121090 -0.724750 9 -1.649203 -1.736800 0.011673 1 0.038591 -0.771687 -1.500292 8 -0.050792 2.012981 -0.063196 8 1.109280 0.846809 1.238793 8 0.109378 1.162868 -1.047026	**Frequencies (cm^{-1}):** -427.7395, 35.8602, 87.9803, 150.7817, 181.765, 194.2302, 251.8004, 333.1821, 371.9532, 426.8579, 471.0786, 529.0943, 548.9584, 577.722, 646.8298, 668.8404, 768.7379, 890.2811, 934.0925, 1041.2998, 1097.8373, 1158.429, 1170.6736, 1231.6597, 1245.4624, 1263.6583, 1424.809, 1480.9921, 3014.9339, 3181.9463
IRC	



Compound: *E*-$CF_3CHCHCl$ + O_3 CPr_{SYN} 2	**Energy (kJ mol^{-1}):** -1099.786602698660
Reaction Coordinates: 6 -2.119779 -0.416894 -0.093052 6 -1.575344 0.575581 0.914608 1 -1.851829 0.505679 1.957069 8 -0.798593 1.515409 0.622578 8 -0.381795 1.681657 -0.648583 9 -2.864173 0.186193 -1.024296 9 -2.907370 -1.278730 0.578051 9 -1.153794 -1.115113 -0.690820 6 2.249947 0.093683 0.134454 17 3.933559 -0.331491 -0.309989 1 1.833235 0.814174 -0.574618 8 1.698787 -0.363303 1.074117	**Frequencies (cm^{-1}):** 13.1291, 24.0652, 38.7694, 57.8792, 67.3713, 82.9336, 112.2987, 182.9539, 249.4797, 326.2852, 447.7082, 478.5895, 505.9983, 535.5461, 588.9915, 710.0088, 757.9938, 797.2082, 882.2556, 926.6446, 972.7186, 1156.541, 1178.7399, 1243.144, 1321.9454, 1368.3674, 1556.7146, 1825.3675, 3070.4585, 3216.0234

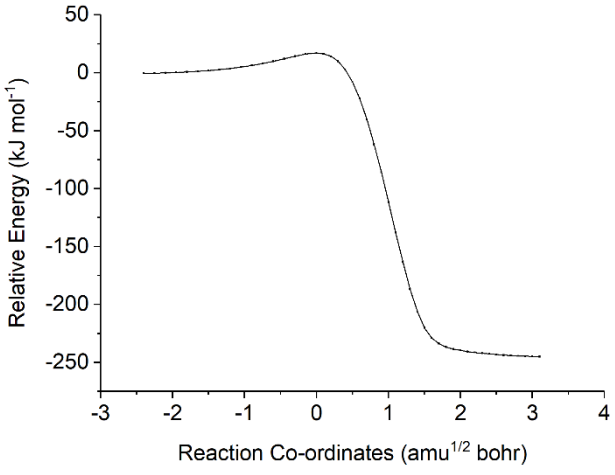
Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{POZ} 1	**Energy (kJ mol^{-1}):** -1099.777915798650
Reaction Coordinates: 6 -1.554608 -0.311060 0.007736 6 -0.124880 -0.173888 -0.546634 6 0.961849 -0.287146 0.524577 17 2.518143 -0.889302 -0.215338 1 0.735359 -0.956966 1.347822 1 -0.005809 -0.910056 -1.338516 9 -1.834292 0.560280 0.981471 9 -2.447764 -0.140568 -0.975975 9 -1.715367 -1.557615 0.504412 8 0.655787 1.910990 -0.031039 8 1.052487 0.986151 1.033607 8 0.134808 1.085215 -1.109044	**Frequencies (cm^{-1}):** -103.3462, 47.6043, 101.2299, 154.7137, 216.1124, 249.6566, 305.936, 381.9277, 395.367, 525.577, 552.3956, 653.7009, 711.5524, 750.9223, 777.5247, 858.0185, 886.6158, 896.6152, 973.0663, 1029.1639, 1094.289, 1144.5436, 1166.8418, 1243.2344, 1275.0457, 1281.9467, 1304.8115, 1378.8911, 3120.9837, 3142.8577
IRC Energy too low for IRC to take place	

Compound: *E*-$CF_3CHCHCl$ + O_3 TS_{POZ} 2	**Energy (kJ mol^{-1}):** -1099.770978070750

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.492268 -0.246953 0.004625 6 -0.155696 0.349271 -0.445698 6 1.056720 -0.074536 0.394229 17 1.809813 -1.595163 -0.132458 1 0.825670 -0.163638 1.453717 1 0.004953 0.104353 -1.498625 9 -1.707888 -0.073368 1.316505 9 -2.508777 0.316409 -0.662221 9 -1.507930 -1.565273 -0.248918 8 1.174508 2.167747 -0.051305 8 1.973438 0.961269 0.128818 8 -0.214026 1.734791 -0.211333	-212.1692, 47.7097, 101.9347, 138.5123, 219.3175, 235.7448, 330.6151, 379.1897, 408.5841, 486.5508, 555.2157, 576.5386, 685.5788, 708.603, 825.7592, 853.1021, 892.158, 906.8044, 1036.0657, 1071.1545, 1098.5329, 1155.6675, 1180.0767, 1256.3015, 1272.2581, 1304.4443, 1343.0164, 1404.4052, 3051.7001, 3097.6386
IRC Energy too low for IRC to take place	

6.16 Ozonolysis of HFO-1234ze(E) (Alkene 14)

Compound: *E*-CF_3CHCHF + O_3 PRC1	**Energy (kJ mol^{-1}):** -739.703284627850
Reaction Coordinates: 6 -1.650945 -0.306763 -0.018338 6 -0.622713 0.630474 -0.552478 6 -0.026733 1.520569 0.219237 1 -0.198987 1.661027 1.276314 9 0.891810 2.358963 -0.274156 1 -0.402806 0.545570 -1.606650 9 -2.844800 -0.116720 -0.626706 9 -1.308519 -1.592769 -0.238216 9 -1.853623 -0.165119 1.306934 8 2.877900 -0.503195 -0.013235 8 2.313009 -1.046946 -0.993731 8 2.364132 -0.653793 1.123104	**Frequencies (cm^{-1}):** 4.8985, 12.6292, 22.7111, 26.1432, 38.8796, 94.8339, 105.985, 192.7761, 197.2378, 386.3606, 409.556, 419.2781, 555.1565, 577.4032, 691.3705, 745.1057, 868.5119, 879.7539, 961.8078, 1085.1441, 1119.6771, 1183.819, 1187.2852, 1241.4821, 1257.0108, 1318.8819, 1346.3541, 1735.9967, 3210.6938, 3219.0963

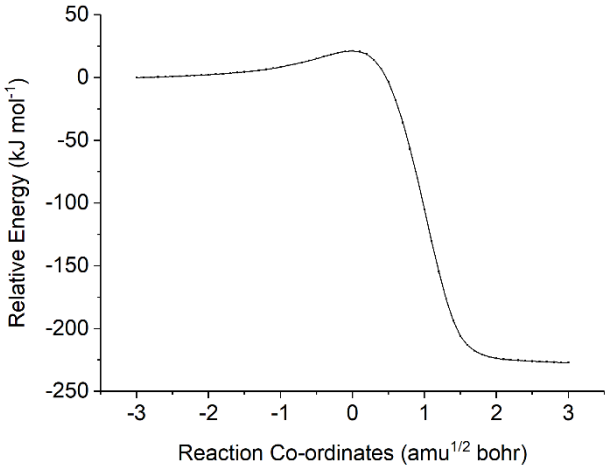
Compound: *E*-CF_3CHCHF + O_3 TS_{OZO} 1	**Energy (kJ mol^{-1}):** -739.689682804154
Reaction Coordinates: 6 1.419285 0.000042 0.014336 6 0.121245 0.471323 -0.570493 6 -0.766906 1.180052 0.183779 1 -0.637305 1.462953 1.215825 9 -1.751348 1.819674 -0.442068 1 0.073493 0.518754 -1.647519 9 2.373955 0.947162 -0.164839 9 1.333429 -0.231185 1.333889 9 1.862919 -1.114508 -0.581161 8 -2.020015 -1.102080 -0.174688 8 -1.914301 -0.509286 0.971199 8 -0.871751 -1.473697 -0.627314	**Frequencies (cm^{-1}):** -290.2803, 47.0046, 95.7327, 118.2241, 158.6037, 203.431, 240.3109, 344.6385, 375.0973, 411.3633, 456.6927, 531.2139, 563.8075, 576.1881, 696.1778, 753.3623, 876.707, 886.713, 923.5971, 1061.2793, 1095.4794, 1104.8871, 1130.8382, 1201.8657, 1255.8713, 1279.9515, 1330.5348, 1586.3292, 3220.608, 3238.2387
IRC:  	

Compound: *E*-CF_3CHCHF + O_3 POZ1	**Energy (kJ mol^{-1}):** -739.799128467212
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 1.378940 0.046561 0.016352 6 -0.045567 -0.055917 -0.521609 6 -1.089193 0.741031 0.310137 9 -1.740430 1.620513 -0.524531 1 -0.696608 1.303143 1.155006 9 1.455821 -0.276226 1.314758 9 2.211038 -0.752440 -0.663023 9 1.810520 1.315649 -0.121266 1 -0.064039 0.299359 -1.553098 8 -1.884992 -1.263432 -0.211684 8 -1.933807 -0.229064 0.812425 8 -0.473322 -1.402506 -0.411321	60.5452, 74.3865, 153.9635, 210.8506, 296.1848, 335.8249, 351.2962, 409.1283, 524.5177, 551.6113, 579.1047, 686.6407, 695.0589, 746.9879, 785.5228, 909.644, 938.9818, 1006.7012, 1037.1033, 1049.0572, 1070.631, 1153.7667, 1181.9293, 1271.4541, 1294.8085, 1307.7155, 1365.0142, 1403.4662, 3075.4681, 3120.7504

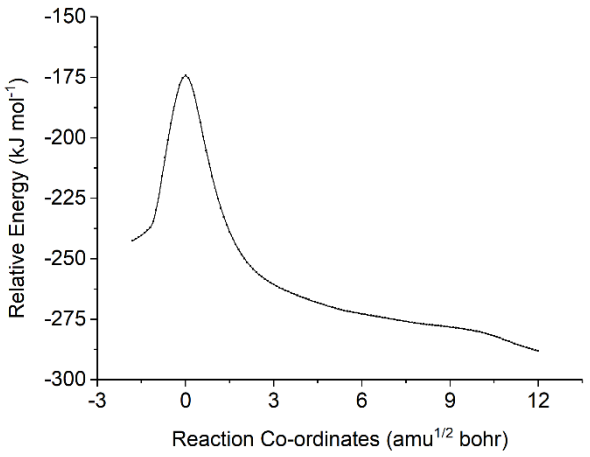
Compound: *E*-$CF_3CHCHF + O_3$ PRC 2	**Energy (kJ mol^{-1}):** -739.704017975154
Reaction Coordinates: 6 -1.514689 -0.376320 -0.023964 6 -0.663542 0.727051 -0.546537 6 -0.116785 1.626999 0.251828 1 -0.221380 1.665919 1.326106 9 0.641800 2.611457 -0.232782 9 -2.734903 -0.374353 -0.602646 9 -0.967756 -1.587414 -0.288741 9 -1.702803 -0.311298 1.309252 1 -0.514123 0.752145 -1.615942 8 2.409322 -1.148597 0.081561 8 2.382160 -0.359206 1.058701 8 2.380838 -0.658442 -1.073244	**Frequencies (cm^{-1}):** 15.9838, 16.9449, 23.9948, 30.1793, 47.1775, 94.6072, 119.9059, 192.6354, 198.3263, 387.002, 410.2886, 419.0111, 554.4183, 577.7799, 690.5176, 746.3248, 867.8081, 880.1144, 964.0518, 1085.004, 1113.9461, 1185.2165, 1193.6168, 1242.6261, 1258.1543, 1319.2618, 1347.6728, 1734.5187, 3210.5021, 3218.7069

Compound: *E*-$CF_3CHCHF + O_3$ TS_{OZO} 2	**Energy (kJ mol^{-1}):** -739.690068045272
Reaction Coordinates: 6 -1.381382 0.040928 0.020532 6 -0.110613 0.560985 -0.578236 6 0.827376 1.166245 0.205938 1 0.749638 1.303086 1.273748 9 1.770388 1.899755 -0.366997 9 -2.286569 1.039725 0.163952 9 -1.955346 -0.894030 -0.747418 9 -1.179123 -0.485408 1.245098 1 -0.110544 0.723826 -1.644402 8 1.415496 -1.492591 0.269456 8 2.156601 -0.496680 0.631215 8 0.953462 -1.345256 -0.921980	**Frequencies (cm^{-1}):** -274.3861, 44.2128, 93.1095, 114.6889, 162.2493, 199.2836, 257.7032, 343.0079, 382.5817, 415.0421, 443.5211, 507.8723, 559.9715, 579.4966, 694.7123, 751.4404, 874.9654, 882.5186, 928.2225, 1068.6525, 1096.9421, 1109.6482, 1132.1699, 1206.8847, 1243.4937, 1286.2774, 1339.7591, 1589.1863, 3222.0994, 3226.0896
IRC:	



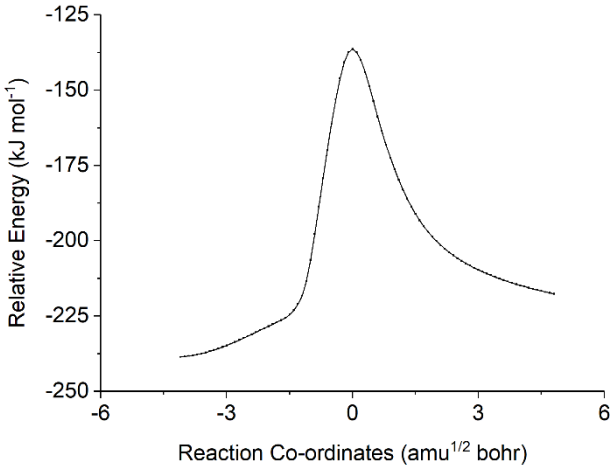
Compound: *E*-CF_3CHCHF + O_3 POZ 2	**Energy (kJ mol^{-1}):** -739.794731182167
Reaction Coordinates: 6 1.315638 0.126925 0.031010 6 −0.073099 0.211842 −0.618313 6 −1.181687 0.712690 0.319279 9 −2.133647 1.366200 −0.440351 1 −0.868015 1.394614 1.108504 9 1.325804 −0.538631 1.191189 9 2.185395 −0.462120 −0.798330 9 1.752457 1.382846 0.273165 1 0.007280 0.843175 −1.500583 8 −1.146873 −1.584141 0.150953 8 −1.714493 −0.426970 0.885602 8 −0.597941 −1.024038 −1.040408	**Frequencies (cm^{-1}):** 44.4138, 87.2889, 150.7713, 166.3573, 261.6313, 309.1999, 331.0583, 409.467, 488.7195, 528.8761, 567.5762, 685.3726, 709.8818, 768.1759, 870.5373, 887.5448, 915.5071, 972.2164, 1016.0725, 1045.1378, 1081.2547, 1142.3652, 1179.0545, 1276.3289, 1285.5176, 1302.1302, 1355.6254, 1393.0225, 3103.7767, 3123.0301

Compound: *E*-CF_3CHCHF + O_3 TS_{ANTI} 1	**Energy (kJ mol^{-1}):** -739.768398521593
Reaction Coordinates: 6 −1.401299 0.066028 0.015534 6 0.017686 −0.243656 −0.421743 6 1.355912 0.781542 0.401632 1 0.791762 1.244267 1.217796 9 1.583311 1.735172 −0.578134 9 −1.594858 −0.212898 1.310689 9 −2.294146 −0.637893 −0.700071 9 −1.646508 1.369905 −0.180485 1 0.271457 0.057819 −1.432879 8 1.662127 −1.658419 −0.404092 8 2.259655 −0.030627 0.652710 8 0.412317 −1.462722 −0.051799	**Frequencies (cm^{-1}):** -448.7486, 42.9496, 95.7915, 132.5415, 195.4736, 250.3922, 310.9982, 388.4779, 403.6771, 471.0522, 512.9073, 578.4309, 581.3856, 603.8158, 639.9277, 715.1346, 894.6684, 940.2153, 956.8633, 1113.3392, 1135.7124, 1161.8294, 1183.4475, 1235.2625, 1262.8909, 1298.824, 1409.8995, 1474.8955, 3035.7092, 3146.7313
IRC:	



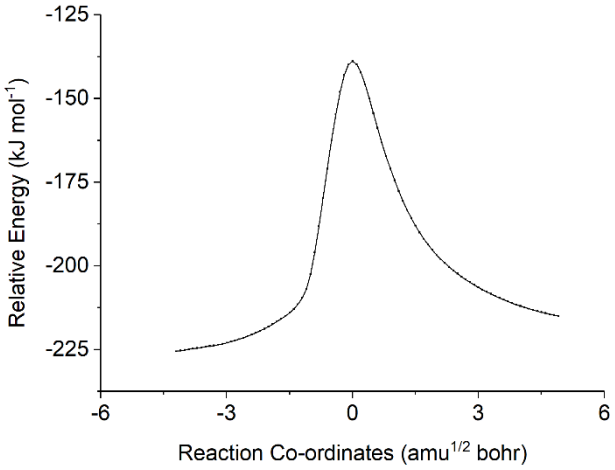
Compound: *E*-CF_3CHCHF + O_3 C_{ANTI} 1	**Energy (kJ mol^{-1}):** -739.811718375671
Reaction Coordinates: 6 1.805191 -0.184764 -0.060805 6 0.428206 0.326315 -0.417713 6 -2.636610 -0.435592 0.419496 1 -3.052729 0.215716 1.187229 9 -3.394008 -0.379769 -0.690955 9 2.252876 0.317518 1.086526 9 2.667010 0.149025 -1.041920 9 1.781650 -1.520950 0.023805 1 -0.111141 -0.062974 -1.271053 8 -1.278176 1.723444 -0.027125 8 -1.700715 -1.158403 0.502437 8 -0.044185 1.249845 0.279794	**Frequencies (cm^{-1}):** 22.8398, 37.3893, 55.0577, 75.5891, 134.8039, 158.4368, 195.9869, 247.5073, 250.6611, 388.0074, 407.923, 419.2533, 552.6533, 562.516, 667.4352, 700.8709, 887.0683, 900.0333, 960.0553, 1004.1026, 1067.3957, 1138.166, 1182.6463, 1270.5522, 1360.2933, 1368.1277, 1563.5239, 1828.7068, 3130.0091, 3204.1543

Compound: *E*-CF_3CHCHF + O_3 TS_{SYN} 1	**Energy (kJ mol^{-1}):** -739.756946242957
Reaction Coordinates: 6 -1.416495 0.056101 -0.032972 6 -0.127186 -0.014331 0.808340 6 1.261974 0.834771 -0.292212 1 0.870740 1.662063 -0.873059 9 2.134453 1.172253 0.641026 9 -1.633453 1.324664 -0.462022 9 -1.382269 -0.742020 -1.100891 9 -2.473154 -0.291889 0.720844 1 -0.073002 0.788436 1.559668 8 1.987626 -1.236023 -0.273504 8 1.517215 -0.240050 -1.005213 8 0.380448 -1.133529 1.056697	**Frequencies (cm^{-1}):** -429.6667, 41.2001, 93.1026, 141.865, 231.2141, 255.1767, 284.3394, 301.5314, 349.924, 434.4559, 509.3386, 530.0464, 566.6337, 647.9882, 699.4884, 777.9475, 841.4563, 876.4437, 1022.7121, 1083.8475, 1125.2987, 1166.0281, 1173.3267, 1250.3008, 1267.0655, 1338.4066, 1414.4067, 1507.834, 2961.687, 3181.4737
IRC:	



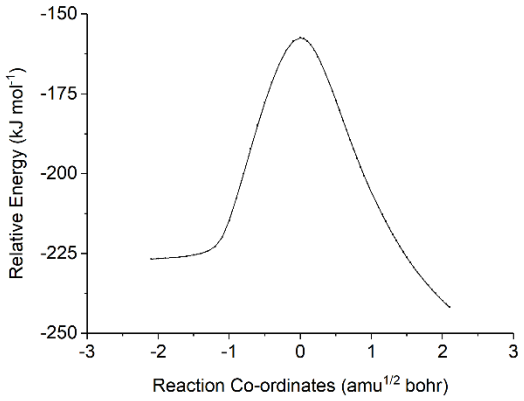
Compound: *E*-CF_3CHCHF + O_3 C_{SYN} 1	**Energy (kJ mol^{-1}):** -739.789802048716
Reaction Coordinates: 6 -1.310437 -0.493076 0.020906 6 -1.370217 0.906600 -0.643638 1 -0.820176 0.978637 -1.593096 8 -2.038622 1.777287 -0.174551 9 -0.257382 -1.210873 -0.431460 9 -1.230472 -0.429326 1.350372 9 -2.423353 -1.182553 -0.301112 6 2.603104 -0.340208 0.374894 1 3.118795 -0.995572 1.062996 9 2.799256 -0.512875 -0.888628 8 1.859035 0.546850 0.816288 8 1.201368 1.375574 -0.084916	**Frequencies (cm^{-1}):** 19.3457, 34.3577, 35.4825, 71.1917, 75.0499, 114.0954, 158.5361, 242.643, 295.349, 341.1491, 424.5251, 480.9683, 518.3991, 529.3147, 695.7802, 765.9299, 828.718, 832.6241, 834.9887, 950.9192, 1136.0438, 1163.6381, 1218.7279, 1271.6573, 1346.4634, 1396.3773, 1609.5661, 1834.244, 2995.2415, 3227.2839

Compound: *E*-CF_3CHCHF + O_3 TS_{ANTI} 2	**Energy (kJ mol^{-1}):** -739.756840898257
Reaction Coordinates: 6 -1.398570 0.016247 0.043500 6 -0.123011 -0.364554 -0.734958 6 1.250024 0.687744 0.236024 1 0.804487 0.648984 1.224417 9 1.408766 1.892765 -0.274657 9 -1.564785 1.357565 0.066062 9 -1.368318 -0.416669 1.311473 9 -2.477337 -0.511969 -0.553350 1 -0.027267 0.185298 -1.682594 8 2.266099 -0.104303 -0.026736 8 2.041987 -1.324586 0.444598 8 0.300313 -1.541879 -0.637233	**Frequencies (cm^{-1}):** -396.643, 49.3117, 75.4729, 141.1118, 228.3769, 242.4132, 310.9741, 358.3716, 408.6798, 440.9006, 488.4629, 516.7019, 556.8361, 596.2169, 620.6364, 693.2856, 834.9736, 913.977, 1080.183, 1114.8132, 1139.9608, 1163.2856, 1208.6758, 1241.5652, 1257.0001, 1354.044, 1387.0695, 1506.0419, 2974.2193, 3159.2806
IRC	



Compound: *E*-$CF_3CHCHF + O_3$ CPr_{ANTI} 2	**Energy (kJ mol^{-1}):** -739.790207230903
Reaction Coordinates: 6 -2.296863 0.008589 -0.000000 6 -0.755354 0.075085 0.000001 1 -0.237568 -0.896832 0.000002 8 -0.169487 1.122934 0.000001 9 -2.708784 -0.666389 1.089023 9 -2.866389 1.209717 -0.000002 9 -2.708782 -0.666391 -1.089023 6 2.895080 0.353330 0.000000 1 1.926361 0.851215 0.000002 9 3.976354 1.082023 -0.000000 8 3.048834 -0.870970 -0.000000 8 1.873458 -1.652846 0.000000	**Frequencies (cm^{-1}):** 22.3429, 28.8256, 61.2297, 82.1805, 98.1211, 110.115, 135.589, 268.577, 275.2861, 325.2231, 344.126, 428.2008, 523.0142, 527.5603, 571.1516, 702.0008, 834.2237, 877.7727, 989.4781, 1011.2292, 1161.4191, 1179.5574, 1223.9844, 1282.7178, 1360.1733, 1401.9915, 1593.874, 1813.3497, 2996.2364, 3119.6762

Compound: *E*-$CF_3CHCHF + O_3$ TS_{SYN}	**Energy (kJ mol^{-1}):** -739.765533937662
Reaction Coordinates: 6 -1.282551 -0.214067 0.017104 6 0.027391 -0.050471 -0.761908 6 1.403451 -0.715691 0.335157 1 0.908935 -1.634662 0.672425 9 2.362872 -1.050219 -0.607069 9 -2.204741 0.623466 -0.483584 9 -1.206690 -0.020417 1.327371 9 -1.707871 -1.478297 -0.191165 1 0.023475 -0.595507 -1.698812 8 0.674637 1.815283 0.194500 8 1.642204 0.204452 1.123585 8 0.556372 1.160358 -0.933799	**Frequencies (cm^{-1}):** -434.2081, 34.4039, 116.7645, 156.4385, 193.5575, 237.7254, 276.0766, 334.2677, 409.8321, 461.3927, 529.5368, 535.0495, 585.6571, 621.1691, 680.304, 768.4757, 892.1492, 915.6366, 966.3998, 1056.5562, 1109.937, 1158.9961, 1175.2459, 1236.5751, 1262.6982, 1294.1239, 1428.3821, 1498.3206, 3013.0146, 3172.9671
IRC	



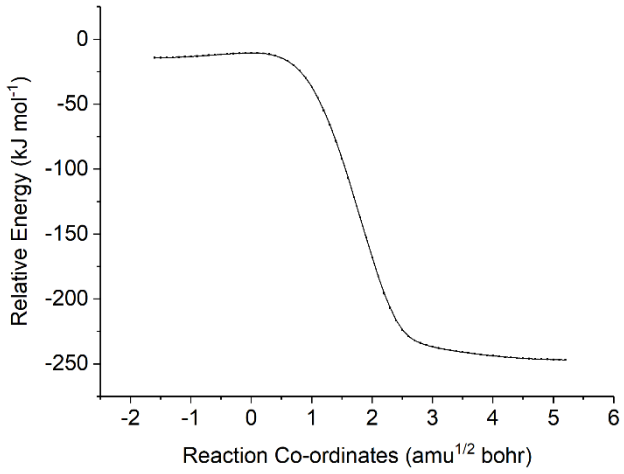
Compound: *E*-CF_3CHCHF + O_3 CPr_{SYN}	**Energy (kJ mol^{-1}):** -739.808552817472
Reaction Coordinates: 6 -1.668374 -0.375948 -0.081651 6 -1.033401 0.513484 0.968627 1 -1.242009 0.356492 2.017354 8 -0.258957 1.463517 0.707067 8 0.080355 1.731184 -0.570521 9 -2.464972 0.322155 -0.896849 9 -2.424746 -1.283152 0.565067 9 -0.765293 -1.031409 -0.810928 6 2.641303 -0.091388 -0.053514 9 3.872676 -0.469362 -0.454036 1 2.259975 0.708035 -0.693338 8 2.101838 -0.592889 0.869194	**Frequencies (cm^{-1}):** 17.9003, 28.7501, 43.7875, 67.6947, 76.6909, 87.9724, 111.7959, 183.141, 249.7382, 326.1957, 478.269, 505.8696, 535.6435, 588.5685, 664.2857, 757.8847, 798.2431, 881.8399, 924.7816, 1053.2791, 1055.5362, 1156.7697, 1178.1369, 1243.8193, 1359.1025, 1370.3575, 1558.5653, 1858.2746, 3102.8712, 3216.4218

Compound: *E*-CF_3CHCHF + O_3 TS_{POZ} 1	**Energy (kJ mol^{-1}):** -739.793338173632
Reaction Coordinates: 6 -1.334396 -0.096672 0.022788 6 0.053824 -0.178773 -0.631213 6 1.132847 -0.767150 0.280120 1 0.796272 -1.512436 0.998880 9 2.118520 -1.331403 -0.502613 9 -1.769863 -1.347417 0.293940 9 -1.337883 0.598684 1.164492 9 -2.210559 0.471886 -0.815755 1 -0.041647 -0.754124 -1.551361 8 0.577421 1.078823 -0.969372 8 1.453071 1.482258 0.132412 8 1.585731 0.313466 0.994678	**Frequencies (cm^{-1}):** -128.2522, 49.2648, 125.4765, 162.6181, 221.4459, 310.6157, 327.5195, 392.1092, 508.0751, 527.2178, 570.2736, 689.1202, 739.3659, 775.2732, 866.6245, 889.781, 903.0577, 974.8389, 1013.5754, 1056.6782, 1102.7176, 1144.1233, 1174.3029, 1276.2206, 1281.8243, 1310.4642, 1352.8677, 1388.5311, 3101.7388, 3115.7315
IRC Energy too low for IRC to take place	

6.17 Ozonolysis of *E*-2-pentene (Alkene 15)

Compound: E-EtCHCHMe + O_3 PRC1.1	**Energy (kJ mol^{-1}):** -421.488584174397
Reaction Coordinates: 6 -1.740295 -0.585099 0.352968 6 -0.821547 0.406185 -0.283648 6 -0.042492 1.277148 0.375218 6 0.879374 2.254667 -0.275745 1 0.800355 2.221132 -1.361982 1 1.919934 2.051895 -0.004605 1 0.668871 3.274713 0.055365 1 -0.083216 1.293729 1.459895 1 -0.820252 0.430588 -1.370554 1 -1.398157 -1.590734 0.089446 6 -3.198945 -0.421645 -0.094226 1 -3.830124 -1.186904 0.358681 1 -3.291167 -0.513038 -1.177907 1 -3.592572 0.554398 0.192215 1 -1.667685 -0.508530 1.439462 8 1.721210 -0.751239 1.069423 8 2.111483 -0.862851 -0.130930 8 1.271987 -1.337759 -0.954420	**Frequencies (cm^{-1}):** 52.4086, 57.2729, 66.6782, 77.0619, 88.0584, 132.2452, 174.7364, 205.5678, 236.3251, 306.0925, 314.2166, 421.6036, 487.3069, 739.6599, 765.9261, 820.7085, 886.3627, 951.3048, 986.9944, 1028.1856, 1061.251, 1083.1677, 1103.0857, 1150.6436, 1170.3659, 1184.5195, 1274.1852, 1317.4957, 1330.4383, 1371.7929, 1410.1721, 1413.2998, 1475.8246, 1481.3627, 1488.8285, 1498.5984, 1505.9748, 1676.2265, 3010.4833, 3012.2186, 3025.559, 3050.2003, 3053.0606, 3087.1634, 3091.3595, 3094.7107, 3114.747, 3135.6153

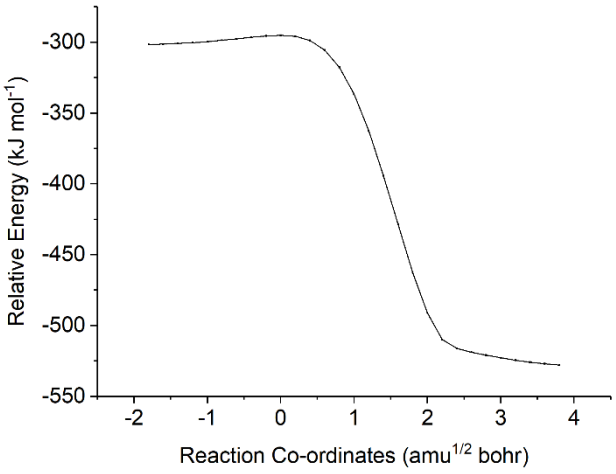
Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -421.484335971544
Reaction Coordinates: 6 -1.718366 -0.574154 0.285094 6 -0.639754 0.237996 -0.353853 6 0.180217 1.093402 0.332080 6 1.103712 2.059269 -0.336882 1 0.022995 1.211389 1.397100 1 2.010923 2.212969 0.245226 1 0.617601 3.034140 -0.444020 1 1.381633 1.719936 -1.334810 1 -0.644246 0.291379 -1.437517 1 -1.666646 -1.594651 -0.099247 6 -3.118478 -0.002846 0.012326 1 -3.882824 -0.638414 0.460343 1 -3.319145 0.055755 -1.058696 1 -3.226870 0.999673 0.427713 1 -1.540336 -0.634437 1.359943 8 1.696959 -0.485874 0.992779 8 1.895429 -0.959539 -0.192650 8 0.832978 -1.497054 -0.693708	**Frequencies (cm^{-1}):** -182.4056, 50.674, 77.3901, 97.0598, 140.42, 173.6853, 186.9526, 215.7021, 304.428, 326.4952, 454.0231, 474.6626, 502.8197, 739.7116, 780.9772, 836.0153, 885.2628, 951.9061, 956.6578, 1026.3492, 1046.9444, 1070.384, 1075.1744, 1104.4707, 1111.0102, 1187.1344, 1266.6054, 1304.4992, 1325.2135, 1362.7527, 1409.7649, 1410.2171, 1477.8087, 1487.8987, 1489.4171, 1498.4953, 1508.4053, 1597.7509, 3013.6713, 3026.5842, 3034.6722, 3065.5839, 3073.6044, 3091.0164, 3093.9823, 3110.3225, 3138.6547, 3161.7992
IRC:	



Compound: E-EtCHCHMe + O_3 POZ1.1	**Energy (kJ mol^{-1}):** -421.583943608976
Reaction Coordinates: 6 1.684696 -0.747268 0.211792 6 0.336624 -0.357350 -0.374311 6 -0.459868 0.737737 0.400490 6 -0.737339 1.988452 -0.413917 1 -1.311431 2.705640 0.171337 1 0.198448 2.463131 -0.715365 1 -1.301201 1.739134 -1.312539 1 0.031988 0.980075 1.343922 8 -1.666857 0.062812 0.784102 8 -1.826031 -0.915616 -0.266353 8 -0.518569 -1.502830 -0.308473 1 0.442560 -0.048565 -1.419504 1 1.547106 -0.997698 1.265563 1 2.019946 -1.658462 -0.287556 6 2.742814 0.344078 0.050703 1 2.463597 1.261807 0.571011 1 3.696943 0.014228 0.460521 1 2.902136 0.591894 -1.000135	**Frequencies (cm^{-1}):** 62.7112, 101.383, 192.4928, 225.0404, 233.675, 281.8098, 315.9847, 396.9137, 454.7088, 508.7768, 673.6165, 714.3245, 742.6936, 772.8453, 846.0353, 896.29, 930.1265, 953.2512, 997.072, 1037.6462, 1052.322, 1078.7669, 1116.089, 1153.23, 1180.432, 1279.9769, 1303.2886, 1322.6638, 1355.5458, 1377.9123, 1404.2388, 1410.0608, 1420.3887, 1487.3178, 1493.232, 1497.1963, 1503.9087, 1509.9617, 3003.7074, 3027.4916, 3032.9267, 3035.0219, 3054.828, 3063.7956, 3089.2092, 3095.8308, 3097.7117, 3113.6228

Compound: E-EtCHCHMe + O_3 PRC1.2	**Energy (kJ mol^{-1}):** -421.491497949549
Reaction Coordinates: 6 1.875424 -0.385929 0.681715 6 0.753230 0.601364 0.762251 6 0.205555 1.283753 -0.255317 6 -0.925875 2.247326 -0.106958 1 -1.211279 2.377239 0.936618 1 -1.806563 1.905648 -0.659437 1 -0.666102 3.225766 -0.518873 1 0.602744 1.156837 -1.255559 1 0.371957 0.787764 1.762276 1 2.655008 -0.070267 1.384374 6 2.484782 -0.613142 -0.698072 1 3.289683 -1.345934 -0.639777 1 2.904659 0.306849 -1.108124 1 1.742257 -0.989644 -1.401468 1 1.505578 -1.337055 1.079948	**Frequencies (cm^{-1}):** 49.8705, 67.3768, 68.5854, 79.7483, 94.9353, 143.7213, 204.7577, 220.0862, 240.4633, 297.909, 318.817, 370.4692, 584.556, 715.9404, 739.6891, 836.9793, 856.637, 952.6201, 991.5418, 1041.6325, 1060.6622, 1086.8529, 1104.2934, 1149.1483, 1150.2937, 1168.6361, 1293.3128, 1323.8404, 1335.8443, 1383.7695, 1412.6411, 1417.242, 1465.8366, 1476.1338, 1489.1991, 1500.8061, 1510.4617, 1674.7055, 2996.4794, 3009.6975, 3012.9957, 3031.5562, 3049.2824, 3088.2777,

8 -1.167912 -0.978271 -1.128868 8 -1.922014 -0.930556 -0.110796 8 -1.378404 -1.193352 1.004454	3094.4037, 3099.1246, 3121.698, 3156.3622

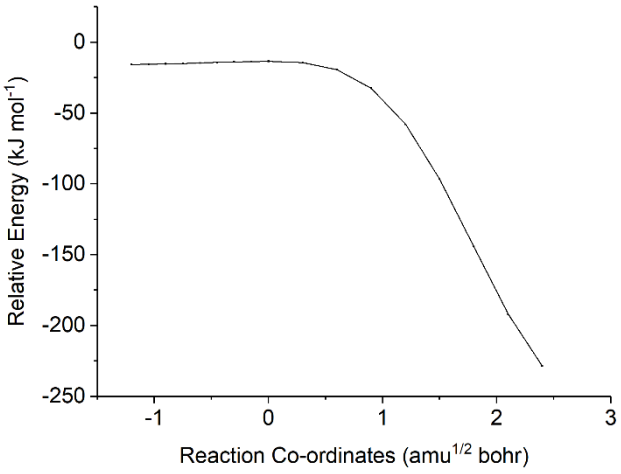
Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -421.483217596223
Reaction Coordinates: 6 -1.888878 0.025477 -0.625756 6 -0.492809 0.543541 -0.778729 6 0.253444 1.140152 0.203555 6 1.553328 1.824888 -0.073644 1 -0.189928 1.297107 1.176883 1 2.057904 1.388743 -0.936185 1 2.221968 1.775100 0.783872 1 1.383729 2.883546 -0.294297 1 -0.124464 0.606182 -1.796706 1 -2.541473 0.647851 -1.249695 6 -2.437538 -0.039153 0.796756 1 -2.512263 0.951273 1.248552 1 -1.804542 -0.656699 1.433065 1 -3.437681 -0.472201 0.793526 1 -1.925402 -0.969082 -1.078262 8 1.065576 -0.780037 1.139263 8 1.502782 -1.269644 0.025471 8 0.550001 -1.502975 -0.816464	**Frequencies (cm^{-1}):** -188.382, 67.2118, 84.8821, 96.1552, 151.1749, 178.3417, 220.713, 229.3139, 284.5453, 350.7869, 392.6666, 487.6771, 584.1714, 733.3562, 740.1909, 845.5988, 856.2946, 955.7994, 960.3943, 1043.1521, 1045.6115, 1071.7736, 1080.1009, 1102.0523, 1110.3965, 1152.4719, 1292.1589, 1304.6886, 1325.0636, 1385.498, 1410.0497, 1418.1713, 1461.4734, 1479.0089, 1488.6231, 1502.4927, 1511.3409, 1595.5623, 2993.8274, 3013.1463, 3030.8338, 3035.5302, 3072.4212, 3089.3299, 3105.5009, 3111.5825, 3143.5866, 3183.9673
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ1.2	**Energy (kJ mol^{-1}):** -421.583028237051
Reaction Coordinates: 6 1.742170 0.570256 -0.553846 6 0.289915 0.126070 -0.693240 6 -0.713617 0.634764 0.387138 6 -1.803817 1.528171 -0.177019 1 -2.483498 1.847771 0.611838 1 -1.366466 2.419604 -0.632017 1 -2.375119 0.998124 -0.938734 1 -0.193884 1.123839 1.210927 8 -1.237097 -0.574410 0.954214	**Frequencies (cm^{-1}):** 59.1461, 89.215, 188.0411, 205.7193, 233.5142, 279.2846, 341.1988, 344.4109, 481.2354, 579.3189, 658.7938, 718.1129, 739.6046, 776.8728, 824.8245, 888.694, 925.8271, 943.0479, 958.8514, 1044.609, 1056.2731, 1093.9126, 1115.3349, 1139.8958, 1165.6845, 1292.2375, 1300.8458, 1347.3392, 1355.8566,

8 -1.125318 -1.511451 -0.141375 8 0.227051 -1.297082 -0.566346 1 -0.090209 0.410446 -1.679110 1 2.297013 0.160058 -1.400472 1 1.759816 1.656057 -0.682502 6 2.432814 0.176414 0.751296 1 2.444175 -0.904234 0.879234 1 3.464272 0.529061 0.749104 1 1.942024 0.608770 1.623817	1377.3026, 1407.1655, 1409.6545, 1425.6182, 1484.1471, 1486.5692, 1497.3083, 1500.8279, 1508.0073, 3007.9717, 3027.2193, 3031.0634, 3039.6811, 3053.8033, 3068.5564, 3093.2509, 3094.1744, 3114.3859, 3115.5146

Compound: E-EtCHCHMe + O_3 PRC1.3	**Energy (kJ mol^{-1}):** -421.488408351414
Reaction Coordinates: 6 -2.110866 0.458300 0.308163 6 -0.847938 0.949138 -0.327617 6 0.195465 1.476283 0.325040 6 1.436338 1.991358 -0.326229 1 0.143456 1.562002 1.406372 1 1.377078 1.929083 -1.412479 1 2.316706 1.427583 -0.001765 1 1.621626 3.032284 -0.049329 1 -0.805724 0.895527 -1.413040 1 -2.008738 0.486640 1.394801 6 -2.519408 -0.947770 -0.147438 1 -3.463460 -1.241606 0.312496 1 -1.760968 -1.680785 0.121748 1 -2.649694 -0.986102 -1.230342 1 -2.918790 1.154244 0.053090 8 1.207538 -1.031768 1.148805 8 1.735970 -1.211056 0.014520 8 0.959863 -1.525016 -0.934958	**Frequencies (cm^{-1}):** 34.1308, 50.7693, 60.3286, 69.4913, 86.4139, 127.4418, 180.2126, 205.1944, 226.1835, 275.1265, 302.7463, 412.7107, 484.0863, 739.8419, 758.852, 823.4271, 889.2012, 952.8856, 988.7214, 1032.253, 1062.896, 1088.0075, 1100.0182, 1158.5671, 1179.2669, 1183.345, 1278.4815, 1318.5258, 1331.8554, 1373.4184, 1411.6999, 1415.2813, 1475.1028, 1477.8603, 1490.1971, 1497.473, 1507.1125, 1684.6269, 2988.5311, 3008.1546, 3030.7855, 3047.8057, 3049.2737, 3087.499, 3093.9553, 3110.3614, 3112.1261, 3130.7571

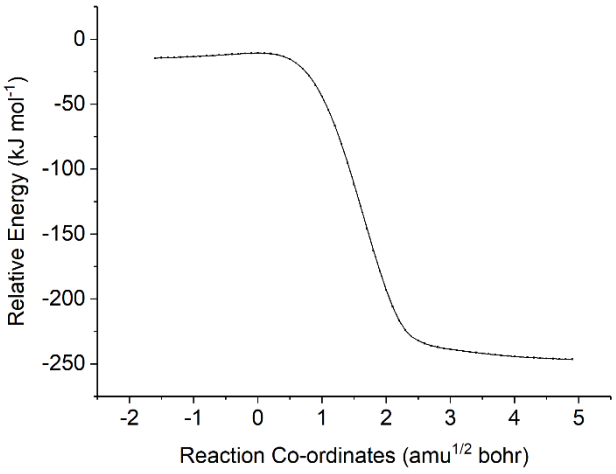
Compound: E-EtCHCHMe + O_3 TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -421.481896887431
Reaction Coordinates: 6 -1.702804 0.538697 0.588966 6 -0.462308 0.785366 -0.214088 6 0.737505 1.144840 0.329903 6 1.919813 1.558527 -0.484472 1 0.792747 1.309526 1.399345 1 1.823893 1.237980 -1.521576 1 2.845680 1.152880 -0.077600 1 2.019097 2.648476 -0.480098 1 -0.565227 0.823107 -1.293423 1 -1.457416 -0.148055 1.402837 6 -2.869610 -0.006710 -0.231163 1 -3.748164 -0.158472 0.395808 1 -2.611754 -0.961585 -0.687778 1 -3.147045 0.684923 -1.029047 1 -2.000778 1.479021 1.066594 8 1.370301 -0.991336 0.939272 8 1.200161 -1.523504 -0.222041 8 -0.031288 -1.509174 -0.605974	**Frequencies (cm^{-1}):** -148.8838, 61.4492, 76.44, 108.7421, 138.1492, 162.8624, 188.6635, 212.2849, 268.2834, 357.7501, 425.4463, 463.5265, 472.9775, 726.2331, 739.2621, 839.8347, 893.3845, 956.0241, 960.0029, 1044.6301, 1053.7135, 1082.6521, 1088.0937, 1100.8369, 1113.12, 1171.5967, 1284.7341, 1294.1423, 1313.8097, 1376.9036, 1410.1944, 1416.4749, 1463.1431, 1477.3757, 1488.7903, 1500.0426, 1506.7703, 1604.6492, 2995.8308, 3014.1377, 3029.6537, 3041.6562, 3072.0552, 3088.1947, 3105.49, 3106.023, 3138.2489, 3157.3772
IRC:	



Compound: E-EtCHCHMe + O_3 POZ1.3	**Energy (kJ mol^{-1}):** -421.584155305522
Reaction Coordinates: 6 1.629291 0.611131 0.480575 6 0.372590 0.147728 -0.235952 6 -0.970943 0.608446 0.403089 6 -1.761042 1.569258 -0.466468 1 -2.691029 1.854075 0.023680 1 -1.182583 2.476873 -0.652675 1 -1.997525 1.108358 -1.425265 1 -0.800178 1.024505 1.397486 8 -1.674675 -0.621463 0.636660 8 -1.100745 -1.515276 -0.347121 8 0.299340 -1.279439 -0.168079 1 0.390160 0.450939 -1.288137 1 1.609371 1.703998 0.505715 1 1.581713 0.268195 1.516576 6 2.920587 0.131701 -0.181100 1 2.986002 0.477972 -1.214188 1 3.791689 0.511118 0.353080 1 2.978124 -0.956191 -0.188830	**Frequencies (cm^{-1}):** 59.3892, 102.8335, 180.5783, 215.2143, 233.7539, 285.572, 301.7684, 395.3131, 479.1007, 503.0922, 646.6847, 723.1593, 748.222, 770.6378, 848.6494, 896.0402, 931.8441, 959.7328, 965.9326, 1045.3307, 1057.3865, 1095.5847, 1117.0301, 1143.4778, 1178.1827, 1286.5304, 1309.4065, 1332.4514, 1354.9259, 1378.5038, 1407.9144, 1410.7469, 1419.7996, 1478.1238, 1486.3193, 1497.4077, 1500.2126, 1507.2973, 3002.6981, 3022.5739, 3030.3067, 3031.3976, 3052.3587, 3058.6103, 3091.0241, 3093.4551, 3104.8712, 3113.9491

Compound: E-EtCHCHMe + O_3 PRC 2.1	**Energy (kJ mol^{-1}):** -421.488412063809
Reaction Coordinates: 6 1.681859 -0.571936 -0.353895 6 0.805693 0.462641 0.277701 6 0.002533 1.302166 -0.393169 6 -0.881277 2.328454 0.230648 1 -1.926017 2.136451 -0.025474 1 -0.641631 3.328518 -0.140125 1 -0.793076 2.329832 1.316366 1 0.001161 1.257089 -1.478366 1 0.853849 0.540585 1.360446 1 1.322762 -1.566587 -0.065024 6 3.153759 -0.447676 0.061350 1 3.263624 -0.520844 1.144560 1 3.570009 0.510285 -0.252155	**Frequencies (cm^{-1}):** 42.2677, 56.9293, 71.5651, 81.5233, 90.0497, 141.0423, 181.9032, 205.4046, 233.5044, 304.4492, 312.2162, 424.0715, 485.2367, 739.641, 763.1984, 822.6074, 888.2298, 951.7223, 986.2725, 1029.2267, 1062.9741, 1084.7685, 1103.6655, 1150.5181, 1170.1679, 1184.1695, 1278.3249, 1316.8326, 1331.7104, 1373.5811, 1409.9642, 1411.1834, 1475.7629, 1479.2856, 1487.3538, 1498.5669, 1505.4007, 1676.1601,

1 3.751840 -1.240636 -0.388617 1 1.591895 -0.515514 -1.440640 8 -1.979848 -0.600018 -0.914386 8 -1.583011 -1.456026 -0.066830 8 -1.383368 -1.031590 1.110368	2992.5755, 3016.4643, 3027.1847, 3047.8093, 3059.5013, 3088.9876, 3093.1187, 3098.3424, 3119.0874, 3131.689

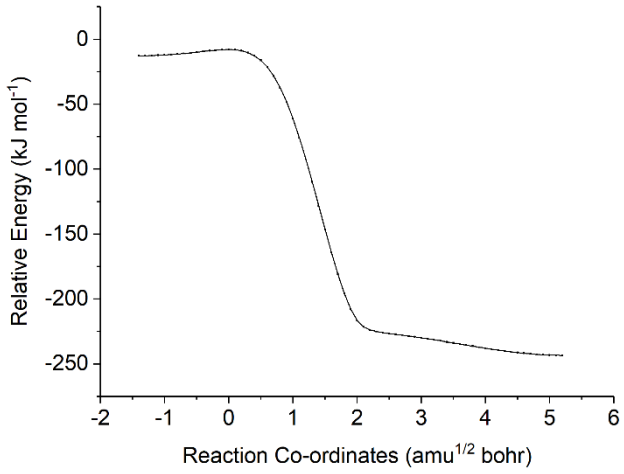
Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -421.482369557796
Reaction Coordinates: 6 1.645376 -0.638019 -0.159314 6 0.615525 0.273427 0.433529 6 -0.181487 1.096196 -0.317003 6 -1.046837 2.165327 0.256795 1 -0.045164 1.096119 -1.392583 1 -0.593052 3.147802 0.095170 1 -1.194373 2.026915 1.326824 1 -2.023640 2.177032 -0.226979 1 0.654259 0.431906 1.504956 1 1.673209 -1.570748 0.405339 6 3.047914 -0.007541 -0.155444 1 3.360648 0.249754 0.857610 1 3.073666 0.903167 -0.754559 1 3.779810 -0.704451 -0.565030 1 1.362792 -0.892004 -1.183115 8 -1.897463 -0.361807 -0.780436 8 -1.407236 -1.429552 -0.243076 8 -1.011690 -1.233869 0.971136	**Frequencies (cm^{-1}):** -181.5449, 46.5181, 77.5772, 120.546, 141.2679, 178.5368, 185.8023, 223.6371, 304.6912, 331.8079, 431.8882, 489.9109, 509.7112, 740.4161, 785.3186, 837.6203, 883.1986, 948.2282, 957.1135, 1024.7894, 1047.0982, 1069.0044, 1075.2178, 1105.2295, 1113.6094, 1186.8217, 1271.8589, 1299.0459, 1335.1025, 1360.8696, 1409.1053, 1410.8902, 1473.216, 1486.127, 1491.3066, 1497.5734, 1509.3064, 1597.8, 3016.6095, 3027.1487, 3033.4601, 3067.7716, 3074.3512, 3091.5597, 3096.3525, 3109.0755, 3144.7551, 3156.3794
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ 2.1	**Energy (kJ mol^{-1}):** -421.583851830179
Reaction Coordinates: 6 -1.588350 -0.805182 -0.142998 6 -0.309421 -0.309630 0.521206 6 0.481308 0.748207 -0.308605 1 0.051145 0.807670 -1.312623 6 0.606487 2.123785 0.313635 1 1.248533 2.761399 -0.293262 1 -0.373905 2.595676 0.378118 1 1.029826 2.054808 1.315280	**Frequencies (cm^{-1}):** 64.7705, 111.9565, 195.1397, 218.8796, 225.1517, 282.1916, 317.9956, 389.4891, 465.4936, 504.4775, 660.794, 729.391, 748.6991, 766.3288, 859.5377, 894.1693, 921.5465, 936.9667, 987.7149, 1037.7992, 1050.9968, 1087.2358, 1131.2113, 1155.5538, 1179.0696, 1268.694,

8 1.793441 0.183975 -0.401706 8 1.518720 -1.219964 -0.432746 8 0.642403 -1.367392 0.709128 1 -0.515247 0.065226 1.526544 1 -1.958642 -1.651192 0.438473 1 -1.340632 -1.187850 -1.135361 6 -2.673298 0.268337 -0.237743 1 -2.934515 0.656609 0.748844 1 -3.580927 -0.140760 -0.680755 1 -2.362503 1.112364 -0.855644	1309.7594, 1338.9998, 1346.9399, 1380.7929, 1399.6796, 1414.5785, 1419.5094, 1487.3651, 1492.8972, 1500.2436, 1504.1552, 1509.6019, 3014.8514, 3025.2587, 3033.5754, 3039.8445, 3042.4624, 3065.1757, 3087.7622, 3094.7033, 3107.0054, 3112.3561

Compound: E-EtCHCHMe + O_3 PRC 2.2	**Energy (kJ mol^{-1}):** -421.487848822016
Reaction Coordinates: 6 1.819178 -0.387187 0.686960 6 0.736668 0.647177 0.758088 6 0.194562 1.308353 -0.275852 6 -0.892398 2.323443 -0.158790 1 -1.770567 2.007508 -0.727119 1 -0.575638 3.284768 -0.571974 1 -1.194900 2.473387 0.876902 1 0.573118 1.126382 -1.275302 1 0.380205 0.878827 1.757246 1 2.609907 -0.098510 1.388360 6 2.425741 -0.649508 -0.688671 1 2.882035 0.251191 -1.101809 1 1.677061 -1.001607 -1.398934 1 3.201189 -1.412469 -0.620452 1 1.420978 -1.324183 1.095078 8 -1.420991 -0.825579 -1.129254 8 -1.346955 -1.500539 -0.057747 8 -1.595290 -0.878753 1.017949	**Frequencies (cm^{-1}):** 52.9397, 58.1826, 68.8945, 81.5961, 89.4161, 153.5717, 204.2447, 219.9466, 239.8108, 292.9988, 317.0631, 369.9358, 583.6526, 716.9881, 739.2529, 835.4286, 855.6535, 951.981, 992.0281, 1041.9454, 1062.6787, 1087.4236, 1103.2847, 1150.3363, 1152.672, 1169.9164, 1290.3102, 1325.8236, 1334.7186, 1381.8094, 1410.6511, 1419.4712, 1469.0045, 1476.2265, 1487.8301, 1501.3044, 1509.7975, 1676.471, 2989.8577, 3005.4093, 3015.7424, 3031.5703, 3058.57, 3090.0874, 3094.7003, 3098.638, 3127.062, 3152.0201

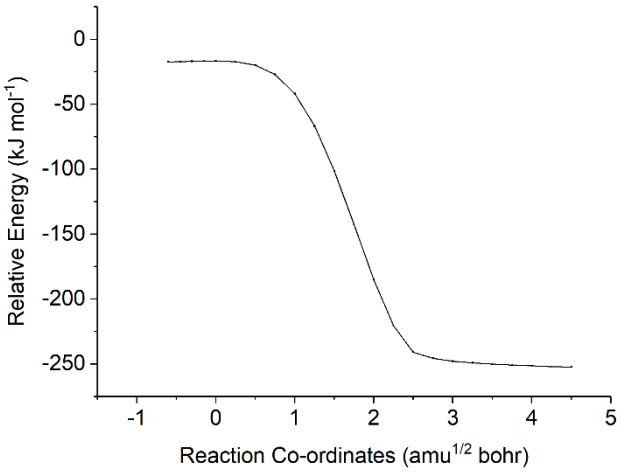
Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -421.482448026458
Reaction Coordinates: 6 -1.816215 -0.235671 0.619683 6 -0.380106 -0.646950 0.772093 6 0.429611 -1.086962 -0.246339 6 1.769338 -1.699437 -0.016006 1 0.008172 -1.191523 -1.237070 1 1.702357 -2.789639 -0.083447 1 2.163014 -1.439293 0.965319 1 2.482332 -1.371165 -0.771989 1 -0.036591 -0.793182 1.788753 1 -2.417865 -0.936440 1.210158 6 -2.363368 -0.170698 -0.804869 1 -2.343689 -1.147539 -1.290325 1 -1.796317 0.524438 -1.423785 1 -3.399359 0.167259 -0.791239 1 -1.949824 0.731610 1.110263 8 1.225177 0.888078 -0.996082 8 0.575284 1.689506 -0.212120 8 0.668565 1.332889 1.030201	**Frequencies (cm^{-1}):** -217.6643, 57.3799, 82.4775, 126.0984, 154.0963, 184.6347, 218.1401, 241.5065, 282.0621, 360.5824, 403.1986, 491.4515, 587.8702, 733.6315, 745.8491, 842.8608, 858.3896, 951.0506, 957.8494, 1040.1506, 1044.4954, 1063.9249, 1080.8622, 1100.2809, 1110.2455, 1157.1246, 1291.9897, 1300.0723, 1320.309, 1381.1644, 1410.3168, 1421.0661, 1465.8541, 1473.1178, 1486.8735, 1503.3542, 1509.2003, 1589.6949, 2997.2193, 3016.1634, 3032.9582, 3039.6326, 3076.2247, 3091.5245, 3101.4563, 3111.7958, 3156.0066, 3178.452
IRC:	



Compound: E-EtCHCHMe + O_3 POZ 2.2	**Energy (kJ mol^{-1}):** -421.583083231273
Reaction Coordinates: 6 1.560747 -0.934347 0.381480 6 0.213357 -0.301243 0.727301 6 -0.880579 -0.433667 -0.370236 1 -0.414426 -0.702243 -1.321203 6 -2.017853 -1.377907 -0.041047 1 -1.639432 -2.396713 0.048429 1 -2.767990 -1.366893 -0.830927 1 -2.493071 -1.096119 0.898147 8 -1.408104 0.891630 -0.470412 8 -0.241943 1.690086 -0.261943 8 0.299643 1.114745 0.956858 1 -0.156607 -0.713723 1.668241 1 1.383012 -1.995889 0.178501 1 2.182000 -0.900162 1.278825 6 2.316762 -0.289796 -0.779642 1 1.777783 -0.370270 -1.723590 1 3.283890 -0.775313 -0.911612 1 2.493462 0.767396 -0.587969	**Frequencies (cm^{-1}):** 60.4282, 102.1048, 195.2891, 214.6022, 226.0847, 272.7123, 333.4032, 345.6821, 475.5063, 571.8655, 646.1119, 717.6559, 743.125, 788.0024, 827.8269, 888.2271, 916.95, 938.3956, 951.2646, 1045.3106, 1076.4613, 1091.3382, 1119.1613, 1158.7106, 1167.8806, 1278.1621, 1318.8674, 1336.854, 1356.0311, 1382.6477, 1406.4529, 1414.8674, 1424.1166, 1483.1315, 1486.7471, 1500.3015, 1502.8651, 1507.0398, 3008.361, 3029.3725, 3038.6341, 3040.7945, 3043.1664, 3053.2218, 3095.0621, 3104.0053, 3110.6241, 3113.2495

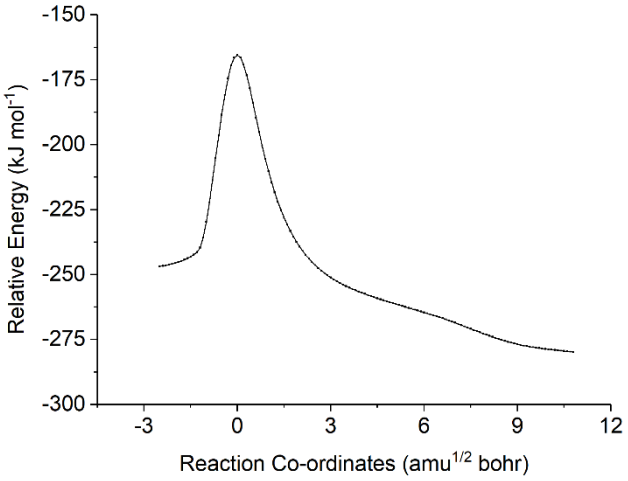
Compound: E-EtCHCHMe + O_3 PRC 2.3	**Energy (kJ mol^{-1}):** -421.488896111931
Reaction Coordinates: 6 -1.916365 -0.608218 -0.502312 6 -0.681455 -1.046188 0.225096 6 0.478477 -1.392176 -0.352774 6 1.677916 -1.900869 0.374601 1 0.553818 -1.342020 -1.435206 1 2.544108 -1.264390 0.182137 1 1.939410 -2.906876 0.035055 1 1.510936 -1.933311 1.450701 1 -0.768964 -1.141122 1.304461 1 -1.666136 -0.356091 -1.535213 6 -2.656328 0.554328 0.168574 1 -2.036251 1.448637 0.217099 1 -2.941552 0.296597 1.189914	**Frequencies (cm^{-1}):** 29.8602, 59.2189, 65.0918, 79.7001, 89.6354, 134.1471, 179.9143, 201.6077, 226.7766, 286.6027, 298.2473, 414.9852, 479.4264, 738.0541, 748.2966, 825.5325, 889.443, 953.489, 987.044, 1036.3263, 1064.2304, 1090.1374, 1098.0935, 1154.8251, 1173.649, 1181.9697, 1278.5475, 1314.1289, 1329.944, 1375.1521, 1410.6442, 1415.5444, 1475.2154, 1476.0086, 1489.1829, 1499.0961, 1504.611, 1676.172,

1 -3.566530 0.800196 -0.378968 1 -2.602063 -1.462594 -0.556227 8 1.676511 1.114686 -0.861086 8 0.870478 1.791045 -0.153699 8 0.655480 1.371733 1.020677	2984.2293, 3016.2331, 3031.541, 3043.7965, 3061.7515, 3089.1881, 3097.1921, 3103.9021, 3114.8445, 3129.56

Compound: E-EtCHCHMe + O_3 TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -421.482791796432
Reaction Coordinates: 6 -1.585661 -0.534244 -0.636299 6 -0.368389 -0.863802 0.173208 6 0.863639 -1.069246 -0.374913 6 2.057215 -1.515920 0.396509 1 0.954642 -1.055699 -1.455450 1 2.920129 -0.889082 0.167492 1 2.324106 -2.542116 0.127620 1 1.878545 -1.474554 1.469911 1 -0.505152 -1.071593 1.227964 1 -1.357548 0.322574 -1.280512 6 -2.827385 -0.241512 0.201065 1 -2.656742 0.611443 0.857840 1 -3.092758 -1.098211 0.823282 1 -3.683079 -0.015175 -0.434806 1 -1.787379 -1.362941 -1.323978 8 1.509216 1.173702 -0.623256 8 0.439761 1.746755 -0.188795 8 0.072113 1.320006 0.969953	**Frequencies (cm^{-1}):** -124.7567, 48.7914, 87.1644, 128.8724, 140.229, 166.236, 190.3325, 220.0948, 276.1717, 351.9511, 425.3763, 465.2244, 474.2651, 726.2648, 738.8533, 839.1315, 895.0763, 958.5987, 959.6939, 1043.4284, 1055.3506, 1083.9675, 1091.6793, 1098.5971, 1116.795, 1172.8786, 1284.3789, 1296.2726, 1308.6784, 1379.2735, 1409.8176, 1416.6383, 1468.3369, 1473.9186, 1485.7609, 1499.2145, 1507.473, 1609.8296, 2994.0737, 3010.3495, 3017.5099, 3030.3872, 3070.2837, 3088.5578, 3101.883, 3106.6534, 3143.0212, 3155.6908
IRC:  	

Compound: E-EtCHCHMe + O_3 POZ 2.3	**Energy (kJ mol^{-1}):** -421.584499116535
Reaction Coordinates: 6 1.535423 0.534084 0.575195 6 0.346354 0.223024 -0.322589 6 -1.030133 0.510142 0.347002 1 -0.873551 0.692253 1.414317 6 -1.848217 1.619904 -0.279454 1 -1.330390 2.572715 -0.164467 1 -2.818764 1.704467 0.208139 1 -2.005024 1.430568 -1.340947	**Frequencies (cm^{-1}):** 61.1127, 104.9018, 189.9569, 217.4095, 231.4799, 276.8662, 293.0606, 396.0192, 482.1328, 509.07, 649.8929, 712.2079, 744.8433, 778.4549, 866.8942, 890.9963, 924.3127, 940.3574, 963.6834, 1049.0934, 1066.1333, 1094.2115, 1121.8497, 1157.7834, 1174.0654, 1279.9548,

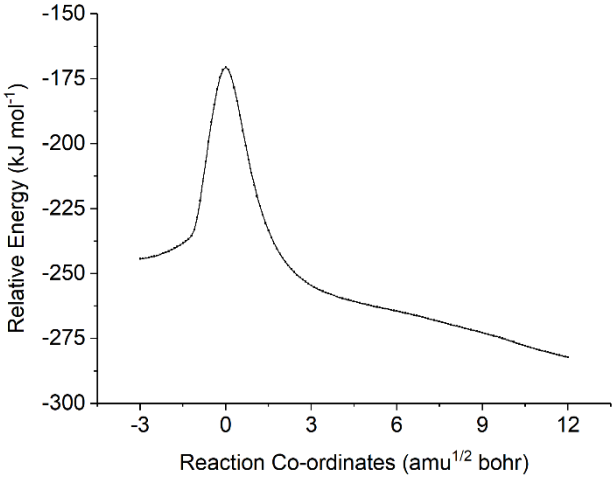
8 -1.741304 -0.720384 0.186806 8 -0.689872 -1.687315 0.280851 8 0.267215 -1.168181 -0.673336 1 0.430336 0.745453 -1.278394 1 1.456382 -0.084383 1.472259 1 1.448129 1.574882 0.903863 6 2.882944 0.313046 -0.107378 1 2.988033 -0.721074 -0.434669 1 3.705455 0.535795 0.572381 1 2.992857 0.955158 -0.983697	1293.1866, 1338.0158, 1356.4399, 1385.1085, 1402.1397, 1415.1632, 1417.5001, 1477.3576, 1486.6657, 1499.5593, 1501.5167, 1507.9329, 3008.1489, 3016.7029, 3028.0805, 3037.0783, 3039.5531, 3057.4536, 3087.9805, 3101.781, 3103.6298, 3112.9225

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.1	**Energy (kJ mol^{-1}):** -421.549380422627
Reaction Coordinates: 6 -1.674635 -0.867488 -0.211761 6 -0.293436 -0.568357 0.307925 6 0.628655 0.924535 -0.483910 6 0.346911 2.099820 0.444357 1 -0.716889 2.246898 0.626862 1 0.740734 3.008086 -0.014597 1 0.862033 1.954738 1.393318 6 -2.686646 0.259819 -0.009643 1 -2.757278 0.552643 1.038751 1 -2.432174 1.144078 -0.592068 1 -3.675009 -0.070092 -0.326809 1 -0.191077 -0.202224 1.325975 1 -2.030226 -1.762642 0.308040 1 -1.601788 -1.131434 -1.267878 1 0.051168 0.914270 -1.422014 8 1.837020 0.515950 -0.574436 8 1.802280 -1.217582 0.421727 8 0.588877 -1.516405 -0.016215	**Frequencies (cm^{-1}):** -476.5859, 69.0866, 98.2151, 173.4452, 193.664, 229.5986, 270.8505, 290.1543, 378.5908, 424.5921, 482.2148, 491.7824, 555.8081, 612.0344, 783.1152, 870.1647, 927.6367, 968.4821, 982.2783, 1035.6195, 1063.2102, 1096.4126, 1116.3377, 1159.6463, 1179.3719, 1246.2126, 1301.2076, 1326.9905, 1330.9384, 1394.4486, 1412.5405, 1424.6189, 1440.1641, 1481.5121, 1484.38, 1496.0891, 1504.9147, 1511.6844, 2926.7104, 3014.8747, 3035.1135, 3038.5385, 3064.6868, 3096.8382, 3099.8153, 3107.9825, 3112.4509, 3116.98
IRC:  	

Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.1	**Energy (kJ mol^{-1}):** -421.595845842666
Reaction Coordinates:	**Frequencies (cm^{-1}):**

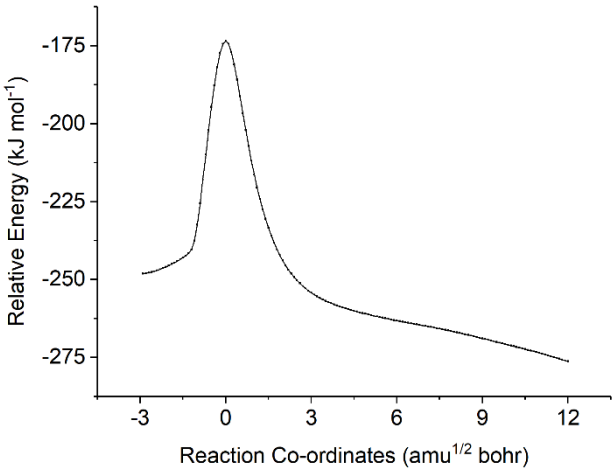
6 2.345438 0.222221 -0.299027 6 1.091165 0.690518 0.331503 6 -1.838594 -0.678247 0.473145 6 -2.793675 -0.576999 -0.676933 1 -3.688025 -1.162361 -0.442143 1 -2.343321 -0.955141 -1.592101 1 -3.102228 0.459887 -0.804976 6 2.569328 -1.284974 -0.097208 1 2.601094 -1.540293 0.961730 1 1.767272 -1.859702 -0.554426 1 3.517937 -1.576978 -0.545557 1 0.842494 0.501716 1.370197 1 3.170568 0.773716 0.167288 1 2.331840 0.486960 -1.355767 1 -2.193111 -0.243742 1.422246 8 -0.773328 -1.262694 0.428725 8 -0.895644 1.760291 0.286137 8 0.275662 1.362506 -0.341785	42.0072, 52.9546, 72.5509, 80.5939, 130.0276, 132.9557, 176.1572, 205.3186, 240.4542, 278.5993, 325.0106, 424.9231, 514.6817, 535.9541, 776.1863, 791.908, 894.1458, 905.9834, 917.5901, 938.0548, 1022.5923, 1096.2713, 1115.3467, 1135.3901, 1182.1924, 1275.1886, 1325.5837, 1373.5271, 1376.2788, 1420.6604, 1424.5671, 1457.0395, 1467.5534, 1474.8352, 1496.5567, 1505.4297, 1579.346, 1748.2871, 2946.591, 2998.441, 3022.0867, 3045.7883, 3086.2788, 3091.8467, 3109.6546, 3129.1972, 3134.5785, 3166.9687

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.2	**Energy (kJ mol^{-1}):** -421.551877987989
Reaction Coordinates: 6 1.666366 0.642755 -0.541622 6 0.349755 -0.078508 -0.629117 6 -0.999481 0.599490 0.510603 6 -1.606280 1.740897 -0.299949 1 -2.171875 1.345797 -1.142784 1 -0.848702 2.438411 -0.661116 1 -2.294521 2.295868 0.338984 6 2.511563 0.313349 0.688201 1 1.972970 0.523072 1.612349 1 2.799428 -0.736249 0.703613 1 3.420597 0.913659 0.686110 1 -0.224692 0.034974 -1.543734 1 1.451169 1.712656 -0.582701 1 2.230486 0.422433 -1.453599 1 -0.341343 0.924790 1.332321 8 -1.731191 -0.422753 0.753028 8 0.368482 -1.333860 -0.172494 8 -0.827923 -1.891302 -0.287802	**Frequencies (cm^{-1}):** -462.5283, 82.4136, 88.4235, 171.3083, 201.7565, 211.3323, 246.1585, 323.1904, 373.8907, 413.9391, 480.548, 518.6697, 582.2787, 644.5958, 780.9312, 866.0714, 906.7746, 978.9033, 987.1634, 1031.6361, 1063.1129, 1093.1427, 1109.2807, 1140.3772, 1184.4143, 1254.9951, 1290.8773, 1335.9625, 1376.5717, 1391.6599, 1396.4297, 1428.3387, 1438.8091, 1477.1805, 1481.0628, 1497.0936, 1501.362, 1507.0533, 2924.3295, 3014.2757, 3028.6568, 3043.7387, 3053.8749, 3090.1287, 3103.0593, 3111.6702, 3114.9935, 3118.6321
IRC:	



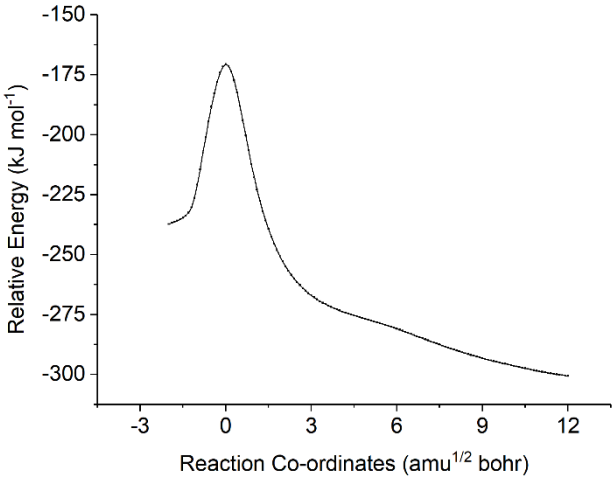
Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.2	**Energy (kJ mol^{-1}):** -421.596815811173
Reaction Coordinates: 6 -2.184680 0.573728 0.600706 6 -0.910369 -0.170058 0.706799 6 1.916700 0.531445 -0.546503 6 3.135941 0.122422 0.222744 1 3.067053 0.440062 1.260873 1 4.010803 0.590736 -0.239407 1 3.269622 -0.956828 0.162797 6 -3.040203 0.254671 -0.620306 1 -2.500942 0.467887 -1.541795 1 -3.331924 -0.794480 -0.638642 1 -3.945139 0.860056 -0.606095 1 -0.215970 -0.019558 1.524974 1 -1.911882 1.634801 0.627165 1 -2.737519 0.401553 1.532005 1 1.852194 0.137387 -1.573831 8 1.084251 1.322246 -0.142246 8 -0.606903 -1.024692 -0.156679 8 0.640073 -1.626912 -0.037160	**Frequencies (cm^{-1}):** 45.1866, 47.8048, 77.6404, 95.1931, 141.8753, 152.7521, 197.381, 201.1667, 261.3593, 269.3164, 299.1753, 425.6257, 513.417, 622.5573, 739.0062, 794.4318, 896.0498, 900.2705, 919.3153, 926.7113, 1027.3958, 1106.5996, 1112.7761, 1125.5387, 1134.0282, 1278.1834, 1350.0074, 1379.2513, 1392.5913, 1423.8789, 1424.2854, 1443.2306, 1457.7398, 1472.2245, 1499.5135, 1504.9112, 1584.3872, 1740.028, 2949.5137, 3001.8195, 3020.464, 3022.7196, 3048.5144, 3090.8625, 3112.5133, 3116.1148, 3134.3129, 3175.6459

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 1.3	**Energy (kJ mol^{-1}):** -421.552487519029
Reaction Coordinates: 6 1.608723 0.567044 0.487635 6 0.419190 -0.075428 -0.161504 6 -1.248708 0.594056 0.437475 6 -1.458189 1.832087 -0.430940 1 -1.662905 1.540740 -1.460181 1 -0.600945 2.506452 -0.402699 1 -2.325086 2.376906 -0.054731 6 2.922789 0.260020 -0.241598 1 3.130878 -0.809526 -0.239758 1 2.888024 0.595633 -1.278868 1 3.754313 0.767964 0.246609 1 0.242296 0.111317 -1.217248 1 1.661182 0.236210 1.525935	**Frequencies (cm^{-1}):** -452.7878, 66.9129, 92.1538, 163.8705, 201.0501, 211.9882, 242.2777, 307.8659, 356.7756, 468.8252, 478.9137, 518.1423, 543.5564, 616.1528, 776.8373, 873.1063, 921.3667, 979.9215, 994.1288, 1018.5205, 1056.6332, 1088.1927, 1129.4007, 1160.9558, 1181.0155, 1244.3065, 1302.2264, 1333.5361, 1353.1717, 1392.384, 1408.2269, 1425.4729, 1439.8994, 1478.3593, 1479.8696, 1498.71, 1499.8182, 1506.3758,

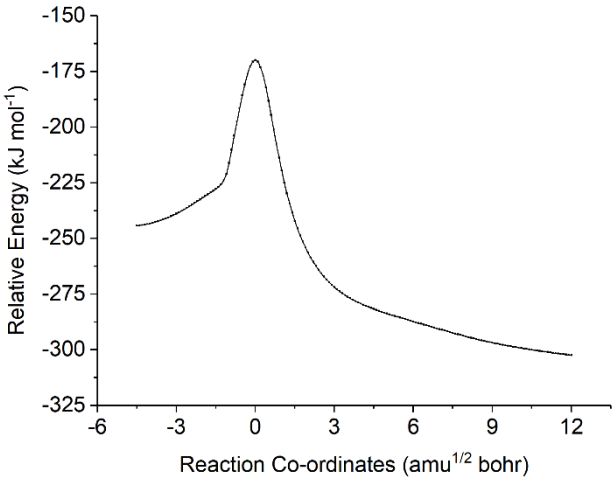
1 1.441345 1.645219 0.504718 1 -0.946270 0.811274 1.475333 8 -2.043900 -0.394257 0.276537 8 0.237678 -1.352436 0.186295 8 -0.824485 -1.859417 -0.418522	2915.4204, 3029.6751, 3034.0878, 3044.2574, 3075.7949, 3091.1753, 3098.096, 3106.6876, 3112.717, 3116.2338
IRC:  	

Compound: E-EtCHCHMe + O_3 C_{ANTI} 1.3	**Energy (kJ mol^{-1}):** -421.592304735529
Reaction Coordinates: 6 2.016574 -0.716811 -0.494140 6 1.159297 0.282047 0.180685 6 -2.235987 -0.253200 0.124467 6 -3.687661 -0.542497 -0.106656 1 -3.862768 -1.606352 -0.249052 1 -4.031299 0.017654 -0.980293 1 -4.268892 -0.174142 0.742828 6 3.305366 -1.003894 0.292526 1 3.932962 -0.115860 0.359619 1 3.084368 -1.342492 1.305043 1 3.875915 -1.787032 -0.204806 1 0.804329 0.164141 1.199658 1 2.235572 -0.375069 -1.505121 1 1.425480 -1.634871 -0.572223 1 -1.961356 0.805128 0.276268 8 -1.372744 -1.105615 0.144719 8 0.815896 1.320266 -0.426163 8 -0.015633 2.217226 0.237291	**Frequencies (cm^{-1}):** 25.9963, 42.2362, 43.6952, 61.1989, 69.7843, 93.3085, 130.927, 163.3971, 204.6656, 209.5304, 326.6427, 417.1765, 511.891, 533.0139, 774.6084, 789.4365, 885.0835, 891.3136, 910.768, 942.1045, 1019.8716, 1093.9921, 1129.6983, 1154.9649, 1181.6657, 1275.0043, 1324.8872, 1374.3865, 1379.2058, 1417.0591, 1448.6431, 1460.828, 1468.1962, 1470.4036, 1500.7651, 1505.5655, 1586.0273, 1765.1542, 2948.6456, 3021.5374, 3021.9536, 3038.7213, 3072.5224, 3086.7386, 3107.2711, 3109.7434, 3131.6861, 3156.9924

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.1	**Energy (kJ mol^{-1}):** -421.553099505068
Reaction Coordinates: 6 1.769289 -0.571468 0.100326 6 0.495268 -0.252246 -0.681838 6 -0.612804 0.819107 0.363802 6 -1.585307 1.469112 -0.577937	**Frequencies (cm^{-1}):** -455.5989, 68.353, 111.5629, 171.092, 189.3761, 240.9539, 254.6737, 288.5137, 334.6834, 392.9801, 486.0785, 548.8001, 609.7895, 697.3704, 786.1673, 860.5998,

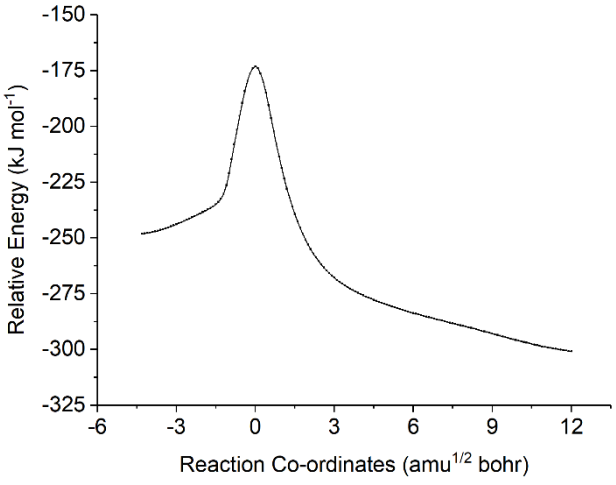
1 -1.938903 0.769859 -1.328851 1 -1.107848 2.320115 -1.060657 1 -2.443677 1.832176 -0.007381 6 2.723626 0.609979 0.254033 1 2.299577 1.411004 0.862387 1 2.985598 1.036243 -0.716817 1 3.650873 0.298629 0.734501 1 0.620287 0.529370 -1.453105 1 1.494892 -0.989215 1.070125 1 2.265334 -1.376574 -0.446590 1 0.002632 1.477237 0.969356 8 -1.044932 -0.190370 1.145452 8 -1.737761 -1.065972 0.436986 8 -0.288457 -1.213126 -1.004098	902.7111, 938.7086, 996.0624, 1029.9804, 1049.1876, 1086.499, 1117.7416, 1145.4926, 1182.2283, 1215.7934, 1282.6978, 1304.0311, 1339.746, 1396.1577, 1417.1522, 1426.2771, 1440.8731, 1474.8601, 1482.88, 1496.5508, 1501.6978, 1503.726, 2892.8746, 3023.4513, 3035.5584, 3036.3321, 3062.4651, 3084.3281, 3093.147, 3103.5192, 3136.1778, 3154.7766
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.1	**Energy (kJ mol^{-1}):** -421.596446137597
Reaction Coordinates: 6 1.885569 -0.150819 -0.613871 6 1.665496 1.204534 -0.009417 6 -1.972738 0.222780 0.629340 6 -2.505478 0.730874 -0.637343 1 -1.689826 0.803151 -1.360245 1 -2.982768 1.697111 -0.502769 1 -3.201655 -0.003897 -1.051955 6 2.849405 -0.995521 0.231089 1 2.413916 -1.228212 1.202733 1 3.798399 -0.482032 0.396531 1 3.061957 -1.937542 -0.271798 1 2.592068 1.783612 0.191557 1 0.929757 -0.656703 -0.751598 1 2.333071 0.018405 -1.600804 1 -2.022408 0.755233 1.571191 8 -1.415518 -0.900272 0.730604 8 -1.272966 -1.641417 -0.425555 8 0.592731 1.689162 0.267246	**Frequencies (cm^{-1}):** 28.6136, 36.8941, 52.8607, 72.3292, 79.5737, 93.7231, 104.2066, 160.6709, 209.1104, 296.3398, 331.5294, 453.4659, 518.627, 669.9734, 763.8095, 768.8914, 876.91, 881.8314, 924.7588, 985.8648, 1006.0905, 1055.4577, 1112.0018, 1135.4342, 1169.5424, 1280.4774, 1344.9298, 1354.1709, 1396.8592, 1410.5811, 1427.5763, 1440.2222, 1461.2682, 1478.0706, 1500.7573, 1505.7463, 1575.2569, 1782.5412, 2860.8282, 2996.6456, 3026.3718, 3031.1418, 3070.7638, 3077.3367, 3095.896, 3107.7674, 3143.4756, 3182.4111

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.2	**Energy (kJ mol^{-1}):** -421.552299326382
Reaction Coordinates: 6 1.739494 -0.878882 -0.138232 6 0.365480 -0.777460 0.531984 6 -0.921916 -0.377036 -0.726895 6 -2.233653 -0.842898 -0.159813 1 -3.047839 -0.364342 -0.709289 1 -2.320595 -1.920814 -0.285104 1 -2.324643 -0.585765 0.890671 6 2.420176 0.453899 -0.434635 1 3.436621 0.289212 -0.792801 1 2.468141 1.068227 0.462979 1 1.884096 1.021577 -1.194564 1 -0.073029 -1.766539 0.754521 1 1.655314 -1.487993 -1.042630 1 2.360908 -1.456954 0.553394 1 -0.620004 -0.803570 -1.679454 8 -0.676627 0.950325 -0.764079 8 -0.940398 1.503191 0.406880 8 0.162468 0.114138 1.433178	**Frequencies (cm^{-1}):** -441.6395, 72.0558, 112.4409, 176.2697, 199.7945, 243.5568, 269.0828, 288.3266, 302.4816, 393.9086, 536.8849, 548.6676, 674.0467, 702.7366, 792.628, 830.1472, 895.7149, 949.8234, 996.661, 1029.9834, 1046.6003, 1089.8941, 1104.8237, 1140.6727, 1188.0164, 1211.9866, 1291.8274, 1303.2324, 1347.7845, 1396.6285, 1409.4898, 1426.2491, 1447.4311, 1475.1692, 1485.7062, 1496.4683, 1497.3326, 1509.382, 2896.7239, 3009.1228, 3034.9724, 3037.0296, 3041.9061, 3098.5974, 3104.584, 3114.0203, 3127.4535, 3154.7772
IRC:  	

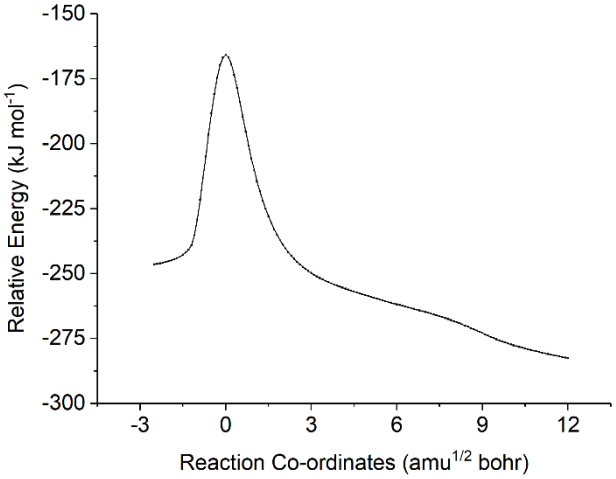
Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.2	**Energy (kJ mol^{-1}):** -421.596944298324
Reaction Coordinates: 6 2.525974 0.303166 -0.239626 6 1.873732 -1.033917 -0.437892 6 -1.967246 -0.653286 -0.256536 6 -2.167952 -0.457495 1.180978 1 -2.871815 0.364363 1.337315 1 -2.509020 -1.371976 1.657590 1 -1.223658 -0.128611 1.622889 6 1.873010 1.205142 0.797464 1 2.435312 2.133195 0.897976 1 1.844147 0.719625 1.773114 1 0.851607 1.452839 0.509622 1 2.358119 -1.675521 -1.202853 1 2.554041 0.780036 -1.226981 1 3.578523 0.098875 -0.005318 1 -2.067663 -1.604421 -0.764995	**Frequencies (cm^{-1}):** 19.6956, 35.2664, 45.7947, 64.0241, 73.9989, 78.1916, 161.7586, 162.9914, 244.9924, 256.2858, 296.2029, 456.0817, 663.7704, 670.7, 674.1578, 760.5124, 848.3052, 881.8958, 912.9134, 984.8543, 1008.7166, 1054.7273, 1113.8124, 1115.9216, 1151.6929, 1284.5835, 1353.5852, 1368.8002, 1395.9662, 1415.2611, 1426.7607, 1440.2789, 1444.9463, 1462.1051, 1499.2891, 1514.8318, 1572.7492, 1788.18, 2871.3864, 2995.4041, 3013.8909, 3025.8389, 3034.7747, 3068.2824,

8 -1.651970 0.285159 -1.033510 8 -1.471712 1.533889 -0.479857 8 0.901844 -1.437806 0.155281	3098.4348, 3105.8516, 3141.7506, 3180.9383

Compound: E-EtCHCHMe + O_3 TS_{SYN} 1.3	**Energy (kJ mol^{-1}):** -421.553488533986
Reaction Coordinates: 6 1.666181 0.206686 0.634242 6 0.528661 0.332833 -0.373832 6 -1.048605 0.630118 0.553826 6 -2.023270 1.206066 -0.432959 1 -1.819805 2.267263 -0.565724 1 -3.036183 1.094724 -0.038376 1 -1.965868 0.697015 -1.389807 6 3.019641 0.106907 -0.073650 1 3.043483 -0.761659 -0.731113 1 3.830207 0.011890 0.649341 1 3.216841 0.993357 -0.680100 1 0.485715 1.309232 -0.889470 1 1.660836 1.070389 1.304994 1 1.494895 -0.685007 1.238496 1 -0.823675 1.225769 1.433932 8 -1.204232 -0.652315 0.940782 8 -1.398053 -1.435076 -0.106369 8 0.234524 -0.677439 -1.106654	**Frequencies (cm^{-1}):** -439.4293, 74.9712, 117.5825, 163.4788, 184.285, 235.5206, 275.1129, 289.9979, 313.9869, 380.3671, 502.319, 543.0404, 634.6056, 710.8916, 794.449, 858.891, 901.3207, 942.9218, 995.5055, 1014.1629, 1050.9656, 1087.6205, 1122.4807, 1148.4039, 1181.6662, 1214.6676, 1288.6972, 1296.2413, 1353.7458, 1395.8603, 1407.3544, 1425.9179, 1446.6551, 1475.2163, 1480.2614, 1496.1689, 1498.1925, 1505.7287, 2894.4403, 3018.7089, 3026.1407, 3035.7987, 3069.8406, 3088.4398, 3103.578, 3103.7855, 3129.1253
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 1.3	**Energy (kJ mol^{-1}):** -421.597591473391
Reaction Coordinates: 6 -2.071139 -0.008893 0.583128 6 -1.163705 0.373705 -0.551253 6 2.411333 0.150460 -0.387143 6 2.396554 0.757853 0.946109 1 3.128683 1.557201 1.019039 1 2.571581 -0.018859 1.694951 1 1.393673 1.147082 1.143291 6 -3.500608 -0.287432 0.103488	**Frequencies (cm^{-1}):** 30.5976, 40.2006, 60.8459, 74.9248, 85.6753, 95.1958, 137.9676, 167.7147, 212.9328, 298.5853, 341.5353, 454.1851, 511.436, 670.4453, 759.3936, 766.0922, 876.0932, 883.7807, 920.2088, 982.1004, 1007.9798, 1058.7137, 1115.3856, 1131.1575, 1162.8557, 1272.0979,

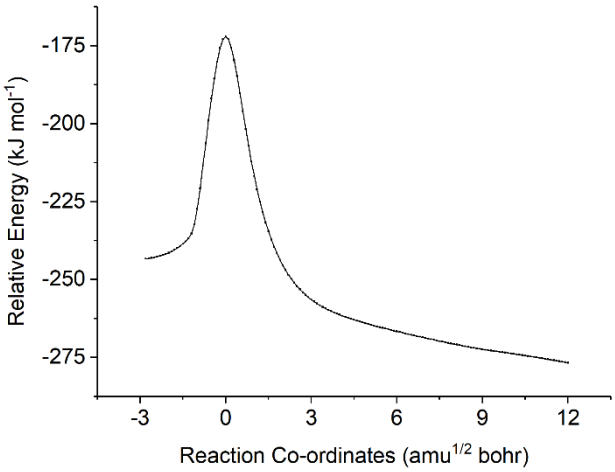
1 -3.964312 0.610141 -0.307410 1 -4.119366 -0.636223 0.929495 1 -3.515255 -1.058226 -0.668707 1 -1.163666 -0.332938 -1.403827 1 -1.645730 -0.916486 1.020457 1 -2.044530 0.777536 1.337300 1 2.987239 0.527548 -1.224372 8 1.758209 -0.885147 -0.678005 8 0.966487 -1.434112 0.307087 8 -0.482562 1.372893 -0.592355	1328.4197, 1353.9243, 1396.7576, 1410.2893, 1427.7266, 1441.3834, 1466.1072, 1469.4499, 1501.8416, 1505.4525, 1573.9096, 1777.975, 2899.6855, 3024.2393, 3029.8981, 3032.8514, 3068.3198, 3077.9606, 3098.1303, 3099.4953, 3139.3665, 3174.061

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.1	**Energy (kJ mol^{-1}):** -421.549557333725
Reaction Coordinates: 6 -1.664114 -0.839665 -0.252087 6 -0.379654 -0.651047 0.563542 6 0.588907 0.781316 -0.282634 6 0.368099 2.146704 0.292157 1 0.830031 2.226736 1.274772 1 0.798600 2.910191 -0.359431 1 -0.695043 2.351155 0.388125 6 -2.650602 0.325306 -0.229662 1 -2.292503 1.188833 -0.791219 1 -3.600525 0.028104 -0.673832 1 -2.858143 0.651674 0.791746 1 -0.511098 -0.127907 1.526224 1 -1.386627 -1.106009 -1.273814 1 -2.145293 -1.726383 0.167538 1 0.213387 0.563089 -1.277724 8 1.823635 0.323408 -0.062243 8 1.974811 -0.901327 -0.539733 8 0.460479 -1.613977 0.561942	**Frequencies (cm^{-1}):** -475.7885, 71.9645, 97.307, 148.3972, 217.6595, 231.5415, 240.4775, 315.4343, 373.572, 393.4528, 477.8707, 514.9309, 562.2577, 623.0975, 770.7675, 862.8957, 907.499, 970.8542, 994.7688, 1032.352, 1054.2595, 1107.4535, 1118.9124, 1151.8491, 1180.4813, 1258.4082, 1286.2032, 1322.8348, 1347.6085, 1384.3431, 1414.9179, 1423.6612, 1443.2128, 1481.5857, 1484.722, 1492.7394, 1503.9163, 1510.0705, 2908.6597, 3025.6522, 3030.5374, 3036.8875, 3059.1189, 3085.5595, 3091.8356, 3102.1467, 3120.6752, 3139.1892
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.1	**Energy (kJ mol^{-1}):** -421.592887336933
Reaction Coordinates:	**Frequencies (cm^{-1}):**

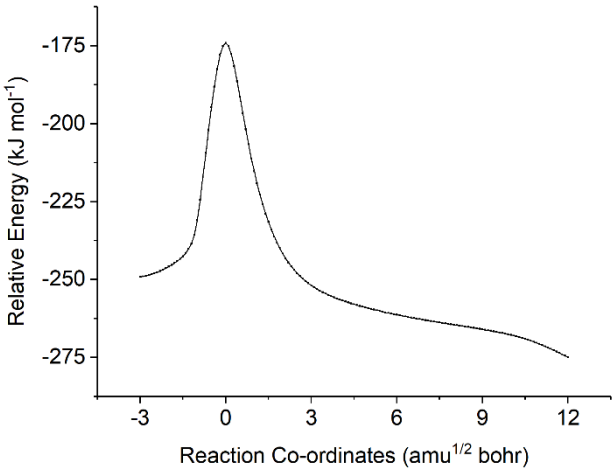
6 -1.947863 0.158963 -0.471952 6 -1.519455 -1.246505 -0.179510 6 1.897034 0.057497 0.405059 6 2.832289 -1.007369 -0.004265 1 3.256843 -0.802066 -0.983818 1 3.635400 -1.100336 0.731554 1 2.297352 -1.959075 -0.022590 6 -3.161713 0.568926 0.373073 1 -2.905281 0.609443 1.431894 1 -3.506494 1.558385 0.077111 1 -3.994879 -0.125967 0.251546 1 -2.326050 -2.007544 -0.238744 1 -1.107399 0.841580 -0.332364 1 -2.230343 0.178646 -1.531966 1 1.362129 0.050766 1.348026 8 1.705659 1.035256 -0.352434 8 0.806679 2.010102 0.061311 8 -0.397716 -1.599471 0.107989	29.436, 50.3859, 71.4122, 76.7841, 100.3718, 104.5291, 132.4944, 197.5896, 210.1367, 269.7783, 325.1018, 332.7315, 521.929, 549.7382, 762.9334, 864.7927, 876.4414, 883.3442, 925.0513, 960.1427, 1008.5452, 1074.129, 1136.0436, 1162.6579, 1170.6192, 1282.8805, 1348.8374, 1359.0674, 1409.2952, 1411.2832, 1428.8512, 1459.2233, 1466.447, 1474.9059, 1500.8704, 1505.9838, 1592.7861, 1776.5071, 2866.0757, 2991.4436, 3026.223, 3029.6772, 3059.2132, 3076.5423, 3090.3431, 3106.7397, 3135.5724, 3171.0259

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.2	**Energy (kJ mol^{-1}):** -421.552392828301
Reaction Coordinates: 6 -1.691598 0.758841 0.326596 6 -0.454064 0.007847 0.850877 6 0.913084 0.490637 -0.349149 6 1.569522 1.794306 -0.020156 1 2.191540 1.700457 0.868359 1 2.190999 2.132992 -0.851193 1 0.813636 2.557186 0.159504 6 -2.413184 0.062354 -0.820870 1 -3.306769 0.620334 -1.101323 1 -2.707097 -0.945609 -0.535715 1 -1.786348 -0.024289 -1.709976 1 -0.012433 0.467067 1.751693 1 -1.418100 1.782713 0.057519 1 -2.366432 0.847062 1.183014 1 0.310269 0.425915 -1.249402 8 1.706425 -0.570024 -0.166955 8 1.066596 -1.690370 -0.460545 8 -0.454499 -1.270573 0.815466	**Frequencies (cm^{-1}):** -455.2172, 74.2402, 97.3318, 162.3392, 178.4687, 230.5036, 249.0991, 322.891, 357.0637, 374.4737, 489.3523, 529.459, 619.809, 637.3621, 786.8566, 826.7009, 906.8747, 983.3953, 1003.2031, 1030.4539, 1050.3595, 1097.0056, 1120.6748, 1152.9465, 1185.9323, 1260.7318, 1288.7282, 1328.7589, 1341.2467, 1385.6545, 1412.5751, 1422.8228, 1454.5993, 1481.296, 1488.7712, 1492.1226, 1495.5713, 1503.4234, 2905.6421, 3015.6992, 3033.5068, 3038.3852, 3041.7651, 3087.3697, 3098.9421, 3118.0155, 3119.3267, 3132.4769
IRC:	



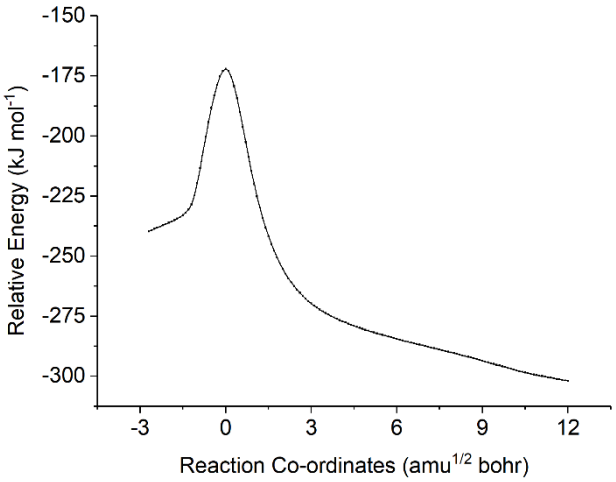
Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.2	**Energy (kJ mol^{-1}):** -421.593046039135
Reaction Coordinates: 6 -2.613139 0.150560 0.059691 6 -1.889859 -1.073793 0.535480 6 1.844747 -0.246405 0.291861 6 2.480589 -1.253799 -0.577504 1 2.838818 -0.806520 -1.501334 1 3.312019 -1.730879 -0.052411 1 1.749937 -2.034690 -0.801232 6 -1.860106 1.019848 -0.936402 1 -2.489897 1.846221 -1.265092 1 -1.570878 0.444626 -1.815956 1 -0.958225 1.436123 -0.487892 1 -2.448241 -1.681606 1.276777 1 -2.887075 0.713851 0.960117 1 -3.572113 -0.202944 -0.341278 1 1.424806 -0.478359 1.264414 8 1.764167 0.941079 -0.094743 8 1.130699 1.853991 0.732763 8 -0.791434 -1.430607 0.177621	**Frequencies (cm^{-1}):** 17.7044, 37.244, 63.1501, 69.0875, 81.6765, 120.1363, 164.4474, 185.5717, 245.9487, 258.7123, 268.921, 324.0153, 550.3206, 662.5874, 673.9513, 848.6607, 868.1376, 878.7414, 913.8014, 960.7304, 1010.075, 1075.2919, 1116.254, 1151.5121, 1162.811, 1284.3917, 1347.7404, 1369.7016, 1409.3151, 1416.1238, 1426.8359, 1444.4297, 1459.827, 1464.4157, 1498.7334, 1518.468, 1592.4816, 1784.2264, 2875.3544, 2992.6708, 3012.7622, 3025.4207, 3034.4261, 3072.6458, 3099.4898, 3105.1407, 3135.32, 3167.9945

Compound: E-EtCHCHMe + O_3 TS_{ANTI} 2.3	**Energy (kJ mol^{-1}):** -421.552491548523
Reaction Coordinates: 6 1.629964 0.405389 0.502142 6 0.537758 -0.165869 -0.407618 6 -1.051420 0.580516 0.307269 6 -1.351633 1.957729 -0.193535 1 -1.669366 1.930035 -1.234334 1 -2.140489 2.419692 0.403258 1 -0.465811 2.585480 -0.112783 6 3.020063 0.107886 -0.064159 1 3.140450 0.534668 -1.061694 1 3.796294 0.531216 0.574297 1 3.182846 -0.966937 -0.136512	**Frequencies (cm^{-1}):** -444.222, 75.0725, 93.6383, 158.9987, 189.7572, 235.3774, 245.3922, 317.6951, 357.7265, 372.9298, 481.4654, 505.9212, 580.698, 621.2213, 788.7839, 869.2352, 909.4963, 988.143, 1008.4051, 1013.6967, 1064.6571, 1116.298, 1123.1731, 1152.4218, 1177.5094, 1262.3428, 1290.7836, 1329.6445, 1356.504, 1387.2132, 1408.9648, 1422.9765, 1448.1919, 1475.3279, 1481.5227,

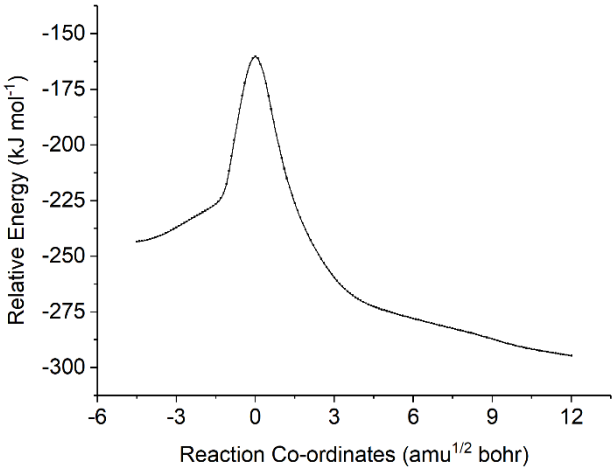
1 0.484523 0.309861 -1.403022 1 1.502651 1.485627 0.613085 1 1.521938 -0.049985 1.487873 1 -0.773636 0.451651 1.348700 8 -1.901059 -0.349686 -0.134539 8 -1.582561 -1.543728 0.337762 8 0.322645 -1.424737 -0.371155	1493.9068, 1496.8241, 1504.4106, 2897.1493, 3017.9865, 3027.6401, 3038.0557, 3066.0305, 3087.2328, 3099.0373, 3104.624, 3119.6249, 3132.3496
IRC:  	

Compound: E-EtCHCHMe + O_3 CPr_{ANTI} 2.3	**Energy (kJ mol^{-1}):** -421.595100791669
Reaction Coordinates: 6 2.051345 -0.085895 -0.564145 6 1.113731 0.329487 0.534249 6 -2.063768 0.010289 0.284461 6 -3.002990 0.914732 -0.403985 1 -3.128914 0.633779 -1.446450 1 -3.970852 0.907611 0.103088 1 -2.613927 1.934069 -0.342819 6 3.513811 0.158197 -0.166771 1 3.765471 -0.363415 0.758158 1 4.184890 -0.205970 -0.944040 1 3.713852 1.220179 -0.019911 1 1.269120 -0.180915 1.500908 1 1.887761 -1.150972 -0.739946 1 1.791156 0.457051 -1.472619 1 -1.812961 0.100396 1.334551 8 -1.527872 -0.922612 -0.357336 8 -0.601271 -1.704633 0.316380 8 0.284345 1.213161 0.436733	**Frequencies (cm^{-1}):** 24.9661, 36.3675, 79.8801, 85.051, 117.7003, 137.1757, 195.3092, 217.8712, 239.7202, 288.5851, 331.0131, 375.8177, 512.8906, 554.0066, 776.215, 864.4793, 876.1346, 883.7518, 919.2619, 965.623, 1002.2612, 1072.2324, 1121.2311, 1162.3308, 1164.7847, 1269.4631, 1326.5173, 1352.6383, 1408.5293, 1410.0875, 1425.6943, 1457.6501, 1463.8446, 1476.3542, 1501.4739, 1505.7525, 1591.5707, 1745.0852, 2930.86, 3026.9634, 3029.4674, 3043.7528, 3074.2145, 3079.3903, 3098.1159, 3101.7584, 3137.5272, 3179.9323

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.1	**Energy (kJ mol^{-1}):** -421.552817024742
Reaction Coordinates: 6 -1.635617 0.320976 0.186542 6 -0.400464 0.081760 -0.647996	**Frequencies (cm^{-1}):** -448.7841, 86.1757, 112.6357, 176.9164, 190.9359, 220.8673,

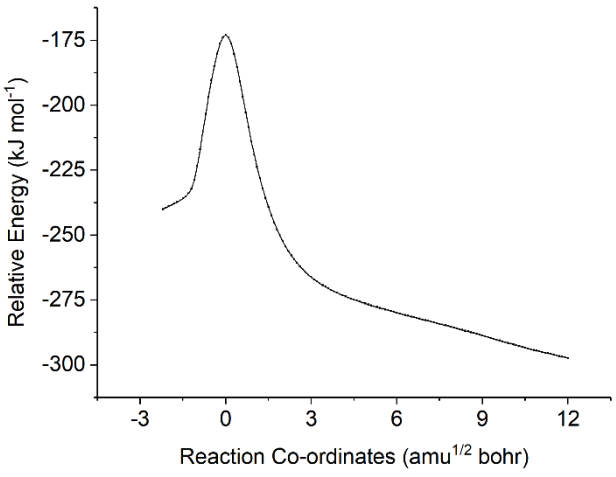
6 0.822811 -0.797904 0.420314 6 1.866751 -1.446277 -0.476205 1 2.444082 -0.687155 -1.001031 1 1.414118 -2.124484 -1.201227 1 2.554405 -2.022456 0.144696 6 -2.636888 -0.827527 0.091746 1 -2.960212 -0.996853 -0.936831 1 -2.219835 -1.762046 0.470543 1 -3.522940 -0.604870 0.685061 1 -0.532483 -0.489920 -1.563843 1 -2.085297 1.247257 -0.185624 1 -1.348678 0.513789 1.217616 1 0.068042 -1.496415 0.819921 8 1.192094 0.121019 1.235628 8 0.660612 1.806113 0.192406 8 0.408449 1.127491 -0.914995	256.763, 277.1845, 372.8064, 385.4061, 488.0973, 537.3276, 593.9945, 710.1754, 785.36, 888.591, 915.6244, 944.5086, 987.6086, 1024.0983, 1064.3556, 1070.3482, 1109.8843, 1143.9378, 1185.5761, 1203.9772, 1282.0755, 1302.0812, 1334.6578, 1398.9077, 1418.786, 1427.2747, 1436.3273, 1482.0907, 1482.7554, 1495.9905, 1503.5483, 1505.0531, 2912.6405, 3019.6992, 3028.5025, 3031.378, 3079.2979, 3090.7257, 3098.7508, 3107.4046, 3117.5508, 3119.6179
IRC  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.1	**Energy (kJ mol^{-1}):** -421.596435832193
Reaction Coordinates: 6 1.675614 -0.282532 -0.537739 6 1.359132 0.628879 0.569750 6 -2.067320 -0.366123 0.514890 6 -2.860736 -0.508619 -0.746878 1 -2.564435 -1.397441 -1.299317 1 -2.712185 0.384495 -1.355852 1 -3.924781 -0.559789 -0.500241 6 2.858441 -1.203731 -0.254214 1 3.771548 -0.639241 -0.060596 1 2.663929 -1.843580 0.606878 1 3.045645 -1.850428 -1.109797 1 1.878408 0.624328 1.522952 1 1.821817 0.339735 -1.428753 1 0.759785 -0.842528 -0.754015 1 -2.317518 0.519016 1.128116 8 -1.220383 -1.144696 0.890183 8 -0.272829 1.588721 -0.652743 8 0.466585 1.513248 0.509531	**Frequencies (cm^{-1}):** 36.853, 45.3465, 67.437, 77.7763, 100.7234, 105.865, 119.8, 180.4349, 204.2004, 220.6665, 360.3963, 457.8005, 512.7642, 685.0171, 703.8188, 782.2635, 847.8696, 875.733, 891.114, 936.0878, 1047.8285, 1105.6493, 1130.5019, 1134.9002, 1141.2588, 1257.1687, 1326.0369, 1374.5668, 1378.0602, 1423.6171, 1425.4559, 1427.2401, 1460.3756, 1470.7763, 1503.4295, 1506.161, 1574.7377, 1781.3528, 2917.5182, 3008.5649, 3025.5961, 3032.4269, 3037.0121, 3086.1893, 3094.7245, 3108.5292, 3131.9677, 3155.8948

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.2	**Energy (kJ mol^{-1}):** -421.548726352612
Reaction Coordinates: 6 1.577500 -0.451707 0.816209 6 0.170544 0.093323 0.972746 6 -0.977975 -0.724066 -0.246747 6 -2.383994 -0.646310 0.331617 1 -2.711107 0.389351 0.406455 1 -2.446191 -1.120664 1.312145 1 -3.067161 -1.167195 -0.340980 6 2.136136 -0.802135 -0.562065 1 2.168382 0.066198 -1.211732 1 3.147948 -1.191511 -0.440904 1 1.541995 -1.567736 -1.057718 1 -0.255127 -0.058067 1.961670 1 1.619932 -1.332926 1.460853 1 2.222974 0.298782 1.287800 1 -0.494698 -1.711422 -0.137348 8 -0.725869 -0.108345 -1.339132 8 0.245417 1.580634 -0.648535 8 -0.127074 1.350282 0.598816	**Frequencies (cm^{-1}):** -440.8988, 60.1082, 128.2652, 176.284, 200.375, 237.5097, 264.7053, 272.3935, 311.1051, 438.1377, 491.3508, 543.1412, 582.4567, 724.3799, 771.9594, 866.5055, 896.6203, 945.2631, 989.2353, 1010.7822, 1059.8268, 1089.1741, 1115.1152, 1130.6905, 1173.1832, 1226.0427, 1305.8307, 1315.8973, 1378.0793, 1397.5886, 1416.7276, 1432.5987, 1443.9895, 1464.6614, 1481.8242, 1495.5263, 1498.1068, 1503.4047, 2896.6268, 3000.2024, 3031.575, 3044.1848, 3048.7751, 3091.464, 3103.5638, 3117.3675, 3121.2128, 3150.0096
IRC  	

Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.2	**Energy (kJ mol^{-1}):** -421.593861868972
Reaction Coordinates: 6 -2.289340 0.667124 0.223020 6 -1.380521 -0.253540 0.928090 1 -1.034271 -0.101662 1.943518 8 -0.921544 -1.308237 0.416618 8 -1.255080 -1.600684 -0.890993 6 -1.558254 1.564742 -0.799842 1 -0.804702 2.180955 -0.313201 1 -1.079911 0.951502 -1.558758 1 -2.284551 2.217254 -1.282739 1 -2.801249 1.280757 0.964262 1 -3.016254 0.049843 -0.311017 6 2.109234 -0.051274 0.033901 6 3.551293 0.003408 -0.369730 1 4.054409 0.857372 0.077369	**Frequencies (cm^{-1}):** 22.853, 26.0031, 43.8889, 49.7757, 70.4458, 80.2237, 112.819, 161.9233, 199.2529, 243.914, 318.6642, 513.2774, 532.5313, 649.5875, 782.8472, 811.6095, 841.0502, 868.4889, 891.6661, 906.886, 1015.0018, 1086.0657, 1131.7504, 1144.6879, 1147.6118, 1290.5496, 1333.8152, 1375.6581, 1380.1994, 1402.8184, 1439.7307, 1460.0967, 1461.2279, 1468.4263, 1492.7702, 1513.9816, 1570.0011, 1785.4563, 2926.4545, 3022.7495, 3030.4738, 3049.5588, 3073.2538, 3086.2388,

1 3.619173 0.052464 -1.459661 1 4.045376 -0.925006 -0.071482 1 1.527310 -0.894233 -0.382797 8 1.574148 0.752421 0.762109	3114.8273, 3134.2045, 3137.9692, 3176.7519

Compound: E-EtCHCHMe + O_3 TS_{SYN} 2.3	**Energy (kJ mol^{-1}):** -421.553174717087
Reaction Coordinates: 6 -1.417198 -0.687853 0.536451 6 -0.316526 -0.462936 -0.469455 6 1.284319 -0.500849 0.472457 6 2.408267 -0.770940 -0.516527 1 2.250192 -1.699999 -1.066422 1 3.346853 -0.857191 0.033091 1 2.505351 0.054950 -1.219141 6 -2.797807 -0.374662 -0.052422 1 -3.008762 -0.985106 -0.931781 1 -3.570739 -0.577433 0.688742 1 -2.873442 0.673658 -0.337320 1 -0.252219 -1.173228 -1.290329 1 -1.229669 -0.077895 1.416367 1 -1.368135 -1.735422 0.838278 1 0.980539 -1.375891 1.071667 8 1.267564 0.617063 1.098731 8 -0.106090 1.675898 -0.004864 8 -0.129760 0.774163 -0.972140	**Frequencies (cm^{-1}):** -444.9487, 74.9216, 124.9824, 167.0417, 185.3857, 215.3436, 260.9597, 275.883, 351.4307, 418.2267, 485.2143, 551.4887, 612.677, 676.3137, 797.9259, 885.7834, 900.547, 945.8479, 990.6047, 991.7042, 1058.9089, 1077.1946, 1105.323, 1141.7259, 1185.9153, 1206.4877, 1298.8354, 1306.8728, 1353.2693, 1398.2586, 1408.5676, 1432.2777, 1436.2517, 1481.7266, 1483.2642, 1496.2087, 1498.6676, 1505.9064, 2912.4073, 3030.8051, 3033.9521, 3050.2013, 3090.1644, 3090.3847, 3108.3851, 3114.4963, 3117.3564, 3128.6289
IRC  	

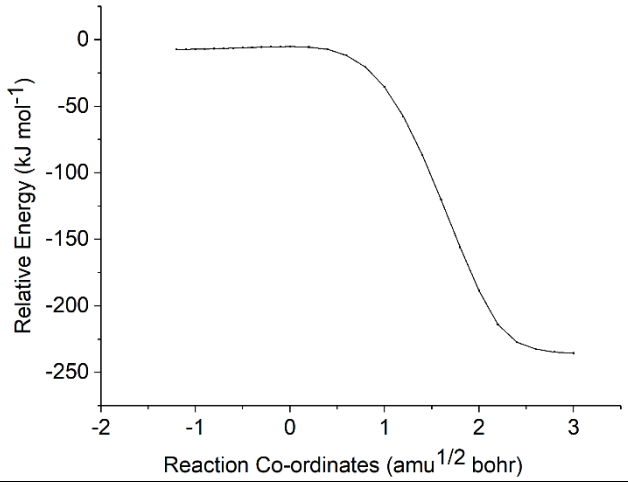
Compound: E-EtCHCHMe + O_3 CPr_{SYN} 2.3	**Energy (kJ mol^{-1}):** -421.597649635912
Reaction Coordinates: 6 1.600425 -0.789202 0.456010 6 1.291458 0.611512 0.790171 6 -2.178308 0.105372 0.327895 6 -2.779359 -0.660224 -0.810701 1 -2.349063 -0.296457 -1.745022 1 -3.854010 -0.462060 -0.850522 1 -2.603423 -1.728080 -0.702155	**Frequencies (cm^{-1}):** 34.3343, 50.4259, 62.445, 78.5207, 93.396, 108.8934, 124.0889, 184.5023, 202.1773, 247.1415, 323.6472, 512.1253, 530.2569, 649.3045, 782.5202, 808.0057, 852.8218, 875.4383, 890.4967, 905.6274, 1008.3437, 1083.7874, 1129.5219,

6 2.750006 -0.889736 -0.571403 1 3.675271 -0.470993 -0.176148 1 2.926937 -1.938067 -0.807636 1 2.485014 -0.365909 -1.486497 1 1.615409 1.096673 1.704856 1 0.698389 -1.231015 0.033449 1 1.860260 -1.314109 1.374492 1 -2.314102 1.201200 0.278710 8 -1.599242 -0.394304 1.265551 8 0.164176 0.904091 -1.152243 8 0.654314 1.395523 0.039772	1134.0319, 1149.4922, 1281.4845, 1331.5976, 1374.3901, 1377.4555, 1402.4769, 1426.9531, 1460.3532, 1466.6299, 1471.1677, 1496.5973, 1511.4618, 1572.4543, 1780.859, 2919.2627, 3025.4484, 3043.2422, 3057.7005, 3085.9501, 3099.8593, 3110.9962, 3131.7359, 3132.6979, 3162.3001

6.18 Ozonolysis of *Z*-2-pentene (Alkene 16)

Compound: Z-EtCHCHMe + O_3 PRC1.1	**Energy (kJ mol^{-1}):** -421.485915987591
Reaction Coordinates: 6 1.690064 -0.580681 -0.464478 6 0.754076 -0.056575 0.581561 6 0.148956 1.144028 0.619170 6 0.239489 2.242063 -0.391680 1 0.853972 1.981390 -1.250184 1 -0.754359 2.507941 -0.757122 1 0.658560 3.143270 0.064103 1 -0.443884 1.374398 1.497639 1 0.609621 -0.711825 1.435080 6 3.109933 -0.792147 0.081851 1 3.105640 -1.471869 0.935629 1 3.550001 0.150149 0.410230 1 3.758551 -1.221211 -0.682782 1 1.723823 0.084451 -1.326579 1 1.307398 -1.537419 -0.828989 8 -2.458488 0.365242 -0.119871 8 -2.355915 -0.852044 0.211952 8 -1.438651 -1.518123 -0.349027	**Frequencies (cm^{-1}):** 16.3461, 33.9606, 62.951, 77.2082, 94.849, 98.7302, 107.8881, 215.0195, 267.3096, 279.4655, 308.9347, 485.8696, 570.9152, 738.2921, 744.9766, 794.9528, 863.127, 935.113, 1005.3333, 1019.9495, 1054.5782, 1062.4593, 1091.283, 1158.4361, 1175.8812, 1179.4621, 1280.6143, 1299.6119, 1338.398, 1405.5231, 1409.8654, 1444.9284, 1481.5746, 1483.5515, 1494.8062, 1498.3462, 1508.3192, 1661.2401, 3021.2104, 3025.3238, 3027.6121, 3063.5139, 3069.8607, 3089.9603, 3092.7421, 3114.6609, 3123.9899, 3147.9352

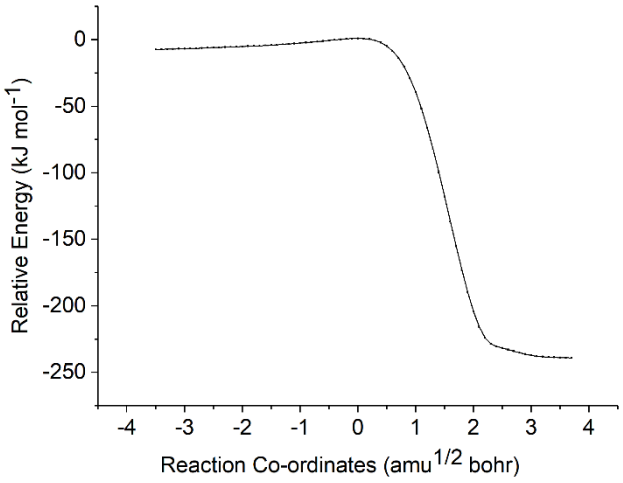
Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.1	**Energy (kJ mol^{-1}):** -421.481920649981
Reaction Coordinates: 6 1.537073 -0.711988 -0.410332 6 0.545964 -0.235037 0.606613 6 -0.041306 1.001289 0.636802 6 0.176339 2.097263 -0.356088 1 0.426058 1.717199 -1.344409 1 -0.712974 2.719312 -0.444805 1 0.994634 2.746859 -0.030281 6 2.987602 -0.466429 0.036310 1 3.685998 -0.858832 -0.703625 1 3.195991 -0.959133 0.987145 1 3.190643 0.597543 0.161642 1 -0.575098 1.276466 1.537311 1 1.360594 -0.226410 -1.369761 1 1.390243 -1.780796 -0.570841 1 0.437240 -0.856941 1.486873 8 -2.157619 0.450121 -0.215537 8 -2.199464 -0.779285 0.158471 8 -1.221338 -1.481568 -0.291568	**Frequencies (cm^{-1}):** -139.2013, 45.7237, 62.0983, 93.8126, 128.9555, 163.8692, 195.094, 217.4619, 293.3005, 303.0398, 432.3547, 523.0694, 571.2071, 738.0359, 781.5139, 794.1595, 861.0797, 933.6821, 993.8774, 1022.4919, 1050.874, 1054.0495, 1088.3243, 1095.0381, 1113.2647, 1176.2111, 1272.7227, 1292.8308, 1340.1243, 1403.2789, 1410.6896, 1446.0296, 1475.2666, 1485.3282, 1497.4079, 1498.7036, 1511.2308, 1586.0258, 3017.3027, 3027.6856, 3046.047, 3073.9682, 3082.8548, 3092.2204, 3097.3822, 3118.8816, 3150.1332, 3171.5845
IRC:	



Compound: Z-EtCHCHMe + O_3 POZ1.1	**Energy (kJ mol^{-1}):** -421.580622944704
Reaction Coordinates: 6 -1.553649 -0.584625 -0.492720 6 -0.244001 -0.561739 0.280899 6 0.517018 0.798878 0.459114 6 0.076409 1.986478 -0.375029 1 0.051749 1.737697 -1.434389 1 -0.908424 2.334351 -0.065086 1 0.777839 2.808751 -0.236077 6 -2.743768 -0.094372 0.333660 1 -2.622607 0.939096 0.659495 1 -3.661693 -0.147624 -0.251103 1 -2.882468 -0.708324 1.224950 1 -0.391742 -1.000074 1.272486 1 -1.456093 -0.007112 -1.411757 1 -1.730050 -1.618896 -0.794525 1 0.523345 1.058280 1.521065 8 1.858646 0.483099 0.044703 8 1.936787 -0.952528 0.168923 8 0.703079 -1.363554 -0.428701	**Frequencies (cm^{-1}):** 39.003, 115.5644, 182.3987, 228.9281, 234.0677, 285.15, 353.1717, 390.0921, 443.0518, 496.8085, 695.2308, 707.2439, 723.3158, 776.0962, 826.4231, 888.076, 938.0483, 942.8503, 996.0758, 1046.2614, 1058.2113, 1070.9476, 1116.9519, 1171.6633, 1188.7505, 1282.578, 1320.2756, 1332.9801, 1367.7061, 1384.4634, 1405.737, 1420.5157, 1424.941, 1483.8785, 1496.5478, 1500.2911, 1505.2034, 1513.4434, 3003.3032, 3025.9169, 3032.7374, 3042.6299, 3046.2986, 3074.0422, 3096.27, 3098.4244, 3106.9382, 3121.0695

Compound: Z-EtCHCHMe + O_3 PRC1.2	**Energy (kJ mol^{-1}):** -421.486538211307
Reaction Coordinates: 6 1.779046 -1.077094 -0.136753 6 1.201636 -0.066142 0.804319 6 1.047226 1.251419 0.611672 6 1.423053 2.050749 -0.594315 1 1.798082 1.439144 -1.411749 1 0.563460 2.617172 -0.960108 1 2.194128 2.783389 -0.340406 1 0.626736 1.824953 1.430786 1 0.885262 -0.465169 1.764430 6 0.926237 -2.347264 -0.245536 1 -0.062625 -2.118669 -0.642859 1 0.792792 -2.814051 0.732065 1 1.400604 -3.078109 -0.901222 1 2.774185 -1.358675 0.228769 1 1.930294 -0.646423 -1.126377	**Frequencies (cm^{-1}):** 17.983, 28.1298, 42.6776, 61.2296, 78.7215, 103.1846, 131.5227, 198.4799, 220.6543, 264.4991, 306.272, 455.65, 579.03, 714.4045, 736.9095, 800.6033, 869.9845, 938.6042, 998.4331, 1029.5138, 1056.1354, 1064.2333, 1092.0364, 1162.117, 1174.8367, 1188.8683, 1280.208, 1298.7537, 1337.3589, 1409.7277, 1412.0548, 1445.9767, 1474.6914, 1482.8954, 1489.5188, 1499.6188, 1506.5024, 1680.477, 2985.2115, 3018.627, 3027.0897, 3057.104, 3065.4498, 3088.5795,

8 -1.571613 1.051512 -0.249519 8 -2.390002 0.246652 0.270933 8 -2.434148 -0.929860 -0.197620	3100.1847, 3110.6328, 3115.4909, 3143.7423

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.2	**Energy (kJ mol^{-1}):** -421.476885591147
Reaction Coordinates: 6 1.679182 -0.864164 0.505697 6 0.487846 -0.127589 1.054031 6 0.013721 1.117827 0.744532 6 0.562756 2.080729 -0.264959 1 -0.032790 2.991119 -0.284867 1 1.592141 2.359835 -0.026312 1 0.560693 1.657530 -1.267710 6 2.027455 -0.701934 -0.976023 1 2.412822 0.288706 -1.207730 1 1.158315 -0.888937 -1.604204 1 2.799567 -1.422369 -1.247952 1 -0.741940 1.514716 1.409354 1 1.522092 -1.924018 0.713736 1 2.545951 -0.580413 1.116799 1 0.064878 -0.582430 1.941426 8 -1.846089 0.511094 -0.601017 8 -2.101812 -0.621288 -0.051518 8 -1.115536 -1.445176 -0.087741	**Frequencies (cm^{-1}):** -126.4689, 30.33, 62.5429, 107.4037, 134.127, 162.5276, 183.0648, 219.4792, 272.8367, 323.0429, 431.8665, 452.6057, 666.4433, 729.0285, 745.6078, 784.0458, 824.6833, 943.34, 980.0162, 1045.4895, 1054.949, 1060.5751, 1096.9769, 1104.239, 1118.7334, 1138.9058, 1282.5462, 1307.8236, 1389.145, 1402.6045, 1413.9986, 1454.5312, 1468.6294, 1483.6732, 1490.7571, 1505.9371, 1517.8441, 1588.1979, 2980.8597, 3026.9433, 3044.3464, 3049.2838, 3090.5147, 3100.3669, 3117.2101, 3121.9256, 3149.0335, 3173.2118
IRC:  	

Compound: Z-EtCHCHMe + O_3 POZ1.2	**Energy (kJ mol^{-1}):** -421.579310920700
Reaction Coordinates: 6 -1.688587 -0.010523 0.557950 6 -0.217169 -0.274690 0.883741 6 0.862963 0.726409 0.365555 1 1.650149 0.783536 1.122288 6 0.434022 2.122044 -0.032372 1 1.298162 2.689194 -0.375997 1 -0.312217 2.114698 -0.822375 1 0.020125 2.638884 0.833691 8 1.396368 0.048574 -0.772207	**Frequencies (cm^{-1}):** 48.1535, 122.0777, 173.958, 206.0727, 238.8542, 266.616, 318.1005, 361.8957, 482.9635, 532.5013, 691.5148, 716.3085, 743.4831, 754.8398, 809.0164, 880.4181, 915.9471, 937.6895, 958.426, 1036.5619, 1081.759, 1098.3757, 1118.9318, 1141.546, 1196.8561, 1282.4425, 1329.8854, 1336.4482, 1370.482,

8 1.497223 -1.282315 -0.268810 8 0.165570 -1.518591 0.272459 1 -0.100472 -0.360650 1.968309 1 -1.936025 0.986245 0.932705 1 -2.282994 -0.704839 1.156222 6 -2.091923 -0.153975 -0.910249 1 -1.931333 -1.172263 -1.257863 1 -3.149444 0.083723 -1.029932 1 -1.525072 0.504536 -1.566333	1398.2098, 1400.5574, 1421.1929, 1428.1523, 1481.424, 1492.9937, 1496.3208, 1503.7782, 1514.2391, 3000.3475, 3021.475, 3030.1411, 3044.2734, 3049.5474, 3050.9091, 3101.7669, 3106.6684, 3118.7516, 3135.9776

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 1.3	**Energy (kJ mol^{-1}):** -421.482637679565
Reaction Coordinates: 6 1.682482 0.473886 -0.305652 6 0.571891 0.390221 0.698002 6 -0.568220 1.137983 0.663222 6 -0.876929 2.170559 -0.372441 1 -0.501858 1.884675 -1.353945 1 -1.949536 2.338345 -0.450695 1 -0.413795 3.126611 -0.107468 6 2.789696 -0.552307 -0.075821 1 3.579534 -0.447913 -0.819632 1 2.397698 -1.567333 -0.138970 1 3.242780 -0.428377 0.909549 1 -1.223136 1.100914 1.523921 1 2.107061 1.484328 -0.280878 1 1.265978 0.354208 -1.309254 1 0.756987 -0.208182 1.581699 8 -2.049920 -0.449790 -0.300061 8 -1.514792 -1.533165 0.129014 8 -0.292192 -1.686961 -0.228726	**Frequencies (cm^{-1}):** -95.8156, 57.1143, 66.6457, 91.4541, 136.9122, 155.0359, 172.306, 206.7368, 244.2774, 351.4562, 420.2222, 450.2199, 599.6161, 706.1163, 739.4924, 803.8615, 878.8389, 948.0656, 983.8884, 1044.4223, 1053.7588, 1055.6652, 1094.9748, 1104.4175, 1122.3205, 1160.0784, 1267.2129, 1290.6675, 1339.7159, 1405.7511, 1416.7323, 1446.1349, 1462.7882, 1476.1303, 1490.8253, 1500.6767, 1506.2546, 1592.7954, 2991.6312, 3013.2051, 3028.7823, 3034.344, 3080.0874, 3088.1929, 3101.249, 3115.3023, 3151.0948, 3173.7999
IRC:	

Compound: Z-EtCHCHMe + O_3 POZ1.3	**Energy (kJ mol^{-1}):** -421.582011869880
Reaction Coordinates: 6 -1.511892 0.691824 -0.147310 6 -0.373175 -0.091623 0.483980 6 1.062248 0.544585 0.463019 6 1.241259 1.893475 -0.203858 1 0.888895 1.879954 -1.233317 1 0.699155 2.662171 0.346934 1 2.296042 2.166362 -0.204986 6 -2.855904 -0.030922 -0.049644 1 -3.119336 -0.233763 0.990104 1 -3.651409 0.575550 -0.482746 1 -2.831120 -0.982260 -0.579720 1 -0.621148 -0.344498 1.519629 1 -1.576970 1.656983 0.360713 1 -1.271151 0.894932 -1.191672 1 1.435759 0.577513 1.490063 8 1.833462 -0.407426 -0.280510 8 1.166717 -1.648477 0.002709	**Frequencies (cm^{-1}):** 40.1952, 106.0324, 182.2964, 221.9801, 232.3694, 289.0288, 330.6208, 409.2705, 458.8236, 475.2868, 696.5606, 705.349, 752.6953, 776.3765, 818.4988, 891.9646, 934.897, 943.3704, 964.1349, 1052.9824, 1056.5677, 1085.6373, 1125.1043, 1167.4514, 1185.254, 1295.6435, 1324.4308, 1338.6855, 1353.5213, 1385.6238, 1411.1699, 1416.9465, 1426.3987, 1475.4189, 1490.2773, 1500.0055, 1504.478, 1507.893, 2998.9044, 3024.0488, 3030.3206, 3030.9631, 3045.4689, 3069.4776, 3091.7494, 3104.8795, 3106.2006, 3122.4955

8 -0.203171 -1.306219 -0.258714	

Compound: Z-EtCHCHMe + O_3 PRC 2.1	**Energy (kJ mol^{-1}):** -421.487538592535
Reaction Coordinates: 6 1.695993 -0.601860 -0.537355 6 0.802956 -0.061714 0.538783 6 0.298439 1.175493 0.647263 6 0.511856 2.338538 -0.271744 1 1.095424 2.085784 -1.154402 1 -0.443809 2.749168 -0.603701 1 1.030152 3.145598 0.253637 1 -0.313757 1.383428 1.517400 1 0.570969 -0.761651 1.334906 6 3.049666 -1.075259 0.011894 1 2.915626 -1.833940 0.784652 1 3.604668 -0.246598 0.453097 1 3.660500 -1.509524 -0.780462 1 1.857573 0.137722 -1.321356 1 1.198398 -1.452722 -1.013520 8 -2.506490 0.462945 -0.036225 8 -2.318500 -0.698359 -0.490110 8 -1.841160 -1.558143 0.300924	**Frequencies (cm^{-1}):** 8.7818, 35.7762, 40.3933, 47.6769, 69.3407, 94.4089, 128.1644, 213.1579, 224.6509, 266.6179, 302.9068, 483.5177, 572.0087, 732.5615, 742.5733, 796.3762, 863.3594, 934.1974, 1008.1776, 1021.2217, 1053.5112, 1065.1447, 1090.9361, 1170.3615, 1174.1367, 1194.8837, 1283.077, 1302.1533, 1339.5978, 1406.4936, 1410.4433, 1444.5333, 1482.8075, 1483.7888, 1494.3507, 1498.2498, 1506.9293, 1677.0231, 3008.7474, 3019.2479, 3025.9334, 3060.1784, 3065.5138, 3089.526, 3091.967, 3110.6595, 3130.262, 3153.3472

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.1	**Energy (kJ mol^{-1}):** -421.478927651676
Reaction Coordinates: 6 1.510495 -0.734284 -0.368736 6 0.544529 -0.235458 0.666017 6 -0.060441 0.998046 0.658017 6 0.085628 2.017463 -0.429575 1 0.071770 1.564395 -1.420826 1 -0.712070 2.755268 -0.381953 1 1.036100 2.551419 -0.331973 6 2.960173 -0.345647 -0.031206 1 3.645525 -0.744472 -0.779909 1 3.256871 -0.743902 0.940031 1 3.087191 0.736779 0.000137 1 -0.516841 1.331927 1.578740 1 1.250357 -0.344752 -1.353762 1 1.439435 -1.819895 -0.431752 1 0.503653 -0.796539 1.589987 8 -2.229954 0.357023 0.197369 8 -1.932415 -0.645526 -0.557170 8 -1.250669 -1.547866 0.062823	**Frequencies (cm^{-1}):** -185.8554, 37.7874, 74.1741, 116.2373, 132.513, 175.4102, 182.9449, 214.9733, 292.3001, 301.6991, 467.0825, 540.8411, 580.5906, 739.7251, 782.7614, 795.5139, 861.8555, 937.0212, 990.7083, 1022.9191, 1047.6194, 1051.6373, 1081.3036, 1088.0966, 1103.5319, 1173.255, 1265.2907, 1293.8288, 1341.2785, 1401.2572, 1411.2227, 1440.3576, 1477.9975, 1486.5151, 1496.2587, 1498.2512, 1510.8248, 1567.8158, 3013.5218, 3028.5461, 3044.9321, 3072.6854, 3075.811, 3091.9832, 3098.5813, 3116.8195, 3167.3658, 3188.293
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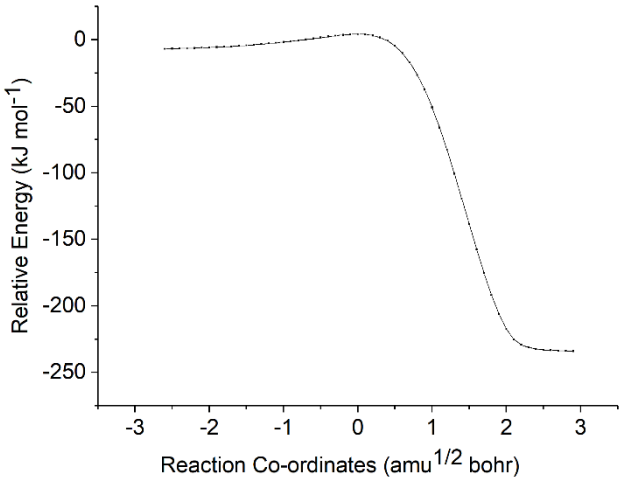
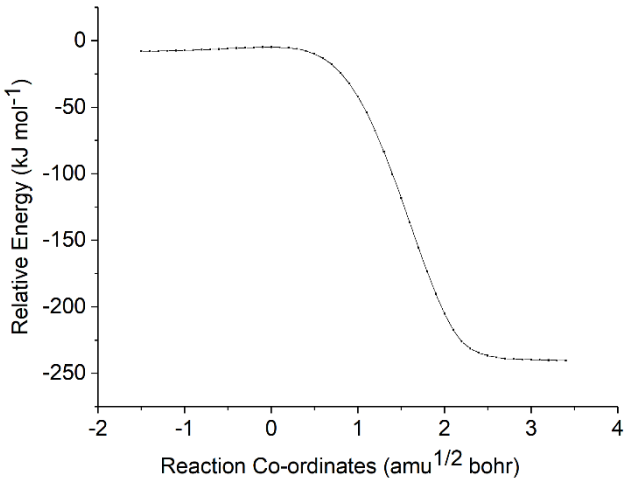


Compound: Z-EtCHCHMe + O_3 POZ 2.1	**Energy (kJ mol^{-1}):** -421.579764023369
Reaction Coordinates: 6 -1.566130 -0.559220 -0.465196 6 -0.302042 -0.569722 0.385547 6 0.489909 0.763607 0.536177 6 0.303965 1.808233 -0.551952 1 0.550045 1.402491 -1.531183 1 -0.719930 2.179691 -0.575661 1 0.964003 2.651451 -0.351839 6 -2.749797 0.112889 0.232966 1 -2.559780 1.164869 0.450353 1 -3.642022 0.064092 -0.390820 1 -2.980579 -0.382448 1.177947 1 -0.539510 -0.946600 1.383871 1 -1.363811 -0.090433 -1.428604 1 -1.818335 -1.599855 -0.675724 1 0.318132 1.193860 1.522950 8 1.839889 0.289147 0.578634 8 1.829515 -0.670169 -0.479286 8 0.672641 -1.490458 -0.150166	**Frequencies (cm^{-1}):** 41.4595, 131.5617, 185.2356, 230.8316, 239.3666, 284.7816, 290.7138, 407.705, 467.6656, 504.4749, 686.9927, 715.1293, 752.6265, 767.4205, 835.9035, 892.262, 910.9456, 947.2209, 977.7365, 1030.1813, 1052.7483, 1068.8779, 1101.892, 1158.7002, 1173.1139, 1276.3252, 1301.076, 1325.7568, 1358.426, 1371.7144, 1401.677, 1415.4427, 1420.0279, 1486.4189, 1497.6168, 1499.8777, 1504.3428, 1512.4406, 3021.4901, 3028.7451, 3044.4945, 3048.185, 3070.3359, 3074.0248, 3092.5004, 3096.024, 3109.4634, 3125.0629

Compound: Z-EtCHCHMe + O_3 PRC 2.2	**Energy (kJ mol^{-1}):** -421.487538592535
Reaction Coordinates: 6 2.078715 -0.278347 -0.065732 6 0.969689 0.298643 0.762733 6 0.297207 1.440079 0.555489 6 0.469563 2.408069 -0.573512 1 1.143653 2.046667 -1.347335 1 -0.492223 2.636527 -1.037528 1 0.867012 3.357607 -0.203171 6 1.980074 -1.797226 -0.242671 1 1.071975 -2.071226 -0.779827 1 1.956174 -2.303406 0.723829 1 2.836259 -2.180284 -0.798854	**Frequencies (cm^{-1}):** 23.5576, 31.0201, 38.0319, 61.8044, 68.3488, 98.3679, 121.1293, 214.3459, 224.723, 264.3391, 314.6344, 458.7348, 580.7507, 708.7569, 741.1838, 800.1846, 868.5019, 938.3971, 1002.6201, 1034.81, 1054.4252, 1063.0705, 1092.505, 1168.4664, 1171.91, 1191.2559, 1281.6948, 1297.8266, 1339.0757, 1409.7959, 1412.4017, 1444.883, 1474.6623, 1483.5566, 1490.9211,

1 -0.434837 1.725535 1.301750 1 3.029307 -0.050332 0.431968 1 2.129209 0.205847 -1.041400 1 0.723065 -0.264352 1.657246 8 -2.410517 0.325180 0.221786 8 -2.109324 -0.677953 -0.481892 8 -1.430294 -1.588464 0.069540	1498.0583, 1504.7358, 1674.3616, 2984.3962, 3016.652, 3028.0911, 3057.1837, 3059.3456, 3089.0117, 3096.8555, 3109.1064, 3129.6205, 3155.8443

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.2	**Energy (kJ mol^{-1}):** -421.475493403939
Reaction Coordinates: 6 1.873971 -0.070063 0.387875 6 0.541612 0.244056 1.021567 6 -0.310895 1.236219 0.587453 6 -0.034170 2.151529 -0.565802 1 0.461818 1.644901 -1.391297 1 -0.953385 2.596264 -0.940775 1 0.618508 2.970101 -0.243440 6 1.857177 -0.985271 -0.845915 1 1.224052 -0.589512 -1.639677 1 1.482443 -1.973555 -0.588865 1 2.867592 -1.086779 -1.242910 1 -1.092257 1.542969 1.267105 1 2.512605 -0.523679 1.146782 1 2.352951 0.874387 0.110979 1 0.365519 -0.152058 2.010474 8 -1.993247 0.034267 -0.288360 8 -1.361093 -1.072279 -0.515636 8 -0.821412 -1.557221 0.554065	**Frequencies (cm^{-1}):** -229.0107, 64.0517, 78.9177, 129.2482, 162.4993, 177.4459, 197.5797, 216.8561, 279.3811, 332.6511, 475.5939, 515.4286, 624.6646, 737.2053, 787.5741, 794.488, 845.2854, 929.7366, 991.7578, 1034.1803, 1045.4619, 1064.2902, 1071.9528, 1088.5727, 1106.9105, 1157.3854, 1263.042, 1299.6186, 1357.4185, 1398.7445, 1414.4435, 1437.4029, 1472.2841, 1485.7327, 1497.1251, 1502.3955, 1512.747, 1555.0945, 3007.4365, 3008.9832, 3039.9373, 3060.6074, 3086.3798, 3098.3772, 3120.8139, 3123.6175, 3180.7038, 3197.9474
IRC:  	

Compound: Z-EtCHCHMe + O_3 POZ 2.2	**Energy (kJ mol^{-1}):** -421.577414763780
Reaction Coordinates: 6 -1.601125 0.417075 0.575694 6 -0.234671 -0.169540 0.951115 6 1.063253 0.553678 0.447193 1 1.741299 0.685514 1.291993 6 0.900861 1.875591 -0.282525 1 1.882377 2.245821 -0.575931	**Frequencies (cm^{-1}):** 47.4175, 118.1233, 195.748, 221.1323, 240.6022, 280.0724, 330.2283, 389.9908, 478.8777, 556.265, 693.249, 708.3074, 748.3374, 783.3273, 818.9452, 866.3148, 911.437, 936.1644, 952.8634, 1040.8849,

1 0.292594 1.773935 -1.177573 1 0.445064 2.622901 0.368660 8 1.707244 -0.438392 -0.372723 8 0.622926 -1.296849 -0.775253 8 -0.057116 -1.508819 0.473687 1 -0.180304 -0.261587 2.036737 1 -1.590133 1.486541 0.799564 1 -2.327193 -0.021049 1.264117 6 -2.089685 0.172915 -0.852861 1 -2.132522 -0.892859 -1.069834 1 -3.094515 0.579906 -0.970799 1 -1.452899 0.635032 -1.604327	1063.5519, 1087.3183, 1101.3445, 1136.0476, 1163.9872, 1278.5798, 1310.0643, 1335.6261, 1353.439, 1389.5589, 1398.8705, 1414.9147, 1423.8093, 1480.2656, 1495.3771, 1497.3148, 1501.359, 1512.4381, 3025.7765, 3041.9281, 3044.0656, 3045.3223, 3052.7977, 3065.0729, 3100.3185, 3102.4637, 3118.4534, 3135.592

Compound: Z-EtCHCHMe + O_3 TS_{OZO} 2.3	**Energy (kJ mol^{-1}):** -421.480940628349
Reaction Coordinates: 6 1.577252 0.593434 -0.331464 6 0.518968 0.454347 0.721638 6 -0.702978 1.073025 0.671916 6 -1.129752 2.008027 -0.417127 1 -0.830936 1.651497 -1.402857 1 -2.208243 2.148454 -0.416754 1 -0.666123 2.990328 -0.276808 6 2.786577 -0.312333 -0.116193 1 3.537722 -0.150681 -0.889296 1 2.491049 -1.360822 -0.141624 1 3.256504 -0.117636 0.849539 1 -1.312354 1.047282 1.563826 1 1.902865 1.640991 -0.360851 1 1.138866 0.404760 -1.316147 1 0.806710 -0.017882 1.651130 8 -2.027569 -0.720797 0.033071 8 -1.120169 -1.416085 -0.560006 8 -0.154320 -1.755031 0.222838	**Frequencies (cm^{-1}):** -164.7987, 49.0223, 78.0182, 130.553, 139.7573, 167.103, 175.635, 211.1543, 246.3096, 351.3945, 460.319, 476.1011, 602.7169, 723.512, 739.3675, 805.6246, 876.8665, 947.5148, 985.2007, 1046.5174, 1050.9305, 1054.0613, 1085.1637, 1093.3173, 1108.9112, 1161.0518, 1259.1384, 1287.9661, 1338.8972, 1407.7528, 1415.6271, 1440.8839, 1464.2203, 1478.7768, 1489.8112, 1499.3211, 1507.9139, 1571.0574, 2980.7896, 3008.0896, 3019.543, 3031.3402, 3072.8116, 3089.0237, 3103.8828, 3117.3074, 3169.1895, 3189.7965

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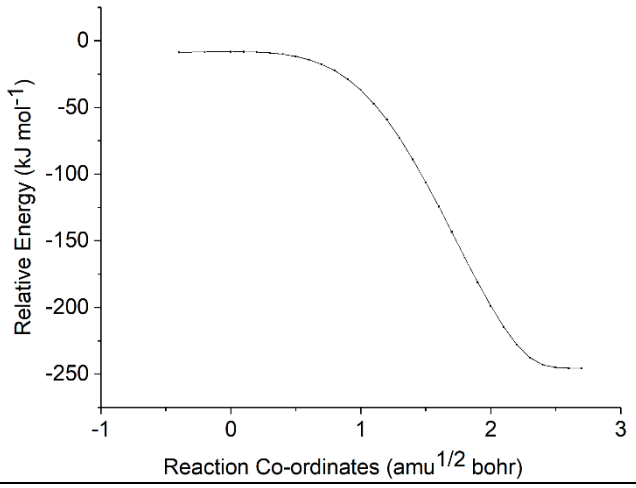

Compound: Z-EtCHCHMe + O_3 POZ 2.3	**Energy (kJ mol^{-1}):** -421.581360460904
Reaction Coordinates: 6 -1.422163 0.686450 -0.239577 6 -0.380240 -0.044094 0.597870 6 1.086067 0.514640 0.554928 6 1.335760 1.735640 -0.314006 1 1.060509 1.549666 -1.350365 1 0.774462 2.597753 0.047736 1 2.394933 1.987217 -0.280178 6 -2.819409 0.090063 -0.075765 1 -3.156240 0.150062 0.961291 1 -3.543262 0.624669 -0.690930 1 -2.834134 -0.958101 -0.372655 1 -0.718225 -0.117995 1.633497 1 -1.435344 1.738560 0.054977 1 -1.122536 0.654705 -1.288104 1 1.439131 0.696229 1.570751 8 1.853935 -0.613245 0.104495 8 0.909055 -1.329990 -0.709328 8 -0.220413 -1.409136 0.176493	**Frequencies (cm^{-1}):** 38.1236, 106.4651, 194.9527, 222.8799, 247.6416, 286.9838, 309.4444, 433.3448, 457.2585, 514.6987, 695.0401, 716.5112, 758.7964, 764.8899, 845.3108, 882.7421, 917.5293, 938.6717, 965.0015, 1049.1385, 1054.262, 1059.2291, 1105.7839, 1142.7719, 1169.6196, 1289.5342, 1291.9887, 1315.4559, 1351.1668, 1379.0314, 1401.1074, 1413.0908, 1417.6865, 1475.6873, 1493.3709, 1498.9986, 1502.2109, 1508.9637, 3027.9321, 3029.4778, 3042.1709, 3043.8476, 3062.0927, 3070.1698, 3089.9162, 3103.1012, 3105.1662, 3122.2873

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.1	**Energy (kJ mol^{-1}):** -421.552501616669
Reaction Coordinates: 6 -1.667754 -0.596109 -0.421243 6 -0.295935 -0.670430 0.188979 6 0.586842 0.965512 0.451080 6 0.401005 1.838943 -0.780213 1 -0.648385 2.051277 -0.985626 1 0.855230 1.371828 -1.652551 1 0.908834 2.789035 -0.607947 6 -2.683005 0.120495 0.469411 1 -2.741390 -0.342745 1.455335 1 -2.433124 1.171967 0.606926 1 -3.674861 0.071721 0.022157 1 -0.216907 -1.033382 1.210073 1 -1.607879 -0.124746 -1.402586 1 -2.002406 -1.624118 -0.590942 1 -0.050354 1.230197 1.311364 8 1.768609 0.576760 0.749867 8 1.790088 -1.322453 0.020157 8 0.636843 -1.193245 -0.621809	**Frequencies (cm^{-1}):** -450.0294, 91.4302, 114.878, 172.9944, 179.5044, 206.6829, 258.5214, 317.0113, 346.6393, 422.3487, 482.3502, 514.905, 585.8273, 614.6184, 782.6311, 851.1901, 926.9331, 957.1878, 1023.132, 1035.1318, 1057.1777, 1112.1293, 1116.963, 1160.2349, 1177.8288, 1241.8886, 1299.7796, 1309.543, 1333.3556, 1396.9342, 1411.2643, 1425.1988, 1438.3836, 1478.0755, 1485.5915, 1498.5172, 1504.1062, 1508.7575, 2915.2916, 3018.3756, 3035.7268, 3037.6692, 3071.7089, 3094.3685, 3099.2615, 3106.6701, 3116.9107, 3117.3735
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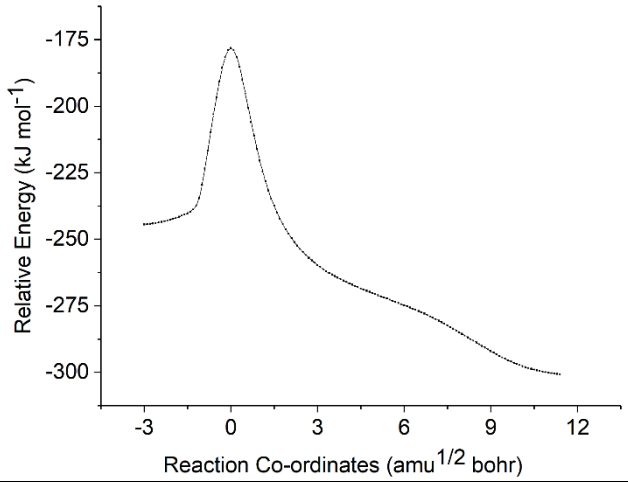
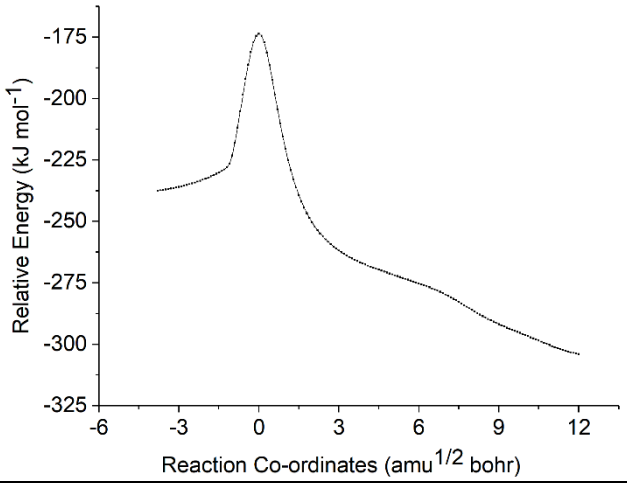


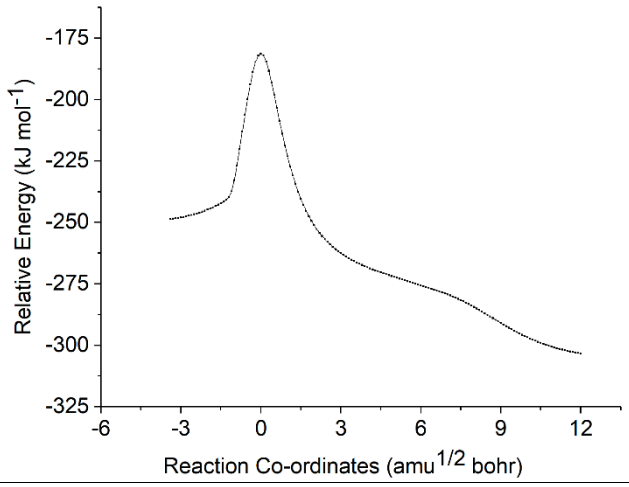
Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.1	**Energy (kJ mol^{-1}):** -421.591705369877
Reaction Coordinates: 6 -2.378148 -0.090769 0.169545 6 -1.188993 0.627316 -0.346030 6 2.215901 -1.228810 0.014316 6 2.866776 0.108015 0.149070 1 3.381974 0.152544 1.113585 1 2.144433 0.920450 0.062945 1 3.645561 0.201178 -0.613786 6 -2.275893 -1.614920 0.024560 1 -2.118895 -1.902579 -1.014956 1 -1.445259 -2.009515 0.604454 1 -3.199963 -2.078395 0.367613 1 -0.735748 0.419205 -1.310197 1 -2.547057 0.205798 1.204589 1 -3.239971 0.265890 -0.409097 1 2.898316 -2.101605 0.072512 8 1.031588 -1.417762 -0.147327 8 0.381686 2.252896 -0.202189 8 -0.690930 1.555121 0.331213	**Frequencies (cm^{-1}):** 18.355, 37.982, 71.8795, 74.4901, 94.6839, 116.6462, 137.8392, 178.2563, 202.1971, 217.8623, 314.0613, 420.1788, 527.4796, 531.8243, 764.5768, 779.8635, 896.2511, 898.8132, 911.4336, 936.8395, 1030.636, 1097.4494, 1145.4745, 1152.5863, 1177.7462, 1276.184, 1325.6832, 1373.589, 1388.2182, 1422.7758, 1425.6546, 1463.6346, 1464.5937, 1481.6193, 1497.9401, 1503.517, 1577.4011, 1783.6574, 2874.266, 2986.8342, 2999.9241, 3045.712, 3059.6874, 3081.3696, 3097.8496, 3106.9369, 3131.1692, 3156.9083

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.2	**Energy (kJ mol^{-1}):** -421.550522919038
Reaction Coordinates: 6 -1.709302 -0.038328 0.767777 6 -0.275448 -0.494166 0.654954 6 1.019442 0.827337 0.468768 6 0.558645 1.895322 -0.512470 1 -0.380188 2.358610 -0.208729 1 0.456986 1.480326 -1.513614 1 1.319782 2.676206 -0.550621 6 -2.475555 0.110415 -0.547290 1 -2.007881 0.830227 -1.215588 1 -2.539849 -0.839411 -1.075705 1 -3.490036 0.450809 -0.342303 1 0.156042 -0.964978 1.532980 1 -1.716663 0.901917 1.323653	**Frequencies (cm^{-1}):** -453.2759, 101.0517, 107.8832, 185.3135, 208.2626, 222.4456, 238.7892, 288.7735, 354.5828, 434.8191, 485.8356, 569.7036, 588.5365, 649.5598, 780.5226, 841.9272, 906.067, 966.8712, 1007.184, 1051.7089, 1072.2076, 1107.9662, 1122.0021, 1131.6047, 1190.8897, 1250.5314, 1293.2576, 1309.984, 1375.7417, 1392.7874, 1397.6494, 1427.946, 1432.2042, 1480.6771, 1482.417, 1498.675, 1501.987, 1510.5701,

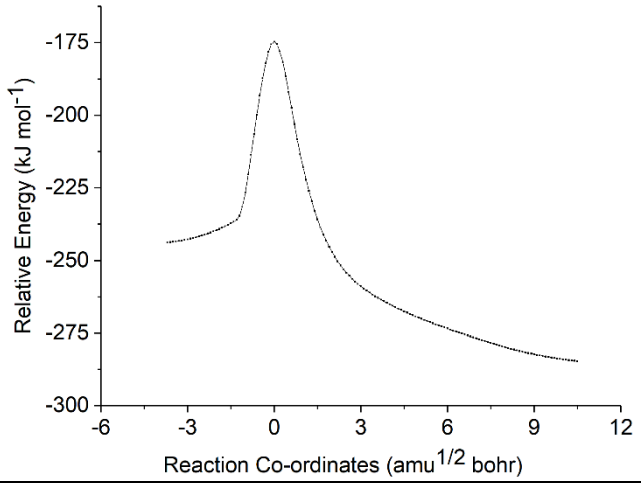
1 -2.225703 -0.759539 1.408247 1 0.948658 1.124642 1.528922 8 2.059649 0.138297 0.166908 8 1.265565 -1.612562 -0.424956 8 0.021305 -1.158521 -0.476660	2906.7921, 3018.6873, 3035.1643, 3049.2286, 3051.1604, 3092.6788, 3108.855, 3119.5132, 3120.2971, 3122.6671
IRC:  	

Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.2	**Energy (kJ mol^{-1}):** -421.593801885446
Reaction Coordinates: 6 -1.962661 -0.783962 -0.499882 6 -0.991550 0.313241 -0.709935 6 2.369011 -1.065233 0.062503 6 2.788974 0.328495 0.394386 1 3.139895 0.352472 1.430609 1 1.981981 1.048227 0.249032 1 3.654100 0.591118 -0.222149 6 -2.695095 -0.771443 0.837496 1 -1.994856 -0.847259 1.668035 1 -3.269532 0.144435 0.969040 1 -3.380959 -1.615551 0.891854 1 -0.393392 0.397662 -1.611067 1 -1.403044 -1.714664 -0.638464 1 -2.670007 -0.749035 -1.337712 1 3.148883 -1.843119 0.190555 8 1.269825 -1.393295 -0.324331 8 0.090694 2.204703 -0.094309 8 -0.843662 1.202232 0.156497	**Frequencies (cm^{-1}):** 35.4228, 42.8486, 79.8051, 98.6999, 101.4857, 117.143, 175.1613, 181.173, 195.3352, 223.0269, 281.3285, 416.8592, 533.044, 618.6424, 741.441, 781.7961, 892.989, 896.8663, 905.0053, 927.1014, 1026.6217, 1109.4606, 1124.0407, 1145.4685, 1152.675, 1279.563, 1346.3248, 1389.7477, 1392.3987, 1423.4905, 1425.0139, 1447.3798, 1468.2239, 1480.5158, 1499.0874, 1504.6434, 1588.9356, 1781.9202, 2880.6668, 2997.5999, 2997.9413, 3032.4312, 3047.3283, 3059.688, 3092.8242, 3111.7056, 3113.0959, 3161.5725

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 1.3	**Energy (kJ mol^{-1}):** -421.552964279408
Reaction Coordinates: 6 -1.589612 0.727157 -0.007695 6 -0.449226 -0.186278 0.333972 6 1.216989 0.635842 0.531749 6 1.401594 1.670292 -0.568647 1 0.628827 2.438961 -0.546569 1 1.412995 1.191635 -1.546551	**Frequencies (cm^{-1}):** -442.1928, 80.0073, 110.4935, 161.1972, 184.1964, 210.9157, 248.6438, 286.6601, 350.73, 462.3242, 483.1396, 517.9774, 604.2923, 617.6594, 780.5891, 850.2464, 925.2345, 962.1581, 996.5967, 1037.3785,

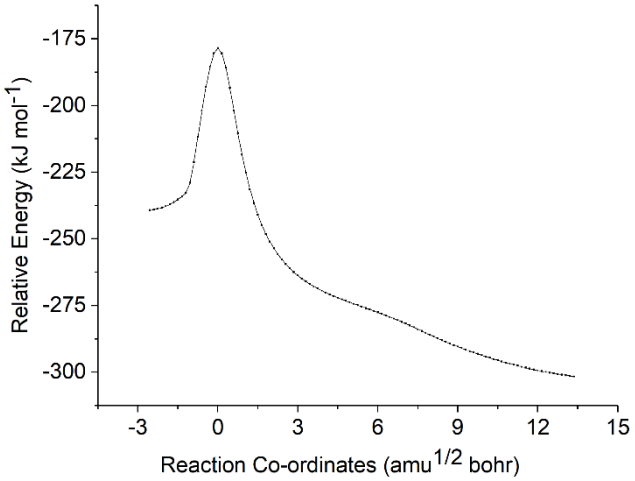
1 2.366566 2.158340 -0.424267 6 -2.953060 0.036203 0.126437 1 -3.034406 -0.806045 -0.559938 1 -3.110710 -0.336648 1.139160 1 -3.755749 0.737517 -0.100832 1 -0.473223 -0.687557 1.297550 1 -1.454698 1.105954 -1.021054 1 -1.544594 1.585909 0.664427 1 0.949747 1.053516 1.517791 8 2.007267 -0.370882 0.561018 8 0.860037 -1.840398 -0.259478 8 -0.085412 -1.006330 -0.665868	1054.745, 1115.3351, 1124.477, 1159.4245, 1172.1227, 1240.4848, 1300.2444, 1315.9062, 1345.5932, 1397.1244, 1406.7005, 1424.0185, 1436.7811, 1479.4835, 1483.0613, 1497.643, 1499.5715, 1506.4466, 2903.9589, 3034.7796, 3035.3372, 3044.8617, 3079.5011, 3094.8024, 3099.4746, 3107.4466, 3117.3383, 3118.9542
IRC:  	

Compound: Z-EtCHCHMe + O_3 C_{ANTI} 1.3	**Energy (kJ mol^{-1}):** -421.592763619681
Reaction Coordinates: 6 -1.927792 -0.599929 0.477028 6 -0.989512 0.332694 -0.185640 6 2.392000 -1.186273 0.004957 6 2.939923 0.202329 -0.022783 1 3.519493 0.369624 0.890222 1 2.154969 0.953953 -0.117845 1 3.651679 0.283175 -0.850013 6 -3.231439 -0.772388 -0.319525 1 -3.782072 0.165492 -0.384478 1 -3.033080 -1.122134 -1.332974 1 -3.868752 -1.508206 0.169123 1 -0.627999 0.189175 -1.198713 1 -2.126194 -0.246771 1.488388 1 -1.415704 -1.563545 0.551690 1 3.144611 -1.995392 0.097604 8 1.219548 -1.479365 -0.064128 8 0.289236 2.200520 -0.235549 8 -0.598289 1.355849 0.420025	**Frequencies (cm^{-1}):** 36.2591, 45.1843, 69.7326, 83.0776, 101.8862, 111.8572, 146.8604, 179.9158, 205.4241, 221.5528, 331.091, 417.7094, 531.2702, 535.5493, 777.3848, 781.8696, 893.7283, 897.3574, 911.2546, 940.9086, 1018.62, 1093.6334, 1145.2497, 1152.1486, 1181.2257, 1276.3212, 1324.1559, 1372.9321, 1389.7383, 1416.2506, 1424.9786, 1467.7567, 1472.6765, 1480.4433, 1500.6015, 1505.5614, 1582.0114, 1782.0364, 2880.8381, 2998.7018, 3029.8939, 3038.2448, 3059.9994, 3086.8366, 3093.9029, 3106.7803, 3109.2429, 3159.6008

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.1	**Energy (kJ mol^{-1}):** -421.550754676428
Reaction Coordinates: 6 1.426705 -0.629905 -0.559256 6 0.345583 -0.680722 0.527739 6 -0.783787 0.815501 0.404070 6 -0.111330 2.128327 0.151688 1 0.391981 2.143172 -0.812939 1 -0.849857 2.932501 0.168548 1 0.615847 2.329251 0.935853 6 2.735871 0.004856 -0.093377 1 3.134933 -0.516650 0.778754 1 3.490417 -0.044231 -0.878651 1 2.615246 1.054422 0.177246 1 0.694028 -0.389000 1.535391 1 1.600407 -1.665040 -0.856153 1 1.043050 -0.126043 -1.448716 1 -1.291787 0.678213 1.353241 8 -1.496995 0.360191 -0.637423 8 -2.138709 -0.751898 -0.305444 8 -0.504610 -1.636410 0.500646	**Frequencies (cm^{-1}):** -456.5309, 76.2024, 106.812, 172.8893, 202.5363, 222.4548, 272.4678, 293.2747, 353.7351, 368.2323, 487.0462, 529.9655, 606.7228, 631.8152, 783.1452, 836.0845, 907.3963, 971.5368, 1004.268, 1031.4462, 1084.185, 1114.8078, 1121.7341, 1148.493, 1176.8374, 1260.8923, 1283.2688, 1310.6288, 1339.5636, 1386.2307, 1413.4168, 1421.7528, 1437.4152, 1481.9637, 1484.9268, 1497.9121, 1502.6216, 1505.6484, 2887.3654, 3028.629, 3038.3705, 3039.1503, 3065.7214, 3088.4416, 3093.6681, 3101.1853, 3123.4699, 3137.0609
IRC:  	

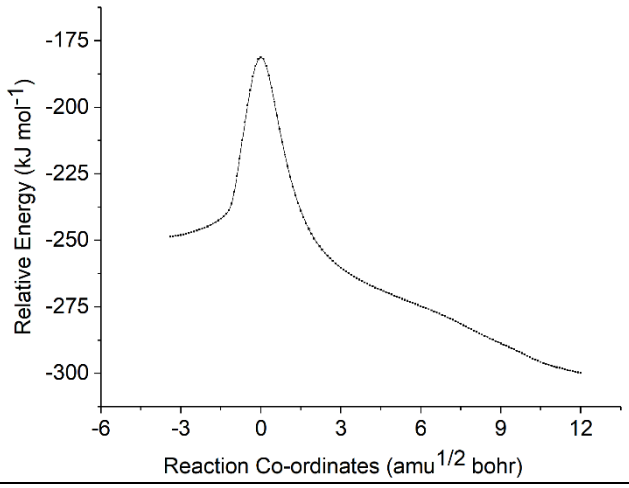
Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.1	**Energy (kJ mol^{-1}):** -421.595241321489
Reaction Coordinates: 6 -2.135609 0.178117 0.487146 6 -1.071013 -0.308518 -0.455432 6 1.964290 -0.025222 0.420383 6 3.104462 -0.892367 0.071376 1 3.582540 -0.564562 -0.848138 1 3.831613 -0.904381 0.886651 1 2.738532 -1.914942 -0.050576 6 -3.529905 -0.227569 -0.014065 1 -3.641865 -1.311969 -0.037424 1 -4.301576 0.177520 0.639985 1 -3.715774 0.152671 -1.019990 1 -1.095001 0.143556 -1.462136 1 -1.942760 -0.230380 1.479017 1 -2.063016 1.265527 0.539933 1 1.369124 -0.156574 1.315738	**Frequencies (cm^{-1}):** 29.5056, 44.9132, 76.0531, 89.7766, 128.5953, 142.2844, 207.5987, 219.6339, 241.4023, 295.8674, 331.1586, 381.4413, 510.2165, 555.8819, 787.3946, 865.3856, 879.6719, 887.4779, 921.5283, 968.107, 999.728, 1071.489, 1115.9627, 1162.1742, 1165.0033, 1270.6198, 1325.3949, 1352.4912, 1407.3042, 1409.7775, 1423.6526, 1457.1875, 1463.9607, 1475.7504, 1501.1711, 1505.9131, 1589.7386, 1737.2285, 2934.4546, 3027.2871, 3029.4081, 3046.0195,

8 1.663199 0.925523 -0.338956 8 0.533593 1.659577 -0.013024 8 -0.291187 -1.210489 -0.210459	3074.7101, 3080.2197, 3097.2101, 3103.4173, 3137.7024, 3182.43

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.2	**Energy (kJ mol^{-1}):** -421.552628851513
Reaction Coordinates: 6 -1.581968 0.732140 -0.359363 6 -0.459488 -0.090414 -0.999764 6 1.191679 0.351509 -0.266992 6 1.400728 1.804045 0.027122 1 0.785329 2.134801 0.861158 1 2.448513 1.989159 0.271454 1 1.154628 2.399516 -0.850773 6 -2.026007 0.253685 1.019853 1 -1.240990 0.380909 1.765037 1 -2.900464 0.813027 1.353119 1 -2.283720 -0.803561 0.993152 1 -0.169915 0.279255 -2.000226 1 -1.301235 1.787750 -0.340173 1 -2.424357 0.663922 -1.055143 1 1.806883 -0.100186 -1.038936 8 1.096809 -0.420212 0.830338 8 0.997739 -1.694751 0.485354 8 -0.472590 -1.366335 -0.876167	**Frequencies (cm^{-1}):** -438.7923, 63.812, 111.6364, 186.2891, 188.6131, 236.8966, 245.5334, 324.8111, 342.0849, 372.7971, 519.2866, 527.0752, 622.721, 683.251, 790.9445, 801.4111, 900.4654, 973.6562, 1009.0764, 1031.1071, 1077.2358, 1105.7587, 1121.034, 1147.4765, 1189.2073, 1262.2017, 1292.9759, 1309.6959, 1347.3079, 1387.5792, 1409.2023, 1421.62, 1449.473, 1477.2059, 1489.3336, 1494.4392, 1497.5487, 1510.0199, 2886.5649, 3013.9567, 3039.0285, 3040.2595, 3045.8022, 3096.9794, 3099.5492, 3115.2202, 3119.9478, 3134.0814
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.2	**Energy (kJ mol^{-1}):** -421.596921970227
Reaction Coordinates: 6 -2.362459 0.260935 -0.255183 6 -1.105422 -0.112448 -0.990552 6 1.737710 -0.120585 0.479878 6 2.929029 -0.920829 0.141533 1 3.554928 -0.409254 -0.585172 1 3.505713 -1.136751 1.044029 1 2.599968 -1.879222 -0.267998	**Frequencies (cm^{-1}):** 36.3684, 49.7967, 78.127, 106.1801, 133.0478, 142.5792, 202.0803, 231.6806, 255.3723, 278.2227, 295.6679, 332.6072, 554.7849, 657.2547, 697.5214, 849.9052, 866.1274, 885.2998, 910.1057, 966.9598, 1007.964, 1071.5065, 1109.78, 1134.7997,

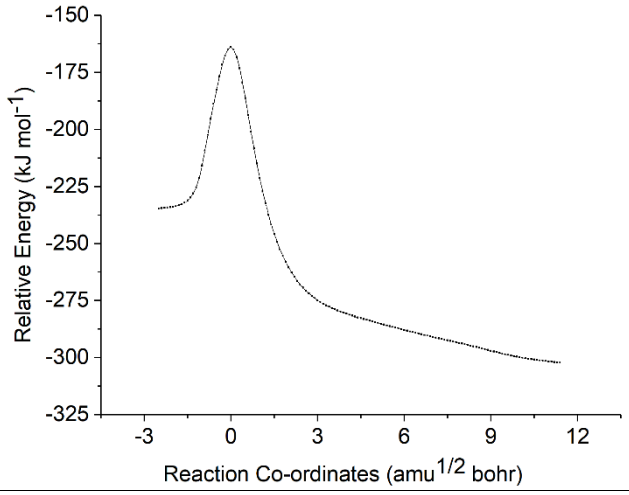
6 -2.622428 -0.527101 1.020509 1 -1.842075 -0.336576 1.756825 1 -3.577086 -0.239823 1.460855 1 -2.642810 -1.598805 0.826148 1 -0.874391 0.522917 -1.862145 1 -2.315303 1.335577 -0.065839 1 -3.180466 0.127085 -0.975268 1 0.996889 -0.434264 1.205096 8 1.562691 0.985162 -0.083141 8 0.390905 1.666743 0.207767 8 -0.414089 -1.080744 -0.738830	1164.6349, 1284.216, 1352.507, 1369.4147, 1408.3148, 1409.8591, 1422.7164, 1449.8084, 1457.5247, 1463.8707, 1493.8912, 1503.508, 1590.6049, 1743.5182, 2939.8785, 2992.6478, 3026.8335, 3040.2196, 3057.7379, 3073.9362, 3099.8241, 3105.676, 3137.4574, 3182.1094

Compound: Z-EtCHCHMe + O_3 TS_{ANTI} 2.3	**Energy (kJ mol^{-1}):** -421.553201394595
Reaction Coordinates: 6 1.428450 0.549724 -0.425231 6 0.532521 -0.128511 0.606236 6 -1.234949 0.443148 0.372601 6 -1.409582 1.903347 0.095848 1 -1.039287 2.167285 -0.892443 1 -2.466156 2.171811 0.156531 1 -0.874840 2.489451 0.841724 6 2.897028 0.180308 -0.196960 1 3.035764 -0.897659 -0.271146 1 3.537417 0.661128 -0.936982 1 3.235881 0.495855 0.791962 1 0.594157 0.304438 1.621514 1 1.115912 0.229203 -1.420082 1 1.310643 1.634233 -0.369422 1 -1.626431 0.050357 1.305554 8 -1.504983 -0.349046 -0.676895 8 -1.414121 -1.623687 -0.329000 8 0.406121 -1.401541 0.563124	**Frequencies (cm^{-1}):** -435.7698, 74.7693, 110.9366, 171.9122, 191.1959, 237.8586, 250.4272, 309.4136, 350.531, 365.7514, 507.8113, 518.1431, 624.4095, 628.5492, 790.8912, 840.832, 905.666, 972.7448, 1006.3154, 1015.6856, 1079.4347, 1118.0988, 1140.6912, 1149.3417, 1174.4585, 1261.6082, 1290.2781, 1305.1364, 1353.0096, 1387.7668, 1407.5843, 1421.989, 1449.0227, 1480.4676, 1483.1515, 1494.0364, 1498.1887, 1506.3233, 2886.8147, 3026.4462, 3028.9737, 3038.1568, 3070.2946, 3087.8145, 3098.887, 3105.7428, 3121.9309, 3135.8716
IRC:  	

Compound: Z-EtCHCHMe + O_3 CPr_{ANTI} 2.3	**Energy (kJ mol^{-1}):** -421.595100791669
Reaction Coordinates:	**Frequencies (cm^{-1}):**

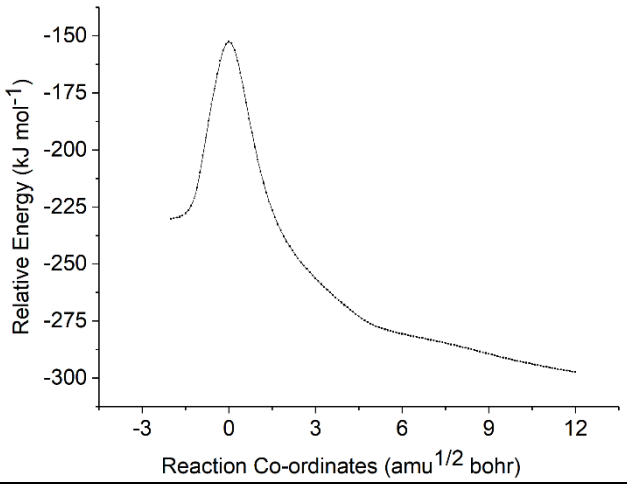
6 2.051350 0.085931 0.564133 6 1.113728 -0.329468 -0.534248 6 -2.063766 -0.010296 -0.284463 6 -3.002986 -0.914745 0.403978 1 -3.128924 -0.633789 1.446440 1 -3.970844 -0.907636 -0.103105 1 -2.613913 -1.934078 0.342820 6 3.513809 -0.158229 0.166770 1 3.765488 0.363334 -0.758181 1 4.184899 0.205947 0.944025 1 3.713812 -1.220225 0.019957 1 1.269107 0.180924 -1.500914 1 1.887803 1.151020 0.739892 1 1.791142 -0.456971 1.472628 1 -1.812955 -0.100401 -1.334551 8 -1.527878 0.922607 0.357338 8 -0.601277 1.704632 -0.316374 8 0.284352 -1.213150 -0.436718	24.97, 36.3681, 79.8813, 85.0518, 117.7021, 137.1761, 195.3116, 217.8739, 239.7259, 288.5853, 331.0133, 375.8215, 512.8901, 554.0073, 776.2214, 864.4798, 876.1359, 883.7525, 919.2635, 965.6231, 1002.2593, 1072.2316, 1121.2301, 1162.331, 1164.7844, 1269.4636, 1326.5168, 1352.6407, 1408.5293, 1410.0894, 1425.6937, 1457.6505, 1463.8441, 1476.3559, 1501.4738, 1505.7527, 1591.5727, 1745.0838, 2930.8569, 3026.9663, 3029.4667, 3043.753, 3074.2177, 3079.39, 3098.1153, 3101.7586, 3137.5302, 3179.9309

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.1	**Energy (kJ mol^{-1}):** -421.547763213279
Reaction Coordinates: 6 -1.213292 -0.609037 -0.483452 6 -0.219218 -0.453030 0.647084 6 0.899352 1.000321 0.329053 6 -0.039598 2.174568 0.038939 1 -0.567010 2.044926 -0.902825 1 -0.751532 2.328571 0.849562 1 0.577693 3.069724 -0.042200 6 -2.629685 -0.185201 -0.098445 1 -2.689491 0.876196 0.140615 1 -3.314916 -0.374391 -0.924512 1 -2.991951 -0.745119 0.765332 1 -0.624826 -0.330875 1.648881 1 -0.869806 -0.086049 -1.372948 1 -1.192315 -1.670162 -0.748833 1 1.371692 1.079694 1.322229 8 1.644396 0.581197 -0.627482 8 1.347630 -1.455594 -0.490617 8 0.791363 -1.345384 0.701302	**Frequencies (cm^{-1}):** -467.5539, 98.9511, 106.1755, 192.0707, 222.0799, 244.533, 257.5907, 302.6104, 341.7176, 396.3764, 487.1542, 533.4525, 579.8498, 709.6385, 782.0742, 883.7748, 910.6977, 969.4444, 1001.524, 1027.1177, 1073.6382, 1080.0511, 1108.7138, 1146.5508, 1191.767, 1201.6391, 1281.1749, 1333.3232, 1348.2452, 1389.7876, 1416.903, 1425.8669, 1435.9346, 1477.756, 1484.4594, 1500.7022, 1505.9066, 1507.7766, 2913.338, 3028.8068, 3033.5229, 3039.23, 3084.8474, 3098.17, 3101.8014, 3105.5528, 3115.5306, 3131.8946
IRC:	



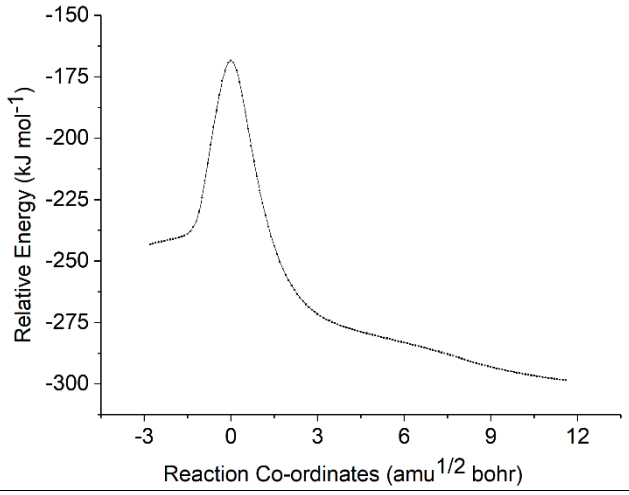
Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.1	**Energy (kJ mol^{-1}):** -421.594302014611
Reaction Coordinates: 6 -1.613697 0.574527 -0.343989 6 -1.874865 -0.587352 0.509903 6 2.214155 0.215268 -0.007807 6 3.703898 0.054287 0.034096 1 4.196776 0.987275 0.297521 1 3.962365 -0.726509 0.754208 1 4.055784 -0.296984 -0.939501 6 -2.573553 1.738351 -0.110783 1 -2.524034 2.095828 0.918532 1 -2.313426 2.573277 -0.758982 1 -3.606439 1.460635 -0.324830 1 -2.597756 -0.593621 1.320237 1 -0.566709 0.870827 -0.174335 1 -1.614616 0.217440 -1.380319 1 1.627739 -0.686464 -0.264227 8 1.641157 1.257921 0.222617 8 -0.331406 -1.800002 -0.604404 8 -1.279166 -1.691943 0.389683	**Frequencies (cm^{-1}):** 31.3852, 48.6145, 68.2796, 73.3178, 85.8861, 103.1177, 120.4182, 166.9355, 199.6125, 219.6591, 359.5018, 470.9166, 514.3039, 685.5906, 716.4343, 798.6364, 850.1149, 878.4964, 890.3537, 937.177, 1050.8862, 1105.2622, 1128.9864, 1143.6434, 1159.6472, 1264.3814, 1334.7979, 1377.1138, 1378.9465, 1424.1461, 1437.1939, 1448.7442, 1461.0831, 1468.8266, 1502.6254, 1505.8906, 1566.056, 1772.4749, 2925.8497, 2950.9292, 3015.3422, 3021.7002, 3034.7808, 3072.2688, 3090.7093, 3109.3763, 3131.008, 3149.5679

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.2	**Energy (kJ mol^{-1}):** -421.542983956151
Reaction Coordinates: 6 -0.945569 1.199696 0.585627 6 -0.278626 -0.089314 1.022906 6 1.340793 -0.394289 0.097491 6 2.036087 0.968064 0.058016 1 1.542786 1.654449 -0.624836 1 2.105067 1.414969 1.050081 1 3.051247 0.801528 -0.304849 6 -1.345894 1.419634 -0.873174 1 -2.145198 0.748251 -1.171583 1 -1.696774 2.446306 -0.990600 1 -0.513560 1.256477 -1.552840 1 -0.014493 -0.099481 2.078391 1 -0.291738 2.005526 0.922050	**Frequencies (cm^{-1}):** -462.2323, 90.9978, 128.6762, 184.9448, 233.2946, 259.5594, 265.1407, 297.4194, 333.8751, 395.9951, 481.5867, 520.6181, 561.8054, 740.9344, 783.2709, 843.1437, 886.8322, 971.485, 997.0958, 1012.4722, 1059.225, 1082.6595, 1114.3745, 1140.4581, 1192.0703, 1222.6964, 1304.0793, 1351.587, 1372.3337, 1393.2254, 1419.0711, 1439.059, 1446.1546, 1469.3424, 1489.2539, 1492.6871, 1500.177, 1511.571,

1 -1.837653 1.272904 1.220122 1 1.802289 -1.078556 0.829818 8 0.957999 -0.917545 -1.005087 8 -1.008021 -1.424951 -0.571934 8 -0.805317 -1.288144 0.726902	2902.8746, 2991.4313, 3036.764, 3042.8423, 3062.8233, 3093.9537, 3109.1742, 3115.1174, 3136.5386, 3143.1911
IRC:  	

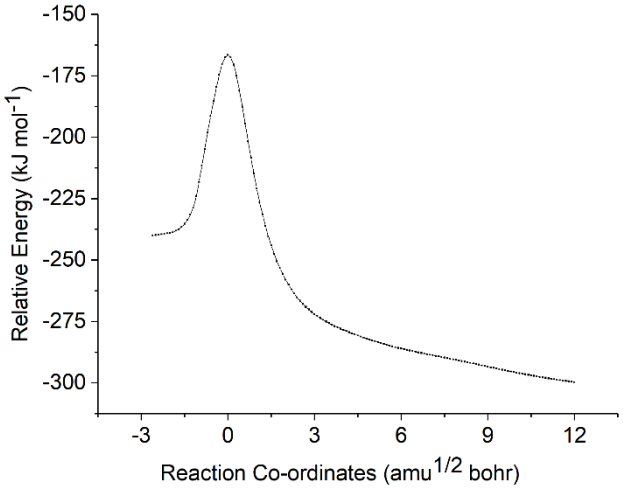
Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.2	**Energy (kJ mol^{-1}):** -421.593861868972
Reaction Coordinates: 6 2.242592 -0.173882 -0.543721 6 1.137718 0.836646 -0.662151 1 0.805370 1.035905 -1.697294 8 0.631297 1.426554 0.265886 6 2.702541 -0.463722 0.877868 1 3.052498 0.442007 1.372212 1 3.515210 -1.189807 0.876760 1 1.886842 -0.868945 1.475396 1 1.880076 -1.076129 -1.046007 1 3.067522 0.191073 -1.167861 6 -1.969147 -0.245984 0.803176 6 -2.612250 0.818160 0.028930 1 -3.324040 1.368093 0.638342 1 -3.085712 0.384315 -0.854957 1 -1.835122 1.494597 -0.340021 1 -2.074461 -0.370898 1.874762 8 -1.235626 -1.128503 0.285476 8 -1.007785 -1.052741 -1.070855	**Frequencies (cm^{-1}):** 34.4011, 39.2154, 66.1622, 84.5421, 88.4878, 98.6929, 171.7936, 172.4224, 245.1941, 255.1205, 300.6495, 454.8323, 668.5725, 671.3097, 672.7391, 764.6795, 850.9917, 884.604, 907.242, 980.9781, 1006.1276, 1058.1955, 1110.3202, 1117.4683, 1142.537, 1285.7294, 1353.0135, 1368.8011, 1395.0399, 1411.8714, 1424.8578, 1441.6054, 1449.6731, 1467.3696, 1494.612, 1501.1559, 1572.6431, 1775.2655, 2917.6717, 3001.9437, 3021.6891, 3039.803, 3041.6395, 3068.314, 3102.3263, 3105.6145, 3138.6306, 3173.1756

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 1.3	**Energy (kJ mol^{-1}):** -421.549091178838
Reaction Coordinates: 6 -1.039768 0.917984 -0.325141 6 -0.320199 0.108530 0.724457 6 1.504685 0.035992 0.289584 6 1.890495 1.481247 -0.035253 1 1.473982 1.796104 -0.988655 1 1.586330 2.171273 0.752341	**Frequencies (cm^{-1}):** -462.0059, 78.6617, 110.5305, 186.7328, 219.9061, 226.174, 260.4617, 306.3856, 358.6679, 406.9177, 481.0186, 543.8094, 588.7721, 675.2071, 802.4534, 877.0357, 896.7579, 967.6062, 987.3409, 1002.8773,

1 2.977916 1.516878 -0.112094 6 -2.560829 0.752689 -0.200735 1 -2.919908 1.064298 0.781183 1 -3.059781 1.366944 -0.950190 1 -2.858306 -0.282212 -0.361688 1 -0.395546 0.462513 1.750122 1 -0.771823 1.964168 -0.184706 1 -0.705568 0.614282 -1.313400 1 1.892509 -0.297317 1.266575 8 1.540186 -0.821720 -0.661389 8 -0.311546 -1.720604 -0.485417 8 -0.486904 -1.227124 0.727185	1058.0108, 1080.4393, 1104.4544, 1163.1897, 1187.3988, 1206.2578, 1306.7073, 1336.7326, 1358.5944, 1387.171, 1408.4392, 1430.4143, 1437.8437, 1478.22, 1488.4517, 1498.1817, 1500.3636, 1506.0343, 2912.0228, 3035.0807, 3035.6809, 3070.2728, 3091.9893, 3094.818, 3110.3328, 3114.9711, 3132.3192, 3133.7843
IRC:  	

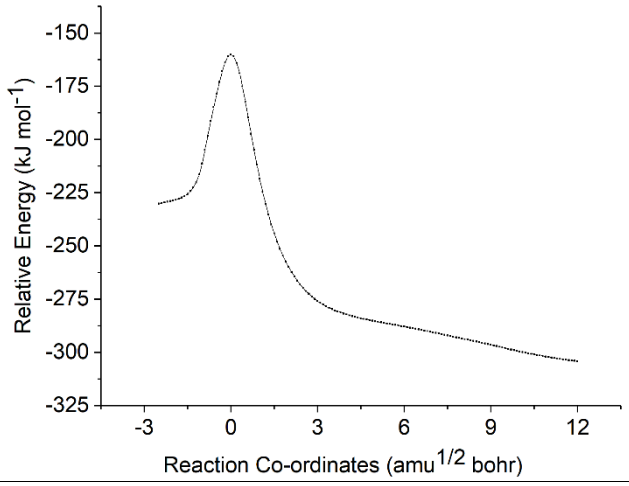
Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 1.3	**Energy (kJ mol^{-1}):** -421.592825799532
Reaction Coordinates: 6 2.248000 0.749929 0.561103 6 0.873717 0.270950 0.330847 6 -3.199591 0.588453 -0.060676 6 -3.116826 -0.892604 -0.258530 1 -2.091552 -1.249737 -0.203226 1 -3.730515 -1.390311 0.497250 1 -3.553872 -1.150112 -1.227139 6 3.057735 0.845713 -0.751412 1 2.614386 1.568221 -1.436079 1 4.072673 1.170122 -0.525520 1 3.101810 -0.126254 -1.236131 1 -0.013050 0.897515 0.322515 1 2.201037 1.723072 1.049401 1 2.736380 0.027802 1.219842 1 -4.220596 1.017382 -0.106164 8 -2.256128 1.316594 0.138057 8 1.621975 -1.858122 0.087626 8 0.597290 -0.941265 0.113975	**Frequencies (cm^{-1}):** 22.9373, 32.1715, 37.327, 59.2534, 71.561, 93.8392, 118.8651, 164.6629, 198.9975, 246.9829, 324.8511, 516.2707, 542.1093, 654.1262, 777.949, 812.6897, 873.4806, 891.0133, 891.654, 909.0511, 1012.3516, 1087.4547, 1138.2663, 1140.4523, 1146.4308, 1289.0478, 1335.2074, 1383.9711, 1385.9446, 1401.8166, 1426.1193, 1461.052, 1461.9211, 1471.5507, 1495.7878, 1511.8383, 1562.8442, 1792.5829, 2888.2096, 3021.8259, 3032.7374, 3043.8229, 3070.8711, 3088.0617, 3105.6064, 3133.7957, 3139.5042, 3153.9733

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.1	**Energy (kJ mol^{-1}):** -421.549271906827

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.736066 -0.482490 -0.451520 6 0.393698 -0.841356 0.215327 6 -0.492103 0.791587 0.471927 6 -0.491085 1.544633 -0.827466 1 0.447071 2.079958 -0.951617 1 -1.302334 2.276519 -0.795498 1 -0.659563 0.888348 -1.674857 6 2.670220 0.354013 0.417238 1 2.308640 1.373453 0.559293 1 3.657523 0.421464 -0.039823 1 2.798360 -0.094099 1.404352 1 0.520472 -1.141450 1.270566 1 2.206208 -1.446023 -0.660698 1 1.553337 -0.018212 -1.419160 1 -0.043612 1.278804 1.332454 8 -1.647775 0.222159 0.863823 8 -2.198095 -0.439853 -0.136657 8 -0.452489 -1.509442 -0.474422	-463.2804, 95.0495, 113.2382, 191.1886, 202.3046, 234.5614, 266.1292, 308.0648, 336.0689, 406.3467, 484.428, 528.4982, 580.6257, 702.0924, 777.3758, 859.563, 897.4619, 945.3965, 1019.3711, 1025.0573, 1053.6429, 1089.7359, 1113.2695, 1150.3938, 1195.9869, 1214.5781, 1280.2288, 1332.6324, 1357.7014, 1395.4697, 1415.3882, 1428.528, 1435.4679, 1472.2276, 1487.783, 1496.4134, 1503.6249, 1506.0536, 2896.2426, 3027.7849, 3036.3855, 3038.3606, 3076.3835, 3091.763, 3098.4442, 3111.6904, 3133.6415, 3157.73
IRC  	

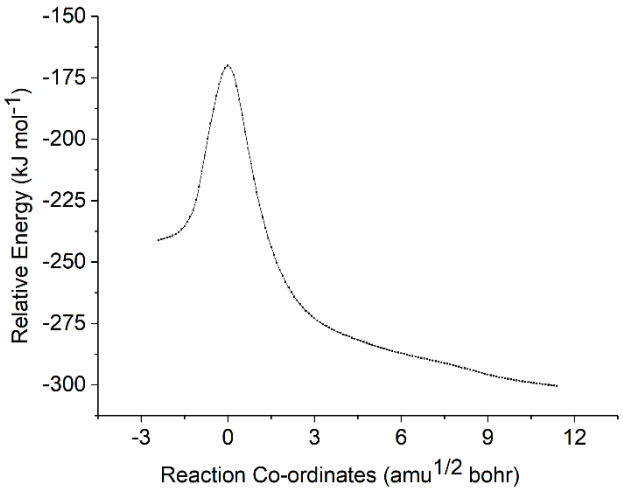
Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.1	**Energy (kJ mol^{-1}):** -421.598002966569
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.262030 0.376069 -0.407011 6 -1.126531 1.008893 0.352349 6 2.112765 -0.134127 -0.653402 6 2.657194 0.443484 0.577728 1 3.555466 1.019700 0.373946 1 2.844213 -0.356886 1.297646 1 1.893728 1.086303 1.025508 6 -2.748147 -0.940444 0.198393 1 -1.951734 -1.682670 0.190605 1 -3.598595 -1.329059 -0.361245 1 -3.068994 -0.802613 1.232629 1 -1.133588 0.834618 1.445676 1 -3.073461 1.115202 -0.394833 1 -1.958903 0.265739 -1.448634 1 2.471889 0.100220 -1.648907 8 1.178475 -0.977358 -0.665059 8 0.620769 -1.325469 0.545740	36.1159, 43.5273, 69.6185, 81.0122, 86.0921, 93.5975, 164.707, 169.4145, 215.2777, 301.8551, 320.6325, 453.5753, 520.3452, 670.2184, 699.816, 765.3163, 879.8852, 886.6142, 917.8593, 981.4554, 1026.7299, 1058.5703, 1117.1084, 1130.3546, 1157.4048, 1277.5943, 1331.6724, 1353.1368, 1395.0174, 1414.2266, 1428.5259, 1441.7608, 1452.4014, 1467.1711, 1497.9546, 1512.5515, 1574.1802, 1773.1909, 2900.3553, 2992.4337, 3024.0757, 3032.209, 3070.0018, 3071.9048, 3092.2088, 3114.4803, 3138.8741, 3173.8597

8 -0.271685 1.706102 -0.145772	

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.2	**Energy (kJ mol^{-1}):** -421.546725604641
Reaction Coordinates: 6 1.780302 -0.024703 0.689968 6 0.384315 -0.697603 0.638887 6 -0.869276 0.676408 0.643693 6 -0.521350 1.696509 -0.402076 1 0.330648 2.292068 -0.084721 1 -1.377917 2.366501 -0.515531 1 -0.316387 1.233750 -1.360309 6 2.477907 0.153570 -0.653052 1 2.548870 -0.797006 -1.178271 1 3.486145 0.539148 -0.496635 1 1.955774 0.847353 -1.308393 1 0.121222 -1.148874 1.610257 1 1.731948 0.915663 1.243079 1 2.375775 -0.699949 1.310879 1 -0.939790 1.034060 1.667706 8 -1.922846 -0.130517 0.403393 8 -1.826283 -0.668760 -0.799714 8 0.070669 -1.376698 -0.402753	**Frequencies (cm^{-1}):** -465.3972, 83.1955, 112.7145, 173.4238, 205.0201, 245.1094, 263.6383, 306.5101, 315.0381, 371.0628, 523.2907, 552.3252, 640.4458, 698.5914, 779.0574, 819.1216, 889.9091, 960.8098, 1005.3205, 1030.7925, 1059.9733, 1090.2942, 1104.1572, 1157.3531, 1207.7375, 1210.4091, 1290.5772, 1314.1744, 1360.0036, 1394.7551, 1411.5037, 1423.3327, 1451.7662, 1473.8377, 1486.3895, 1495.7252, 1501.8017, 1506.9454, 2903.75, 3020.1905, 3034.0802, 3044.8696, 3047.9559, 3104.2681, 3113.6435, 3120.9821, 3121.8964, 3170.7739
IRC  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.2	**Energy (kJ mol^{-1}):** -421.598881244841
Reaction Coordinates: 6 2.242592 -0.173882 -0.543721 6 1.137718 0.836646 -0.662151 1 0.805370 1.035905 -1.697294 8 0.631297 1.426554 0.265886 6 2.702541 -0.463722 0.877868 1 3.052498 0.442007 1.372212 1 3.515210 -1.189807 0.876760 1 1.886842 -0.868945 1.475396 1 1.880076 -1.076129 -1.046007 1 3.067522 0.191073 -1.167861 6 -1.969147 -0.245984 0.803176	**Frequencies (cm^{-1}):** 34.4011, 39.2154, 66.1622, 84.5421, 88.4878, 98.6929, 171.7936, 172.4224, 245.1941, 255.1205, 300.6495, 454.8323, 668.5725, 671.3097, 672.7391, 764.6795, 850.9917, 884.604, 907.242, 980.9781, 1006.1276, 1058.1955, 1110.3202, 1117.4683, 1142.537, 1285.7294, 1353.0135, 1368.8011, 1395.0399, 1411.8714, 1424.8578, 1441.6054, 1449.6731, 1467.3696, 1494.612,

6 -2.612250 0.818160 0.028930 1 -3.324040 1.368093 0.638342 1 -3.085712 0.384315 -0.854957 1 -1.835122 1.494597 -0.340021 1 -2.074461 -0.370898 1.874762 8 -1.235626 -1.128503 0.285476 8 -1.007785 -1.052741 -1.070855	1501.1559, 1572.6431, 1775.2655, 2917.6717, 3001.9437, 3021.6891, 3039.803, 3041.6395, 3068.314, 3102.3263, 3105.6145, 3138.6306, 3173.1756

Compound: Z-EtCHCHMe + O_3 TS_{SYN} 2.3	**Energy (kJ mol^{-1}):** -421.549400028304
Reaction Coordinates: 6 1.668858 0.574212 -0.003248 6 0.541350 -0.413522 0.342411 6 -0.955481 0.663123 0.605561 6 -1.101048 1.588553 -0.568885 1 -0.438867 2.443448 -0.457370 1 -2.131631 1.952413 -0.587113 1 -0.900999 1.083276 -1.507761 6 3.018277 -0.147382 0.017056 1 3.210240 -0.602983 0.989955 1 3.828786 0.553183 -0.187856 1 3.045167 -0.935176 -0.734960 1 0.648212 -0.826591 1.361043 1 1.484873 0.991902 -0.991624 1 1.677925 1.393230 0.720208 1 -0.855214 1.118707 1.586977 8 -1.817138 -0.367974 0.701885 8 -1.912647 -0.999098 -0.453420 8 0.154757 -1.228093 -0.567074	**Frequencies (cm^{-1}):** -447.1446, 92.8643, 105.2922, 181.1188, 194.2728, 235.7871, 288.3123, 305.1581, 316.2272, 363.268, 491.0615, 531.8951, 606.4045, 709.3256, 792.075, 862.8779, 901.0758, 953.2958, 998.8875, 1025.8471, 1066.8904, 1097.8707, 1119.9234, 1150.9869, 1189.9971, 1212.4343, 1286.9133, 1331.0319, 1356.592, 1395.3581, 1409.3749, 1424.3784, 1438.2018, 1473.5369, 1482.6427, 1494.4735, 1495.9127, 1504.2816, 2896.6084, 3024.2406, 3028.991, 3036.4732, 3080.7535, 3096.029, 3108.0724, 3113.1669, 3125.1493, 3159.7198
IRC  	

Compound: Z-EtCHCHMe + O_3 CPr_{SYN} 2.3	**Energy (kJ mol^{-1}):** -421.597666248278
Reaction Coordinates: 6 -2.081170 -0.279867 -0.420192 6 -1.126153 0.653042 0.268217 6 2.265923 -0.051798 -0.633879 6 2.682980 0.763726 0.509109 1 3.482446 1.444902 0.231141	**Frequencies (cm^{-1}):** 34.0085, 41.9796, 58.9497, 77.72, 85.0036, 98.3234, 154.1378, 171.5929, 213.2412, 300.7512, 344.636, 455.0148, 512.4946, 669.8224, 756.9535, 765.2295, 875.3512, 884.4651, 919.1895, 981.2262,

1 2.977923 0.106923 1.330928 1 1.816324 1.329332 0.864856 6 -3.486922 -0.215923 0.188174 1 -3.463849 -0.422705 1.259334 1 -4.138253 -0.955291 -0.276480 1 -3.938472 0.766399 0.044302 1 -1.093176 0.554347 1.369949 1 -2.090897 -0.051875 -1.485951 1 -1.668680 -1.284587 -0.288183 1 2.603939 0.104266 -1.651904 8 1.476212 -1.026981 -0.533108 8 0.958650 -1.301327 0.713873 8 -0.436769 1.477459 -0.289087	1009.0809, 1058.5425, 1117.1317, 1129.3386, 1162.4371, 1273.7295, 1329.8178, 1353.1604, 1395.2041, 1410.6231, 1428.8666, 1441.7341, 1467.1374, 1469.9637, 1501.8379, 1505.5438, 1572.7884, 1774.7958, 2906.6795, 3021.7024, 3027.2645, 3031.0964, 3068.0737, 3077.5953, 3097.4632, 3099.4044, 3138.8147, 3173.3747

6.19 Ozonolysis of *E*-2-butene (Alkene 17)

Compound: E-MeCHCHMe + O_3 PRC	**Energy (kJ mol^{-1}):** -382.236446263383
Reaction Coordinates: 6 0.899353 -2.059761 -0.233507 6 1.126348 -0.702981 0.346488 6 1.258616 0.421787 -0.373015 6 1.470945 1.783677 0.195458 1 2.396089 2.225974 -0.183389 1 1.515791 1.763446 1.283676 1 0.656295 2.449612 -0.099113 1 1.235012 0.346561 -1.456194 1 1.204206 -0.641103 1.427355 1 1.663445 -2.764642 0.103887 1 -0.061902 -2.468878 0.091693 1 0.906912 -2.038565 -1.322928 8 -1.456886 0.685232 -0.949545 8 -1.865483 -0.144804 -0.081511 8 -1.433558 0.018479 1.098866	**Frequencies (cm^{-1}):** 58.3586, 69.5577, 81.0762, 90.1568, 126.5186, 163.9061, 242.876, 264.4227, 289.7316, 318.6782, 502.6586, 739.653, 771.3887, 874.9868, 984.0216, 991.5663, 1053.6945, 1069.9653, 1083.077, 1149.6834, 1169.4477, 1174.1439, 1328.1025, 1335.5889, 1410.0842, 1413.3125, 1475.7148, 1475.9204, 1482.5652, 1493.5208, 1679.165, 3011.0538, 3016.6008, 3050.4858, 3059.6857, 3094.4754, 3098.2549, 3125.7921, 3139.1112

Compound: E-MeCHCHMe + O_3 TS_{OZO}	**Energy (kJ mol^{-1}):** -382.225772463065
Reaction Coordinates: 6 -1.046677 1.897412 -0.332661 6 0.059065 1.141408 0.329336 6 1.033198 0.474964 -0.364221 6 2.248105 -0.111637 0.268324 1 3.123758 0.509393 0.056798 1 2.452687 -1.105067 -0.131445 1 2.136225 -0.192016 1.348558 1 1.016920 0.527941 -1.446770 1 0.194916 1.288004 1.393561 1 -0.780048 2.955219 -0.422601 1 -1.242606 1.521364 -1.336818 1 -1.967711 1.845308 0.245864 8 -0.053144 -1.525471 -0.703149 8 -1.197710 -1.224115 -0.185209 8 -1.086182 -0.720791 0.999382	**Frequencies (cm^{-1}):** -188.3547, 81.9622, 90.3163, 135.352, 162.7455, 180.6841, 254.1221, 294.6378, 379.805, 479.5723, 503.7301, 739.6787, 803.6502, 872.6806, 956.0153, 996.0356, 1034.6915, 1053.4335, 1074.5121, 1094.6569, 1106.8957, 1177.6518, 1300.688, 1331.9812, 1409.7198, 1410.9994, 1471.1451, 1477.8972, 1484.5723, 1492.2466, 1602.8403, 3013.7441, 3016.9005, 3073.6073, 3073.8089, 3108.7869, 3109.9587, 3148.9688, 3164.9979

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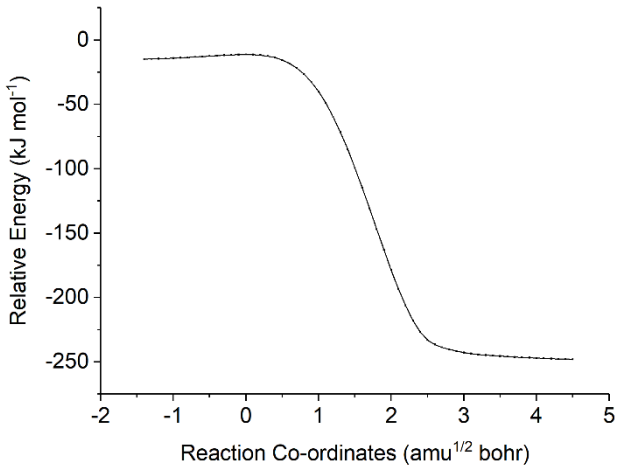
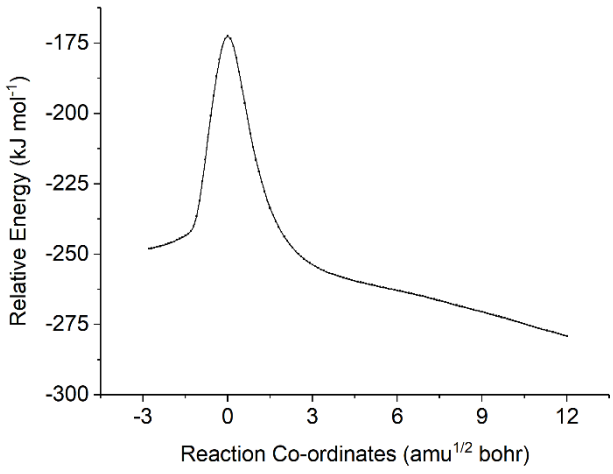


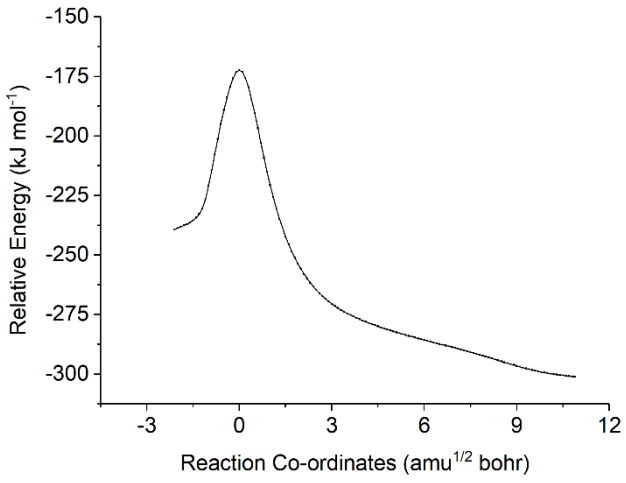
Compound: E-MeCHCHMe + O_3 POZ	**Energy (kJ mol^{-1}):** -382.327078857588
Reaction Coordinates: 6 1.552802 -1.393379 -0.388665 6 0.570268 -0.556745 0.410087 6 -0.755976 -0.254690 -0.350420 6 -2.006228 -0.877494 0.234351 1 -2.126000 -0.592138 1.279081 1 -1.943863 -1.964386 0.171272 1 -2.889129 -0.559370 -0.318865 1 -0.632648 -0.532809 -1.401312 1 0.361936 -1.010346 1.380563 1 1.114307 -2.362878 -0.635399 1 1.816169 -0.887667 -1.317411 1 2.462291 -1.568202 0.184421 8 -0.873681 1.167117 -0.258536 8 0.495158 1.582108 -0.306378 8 1.087491 0.747229 0.718105	**Frequencies (cm^{-1}):** 64.8038, 220.309, 232.5758, 267.1186, 287.8715, 341.1056, 467.6735, 515.0555, 646.2952, 716.2727, 744.8524, 803.9528, 890.906, 899.2291, 937.0789, 1010.3096, 1051.2288, 1090.2497, 1117.0373, 1157.8789, 1172.3666, 1301.6783, 1337.0446, 1366.9887, 1399.4585, 1410.2449, 1415.6693, 1485.2531, 1487.4438, 1497.608, 1501.3611, 3014.0789, 3030.515, 3038.9844, 3052.9045, 3093.5058, 3103.9515, 3112.8106, 3114.6029

Compound: E-MeCHCHMe + O_3 TS_{ANTI}	**Energy (kJ mol^{-1}):** -382.295161272590
Reaction Coordinates: 6 1.982012 0.808100 0.391907 6 0.987127 0.034970 -0.470264 6 -0.686210 0.470036 0.311440 6 -1.266063 1.757674 -0.181327 1 -1.614813 1.657476 -1.207646 1 -0.514404 2.544412 -0.140648 1 -2.103645 2.067487 0.446608 1 -0.344016 0.411206 1.339913 1 0.797515 0.482601 -1.460054 1 2.966448 0.744557 -0.073579 1 1.720916 1.863857 0.478890 1 2.047834 0.362715 1.383574 8 -1.358055 -0.612924 -0.086607 8 -0.789511 -1.715009 0.375186 8 1.015437 -1.241941 -0.423278	**Frequencies (cm^{-1}):** -461.3129, 91.8994, 163.6875, 194.3116, 232.996, 289.5988, 353.4411, 373.2795, 478.6797, 491.976, 547.6361, 622.021, 866.0536, 916.347, 971.0719, 1004.3841, 1020.9138, 1088.6455, 1119.7499, 1152.6565, 1187.8778, 1262.5048, 1340.2856, 1386.3372, 1393.6048, 1423.3211, 1439.6029, 1479.2885, 1480.8882, 1494.1293, 1499.375, 2914.4882, 3030.1394, 3038.0648, 3091.4781, 3098.7484, 3113.2483, 3119.6802, 3132.2864

IRC:



Compound: E-MeCHCHMe + O_3 C_{ANTI}	**Energy (kJ mol^{-1}):** -382.336226600511
Reaction Coordinates: 6 -3.254952 -0.033203 -0.203001 6 -1.786166 -0.012313 0.090147 1 -1.310158 0.981262 0.158031 8 -1.114416 -1.010819 0.245567 1 -3.785193 0.529793 0.569664 1 -3.440921 0.488432 -1.145558 1 -3.635213 -1.050752 -0.254613 6 1.626486 -0.184485 0.340862 6 2.261185 -1.406324 -0.187642 1 2.614081 -1.258390 -1.205145 1 1.531600 -2.219316 -0.163555 1 3.095391 -1.701772 0.453602 1 1.217081 -0.112318 1.342510 8 1.539705 0.830109 -0.384929 8 0.903963 1.950835 0.139721	**Frequencies (cm^{-1}):** 28.4429, 48.3231, 64.7263, 73.094, 87.4988, 122.5109, 163.4894, 188.7282, 264.6646, 323.2547, 512.331, 548.2417, 789.2904, 858.9501, 874.6003, 890.8356, 957.8616, 1075.5635, 1130.1522, 1154.8462, 1163.031, 1350.6001, 1379.4436, 1409.4662, 1448.5499, 1459.1851, 1460.7838, 1464.6933, 1468.236, 1596.7031, 1764.9877, 2949.6237, 3022.0973, 3026.0529, 3072.6207, 3073.4064, 3132.0938, 3136.0207, 3167.7308

Compound: E-MeCHCHMe + O_3 TS_{SYN}	**Energy (kJ mol^{-1}):** -382.296226059565
Reaction Coordinates: 6 2.132171 0.359796 0.464386 6 0.931909 0.400328 -0.468626 6 -0.597681 0.619543 0.556405 6 -1.672387 1.105775 -0.372864 1 -1.644973 0.577929 -1.320843 1 -1.549797 2.174421 -0.540871 1 -2.647102 0.938567 0.091855 1 -0.354940 1.250341 1.406966 1 0.790782 1.361140 -0.992451 1 2.088969 -0.519937 1.104142 1 3.041521 0.295586 -0.135078 1 2.195684 1.256652 1.082583 8 -0.639885 -0.660664 0.979123 8 -0.847443 -1.479948 -0.037499 8 0.651801 -0.640307 -1.163137	**Frequencies (cm^{-1}):** -453.6742, 125.4624, 173.6081, 179.8899, 239.9279, 287.1788, 293.3539, 377.7335, 486.9587, 541.0982, 594.4834, 698.8899, 861.5047, 917.26, 942.6928, 975.2381, 1029.3112, 1072.3249, 1106.1106, 1142.2371, 1184.7656, 1213.9764, 1300.9619, 1395.7229, 1398.5453, 1425.5087, 1434.8039, 1473.7058, 1481.8844, 1495.727, 1496.9769, 2910.6552, 3031.1764, 3036.1403, 3090.7214, 3103.5445, 3117.6852, 3127.8814, 3153.5131
IRC  	

Compound: E-MeCHCHMe + O_3 CPr_{SYN}	**Energy (kJ mol^{-1}):** -382.340232237893
Reaction Coordinates: 6 -2.172479 -0.960228 0.293099 6 -2.286877 0.487923 -0.061300 1 -3.322654 0.867678 -0.177628 8 -1.357784 1.244593 -0.223801 1 -1.136696 -1.275381 0.412009 1 -2.738558 -1.146179 1.210525 1 -2.658302 -1.553438 -0.487401 6 1.530365 0.521866 -0.556862 6 1.830951 1.029386 0.784156 1 0.970935 0.845622 1.432052 1 2.069402 2.088660 0.758532 1 2.651532 0.445553 1.210916 1 1.514447 1.131220 -1.452260 8 1.275161 -0.688463 -0.784525 8 1.237390 -1.540808 0.300663	**Frequencies (cm^{-1}):** 40.5603, 56.762, 67.5313, 81.4719, 99.3918, 104.4479, 161.0049, 178.4108, 296.656, 453.3358, 525.0827, 670.0714, 763.4739, 779.938, 878.408, 893.9095, 985.7711, 1055.5354, 1112.1978, 1143.1897, 1145.9108, 1353.8341, 1388.268, 1396.5767, 1425.9807, 1440.1756, 1461.3315, 1466.1014, 1480.1362, 1575.5534, 1787.6075, 2876.1121, 3009.2685, 3026.5878, 3062.5928, 3071.1226, 3113.9292, 3143.2101, 3181.2549

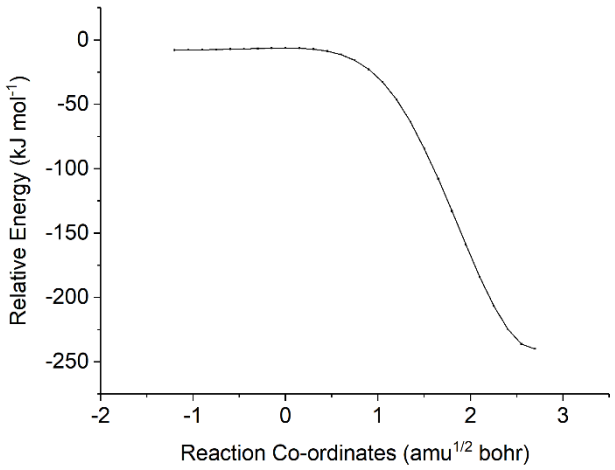
6.19 Ozonolysis of *Z*-2-butene (Alkene 18)

Compound: Z-MeCHCHMe + O_3 PRC1	**Energy (kJ mol^{-1}):** -382.229228168826
Reaction Coordinates: 6 1.594611 -1.581314 -0.370201 6 0.989111 -0.672755 0.651247 6 0.989117 0.672746 0.651251 6 1.594628 1.581305 -0.370192 1 0.866855 2.322125 -0.705141 1 1.963037 1.051473 -1.245483 1 2.431385 2.135662 0.064571 1 0.551279 1.168773 1.510424 1 0.551269 -1.168783 1.510418 1 2.431358 -2.135689 0.064559 1 0.866828 -2.322120 -0.705160 1 1.963032 -1.051480 -1.245486 8 -1.608271 1.076845 -0.254240 8 -2.112165 0.000013 0.180794 8 -1.608294 -1.076839 -0.254221	**Frequencies (cm^{-1}):** 16.2548, 56.2492, 82.7501, 94.2073, 102.5459, 114.1629, 128.3086, 277.87, 301.6874, 411.7046, 574.1599, 720.6377, 741.052, 868.7126, 976.6206, 998.751, 1030.3052, 1058.9184, 1066.0389, 1156.519, 1165.6025, 1176.5569, 1291.1732, 1396.1838, 1416.4702, 1443.1164, 1479.3426, 1482.1056, 1488.2765, 1492.2126, 1663.4207, 3018.9313, 3020.5414, 3066.2352, 3067.0328, 3108.8651, 3121.1368, 3133.9301, 3154.2931

Compound: Z-MeCHCHMe + O_3 TS_{OZO} 1	**Energy (kJ mol^{-1}):** -382.225269220402
Reaction Coordinates: 6 1.460685 1.546710 -0.347977 6 0.775095 0.683188 0.660948 6 0.775100 -0.683186 0.660947 6 1.460697 -1.546701 -0.347978 1 2.509359 -1.696620 -0.071975 1 1.442045 -1.106098 -1.343229 1 0.994053 -2.528700 -0.400661 1 0.391178 -1.182477 1.540972 1 0.391168 1.182475 1.540974 1 2.509354 1.696613 -0.071989 1 1.442011 1.106119 -1.343233 1 0.994051 2.528714 -0.400639	**Frequencies (cm^{-1}):** -126.7195, 58.6512, 92.0451, 92.1884, 156.05, 168.8722, 192.9522, 282.759, 427.4912, 444.997, 579.3511, 733.5891, 751.9695, 880.9069, 956.2804, 1011.7671, 1027.6974, 1040.4947, 1063.9548, 1099.5493, 1118.7908, 1160.4635, 1273.9453, 1393.8061, 1414.0534, 1446.7595, 1473.8856, 1476.0358, 1485.7078, 1495.9745, 1594.0973, 3014.5466, 3014.8489, 3081.2648,

8 -1.369485 -1.074479 -0.266424 8 -1.948857 -0.000005 0.132117 8 -1.369493 1.074473 -0.266425	3082.4632, 3114.3126, 3118.4434, 3158.3962, 3177.8955

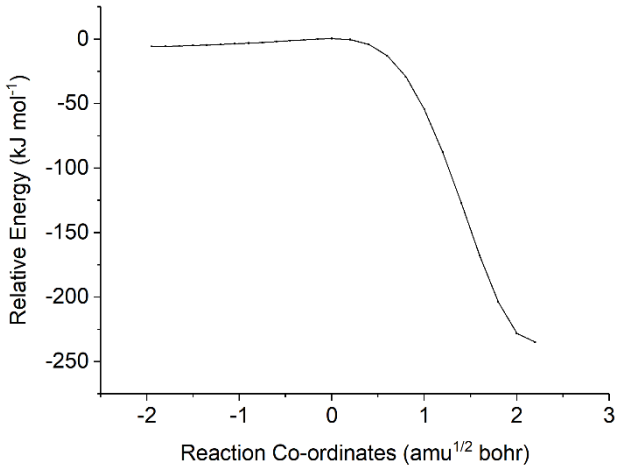
IRC:



Compound: Z-MeCHCHMe + O_3 POZ1	**Energy (kJ mol^{-1}):** -382.325132793566
Reaction Coordinates: 6 -1.392832 1.499076 -0.189052 6 -0.229835 0.785112 0.468761 6 -0.229817 -0.785116 0.468763 6 -1.392793 -1.499109 -0.189059 1 -1.517243 -1.188217 -1.224515 1 -2.315591 -1.297365 0.355138 1 -1.223872 -2.575232 -0.171270 1 -0.108523 -1.126847 1.500178 1 -0.108540 1.126847 1.500174 1 -2.315621 1.297313 0.355154 1 -1.223936 2.575203 -0.171267 1 -1.517285 1.188180 -1.224506 8 0.953256 -1.113052 -0.270391 8 1.818804 0.000023 0.006348 8 0.953225 1.113071 -0.270402	**Frequencies (cm^{-1}):** 42.0681, 217.786, 240.8725, 272.6889, 324.4871, 355.1083, 456.5333, 489.9402, 690.333, 707.6178, 742.0599, 767.8912, 888.6334, 891.9836, 936.8086, 1038.7027, 1038.8919, 1075.434, 1115.7667, 1163.51, 1194.9491, 1328.465, 1341.8476, 1374.6588, 1396.2842, 1418.8497, 1425.166, 1477.6269, 1495.4667, 1496.0745, 1511.8998, 3007.2687, 3029.4442, 3042.5818, 3047.0352, 3103.932, 3106.9928, 3117.9326, 3125.302

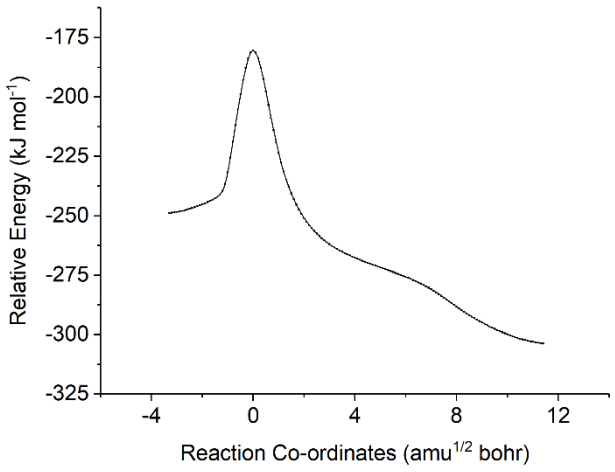
Compound: Z-MeCHCHMe + O_3 PRC 2	**Energy (kJ mol^{-1}):** -382.231445320259
Reaction Coordinates: 6 -1.710958 1.584226 -0.379563 6 -1.072263 0.670414 0.619644 6 -1.072322 -0.670316 0.619695 6 -1.711114 -1.584150 -0.379431 1 -0.988692 -2.310762 -0.756827 1 -2.136706 -1.056951 -1.230670 1 -2.512753 -2.160579 0.091186 1 -0.583786 -1.163590 1.451924 1 -0.583684 1.163709 1.451836 1 -2.512515 2.160805 0.091010 1 -0.988452 2.310711 -0.757046 1 -2.136631 1.056994 -1.230740 8 1.849154 -1.077159 0.127274	**Frequencies (cm^{-1}):** 6.413, 41.3805, 47.2305, 70.6879, 99.9927, 120.8342, 127.4886, 228.7989, 290.0326, 411.0696, 572.9587, 712.183, 742.3021, 866.9998, 976.4639, 1002.2744, 1028.0497, 1061.2945, 1065.6396, 1162.3368, 1169.9433, 1193.5159, 1294.8591, 1395.7512, 1416.9709, 1442.2763, 1480.5241, 1483.9126, 1490.2773, 1493.2641, 1679.781, 3017.2871, 3019.0741, 3058.9747, 3059.3398, 3103.344, 3115.1089, 3140.9575, 3160.6417

8 2.031893 -0.000018 -0.503902 8 1.849349 1.077005 0.127534	

Compound: Z-MeCHCHMe + O_3 TS_{OZO} 2	**Energy (kJ mol^{-1}):** -382.222466209398
Reaction Coordinates: 6 1.387324 1.529584 -0.400625 6 0.775662 0.685788 0.674014 6 0.775681 -0.685766 0.674016 6 1.387375 -1.529550 -0.400614 1 2.478075 -1.540950 -0.302784 1 1.161084 -1.149252 -1.397051 1 1.038530 -2.557876 -0.340926 1 0.494581 -1.183917 1.590545 1 0.494552 1.183934 1.590542 1 2.478025 1.540995 -0.302820 1 1.161014 1.149287 -1.397059 1 1.038467 2.557904 -0.340926 8 -1.451206 -1.073518 0.130315 8 -1.635120 -0.000017 -0.558186 8 -1.451246 1.073478 0.130337	**Frequencies (cm^{-1}):** -179.9205, 43.8862, 124.2775, 137.72, 168.9872, 173.3792, 182.0554, 276.102, 463.5741, 471.5026, 586.5898, 738.3545, 757.4602, 882.7404, 957.6907, 1013.7444, 1023.7251, 1036.9449, 1066.0898, 1084.4722, 1108.6346, 1156.9499, 1262.4221, 1394.0517, 1415.8244, 1441.2058, 1476.8589, 1478.9441, 1483.9517, 1494.4465, 1573.8758, 3007.8466, 3009.2464, 3070.5035, 3071.2607, 3116.4031, 3118.3456, 3178.0145, 3195.2417
IRC:  	

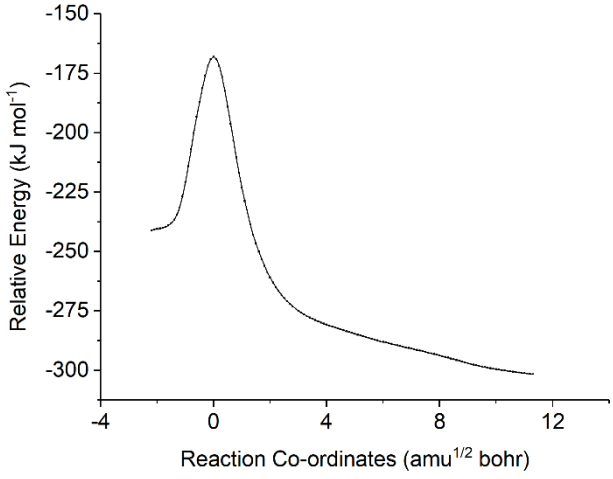
Compound: Z-MeCHCHMe + O_3 POZ 2	**Energy (kJ mol^{-1}):** -382.324192708349
Reaction Coordinates: 6 1.470219 1.296843 -0.298783 6 0.785023 0.254289 0.567603 6 -0.784924 0.254580 0.567607 6 -1.469738 1.297365 -0.298800 1 -1.180615 1.197178 -1.343262 1 -1.227382 2.306792 0.035484 1 -2.549075 1.170177 -0.227928 1 -1.152923 0.312605 1.592608 1 1.153048 0.312155 1.592603 1 1.228241 2.306351 0.035533 1 2.549509 1.169251 -0.227924 1 1.181049 1.196793 -1.343245 8 -1.112008 -1.078196 0.143258 8 -0.000273 -1.416927 -0.703932	**Frequencies (cm^{-1}):** 38.0005, 223.0042, 262.0402, 279.9635, 296.2165, 393.5632, 465.8663, 510.717, 698.1451, 704.8326, 760.4771, 764.8873, 879.3777, 900.4635, 932.0543, 1026.3986, 1043.613, 1047.2818, 1088.068, 1153.8241, 1160.3873, 1304.9292, 1310.2585, 1374.0934, 1382.1807, 1412.317, 1416.8266, 1478.9981, 1491.6342, 1499.5966, 1509.4278, 3039.3843, 3045.313, 3052.3473, 3068.0879, 3100.7529, 3106.1756, 3117.9367, 3125.8741

8 1.111615 -1.078598 0.143220	

Compound: Z-MeCHCHMe + O_3 TS_{ANTI}	**Energy (kJ mol^{-1}):** -382.296039569149
Reaction Coordinates: 6 -0.741319 -1.747586 -0.608345 6 -0.734657 -0.709330 0.503511 6 0.849341 0.284438 0.409615 6 2.086490 -0.511244 0.135651 1 2.087797 -0.906204 -0.878105 1 2.157592 -1.340297 0.838180 1 2.971787 0.113809 0.268115 1 0.759626 0.775905 1.373132 1 -0.483689 -1.104330 1.503252 1 -0.741813 -1.264419 -1.584138 1 0.104154 -2.432462 -0.539282 1 -1.657173 -2.334566 -0.525864 8 0.464558 1.067467 -0.610475 8 -0.585439 1.796425 -0.262622 8 -1.623795 0.210470 0.485862	**Frequencies (cm^{-1}):** -450.9137, 116.6802, 167.919, 191.7874, 227.3382, 280.7835, 340.4079, 366.0788, 482.1771, 519.0225, 582.5343, 624.7029, 844.0629, 913.3318, 960.6072, 1004.8262, 1032.13, 1116.4549, 1117.7743, 1147.9238, 1180.4388, 1261.693, 1310.7033, 1386.1431, 1397.3511, 1421.6919, 1437.8482, 1478.149, 1482.1633, 1493.9688, 1499.6401, 2902.6942, 3035.189, 3038.3987, 3094.1163, 3099.0198, 3117.0922, 3121.6752, 3135.561
IRC:  	

Compound: Z-MeCHCHMe + O_3 C_{ANTI}	**Energy (kJ mol^{-1}):** -382.336899685096
Reaction Coordinates: 6 2.343775 0.721478 0.120516 6 2.169715 -0.758425 0.028389 1 3.097053 -1.356608 0.135989 8 1.118323 -1.331528 -0.149821 1 1.399571 1.256080 0.007787 1 2.805386 0.961770 1.083103 1 3.059259 1.039533 -0.643935 6 -1.455772 -0.146320 -0.358444 6 -2.141036 -1.342437 0.166753 1 -2.517854 -1.169482 1.171743 1 -1.438274 -2.178122 0.172056	**Frequencies (cm^{-1}):** 42.9772, 75.8743, 80.8582, 103.8231, 118.0927, 133.2153, 179.3389, 199.657, 270.7004, 325.2615, 532.6896, 550.0271, 781.9405, 865.21, 876.4563, 896.8721, 960.332, 1074.5883, 1145.2725, 1152.4784, 1162.7796, 1349.0463, 1389.7674, 1409.4093, 1425.1553, 1459.1251, 1466.4471, 1468.0809, 1480.0693, 1592.9126, 1781.7088, 2882.7063, 2999.1247, 3026.4688,

1 -2.968033 -1.617249 -0.493195 1 -1.008267 -0.100555 -1.344954 8 -1.387401 0.884997 0.347305 8 -0.722038 1.986387 -0.176469	3060.1949, 3076.741, 3094.4859, 3135.6023, 3170.0262

Compound: Z-MeCHCHMe + O_3 TS_{SYN}	**Energy (kJ mol^{-1}):** -382.292399119526
Reaction Coordinates: 6 2.174760 0.183728 0.008248 6 0.909299 -0.602714 0.362039 6 -0.401201 0.707424 0.605689 6 -0.369631 1.641351 -0.570465 1 -0.242545 1.107566 -1.506342 1 0.425467 2.372500 -0.447937 1 -1.323311 2.174340 -0.605298 1 -0.244369 1.142285 1.589103 1 0.937517 -1.012702 1.385146 1 2.379704 0.970858 0.734485 1 3.009493 -0.517832 0.027093 1 2.110787 0.605837 -0.991453 8 -1.420990 -0.168444 0.685470 8 -1.592712 -0.781138 -0.470976 8 0.397188 -1.353117 -0.541728	**Frequencies (cm^{-1}):** -465.7696, 104.6257, 190.1491, 226.6786, 263.2551, 304.7061, 309.9565, 361.0558, 483.5747, 527.3944, 574.4322, 702.2875, 862.2176, 907.7514, 951.0997, 1000.5877, 1023.4662, 1078.6887, 1103.5071, 1152.076, 1198.078, 1212.5444, 1344.5156, 1388.517, 1396.7728, 1424.2704, 1436.318, 1470.2561, 1487.4215, 1494.1252, 1502.7881, 2914.2447, 3035.4291, 3037.0332, 3095.3983, 3112.3989, 3125.0849, 3132.9402, 3159.3922
IRC  	

Compound: Z-MeCHCHMe + O_3 CPr_{SYN}	**Energy (kJ mol^{-1}):** -382.341847196068
Reaction Coordinates: 6 -2.575388 -0.475137 -0.224658 6 -1.656799 0.539062 0.382613 1 -1.558708 0.485092 1.481750 8 -1.055700 1.384963 -0.240999 1 -2.640652 -0.350326 -1.303167 1 -2.200388 -1.470587 0.020789 1 -3.567732 -0.382682 0.224597	**Frequencies (cm^{-1}):** 44.5356, 61.3265, 85.2874, 89.2671, 100.2886, 127.2994, 171.6681, 196.4532, 300.2958, 455.0499, 513.2373, 669.8265, 764.9019, 779.3715, 884.3228, 892.1279, 981.2246, 1058.843, 1116.8874, 1127.3066, 1135.3539, 1353.0833, 1374.0802, 1395.2676, 1427.7885,

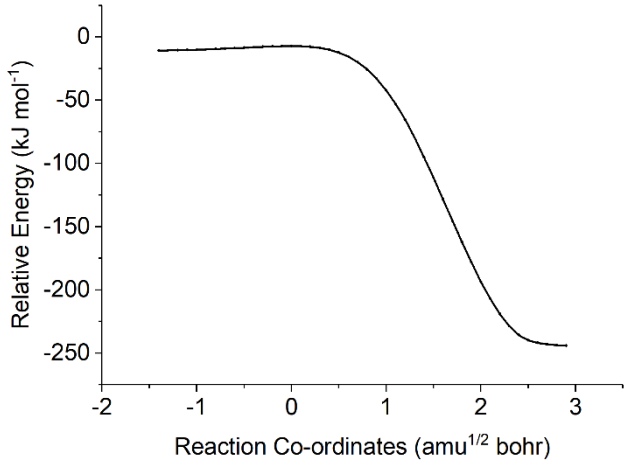
6 1.704683 -0.009558 -0.693935 6 2.140169 0.870844 0.392701 1 1.266121 1.406451 0.775659 1 2.887025 1.579181 0.045049 1 2.513051 0.262837 1.220399 1 1.979315 0.121918 -1.734281 8 0.973295 -1.018077 -0.513133 8 0.538153 -1.267281 0.770243	1441.5812, 1461.2162, 1467.253, 1472.0736, 1572.9701, 1778.6069, 2923.9538, 3021.7811, 3025.2706, 3068.0434, 3084.0704, 3131.4128, 3138.9098, 3173.2592

Compound: Z-MeCHCHMe + O_3 TS_{POZ} 1	**Energy (kJ mol^{-1}):** -382.321485722886
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.182724 1.775886 -0.581804 1 0.216392 1.291005 -1.555960 6 -0.711469 -0.427476 0.455564 6 -2.140921 -0.148666 0.038491 1 -2.184398 0.354061 -0.925402 1 -2.625930 0.477676 0.787747 1 -2.699210 -1.080915 -0.032187 1 -0.683507 -0.965346 1.408878 1 0.203425 1.229747 1.520810 1 -0.735938 2.359624 -0.510990 1 1.025735 2.461374 -0.507721 6 0.262300 0.754210 0.539789 8 -0.101772 -1.220853 -0.559332 8 1.505872 0.057283 0.561212 8 1.336854 -1.067799 -0.364058	-134.2804, 163.7151, 205.7858, 226.8465, 259.4079, 333.162, 408.2272, 516.3173, 673.3651, 710.3546, 779.2753, 804.8931, 853.5614, 888.3796, 962.0843, 1005.0111, 1039.3048, 1087.6986, 1113.4352, 1164.2126, 1180.9661, 1282.1568, 1339.0451, 1369.728, 1387.8416, 1415.3228, 1418.4199, 1483.0492, 1492.0999, 1499.5139, 1507.2902, 3005.7406, 3040.9999, 3046.1081, 3058.5875, 3103.8353, 3108.2972, 3121.6559, 3125.1516
IRC Energy too low for IRC to take place	

6.20 Ozonolysis of 2-methylpropene (Alkene 20)

Compound: $(CH_3)_2CCH_2$ + O3 PRC	**Energy (kJ mol^{-1}):** -382.236083327848
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.824158 -0.601839 1.158834 6 -1.319940 0.285715 0.056344 6 -0.596484 1.385252 0.304018 6 -1.725130 -0.100766 -1.336310 1 -0.270135 2.038674 -0.492606 1 -0.335408 1.675152 1.313372 1 -1.388262 -1.112792 -1.571671 1 -1.314691 0.578560 -2.080906 1 -2.814789 -0.101504 -1.431201 1 -2.917807 -0.602590 1.176838 1 -1.514282 -1.637045 1.000280 1 -1.467942 -0.279619 2.136015 8 2.237554 0.768557 -0.080777 8 2.080016 -0.423044 0.301886 8 1.284628 -1.141640 -0.364538	13.2204, 44.2658, 61.6635, 66.7373, 108.93, 160.9186, 204.0624, 233.4983, 382.3804, 438.6805, 447.2956, 705.214, 742.4158, 814.159, 935.0968, 961.2337, 989.6545, 1014.287, 1085.9076, 1104.8397, 1169.5686, 1195.7772, 1301.4263, 1410.1072, 1414.8522, 1439.8801, 1470.9504, 1480.9185, 1489.411, 1503.1939, 1671.4078, 3013.1628, 3018.4672, 3058.355, 3061.3415, 3104.211, 3110.2042, 3138.3913, 3221.9192

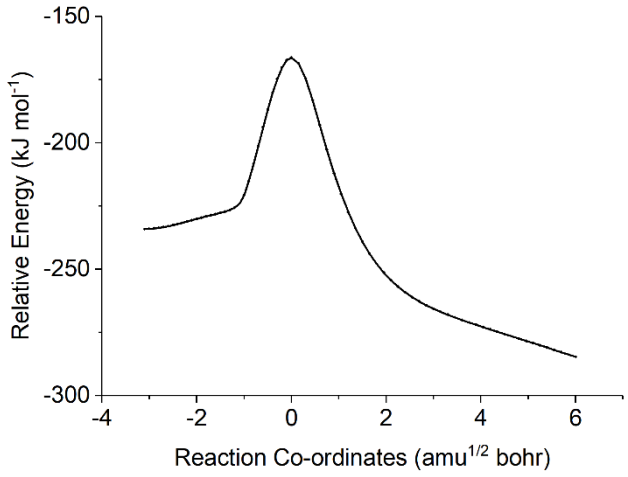
Compound: $(CH_3)_2CCH_2$ + O_3 TS_{ozo}	**Energy (kJ mol^{-1}):** -382.225921208913
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.435640 -0.838117 1.086069 6 -0.976739 0.241742 0.146859 6 -0.197860 1.276256 0.598455 6 -1.650320 0.314019 -1.191081 1 -0.043102 2.156252 -0.006361 1 0.103465 1.335294 1.633905 1 -1.626613 -0.650809 -1.697239 1 -1.183015 1.055588 -1.835653 1 -2.702774 0.585158 -1.061880 1 -2.427837 -0.589263 1.476145 1 -1.518134 -1.799148 0.580955 1 -0.763404 -0.946041 1.936181 8 1.898487 0.685989 0.069088 8 1.737168 -0.592289 0.076333 8 0.829941 -0.982503 -0.753904	-200.6631, 61.9624, 130.0607, 170.9458, 185.1998, 195.7286, 212.0207, 390.6483, 429.2649, 450.2241, 474.3117, 741.9401, 775.7663, 808.4966, 949.5694, 954.9689, 986.7612, 1020.5955, 1067.2692, 1080.8425, 1087.3552, 1122.3664, 1308.4295, 1409.1944, 1409.6658, 1426.1079, 1472.0263, 1480.6726, 1487.4262, 1503.5581, 1582.3866, 3011.6863, 3017.2626, 3076.1051, 3078.4167, 3114.0848, 3118.9519, 3156.4788, 3246.2811
IRC	



Compound: $(CH_3)_2CCH_2$ + O3 POZ	**Energy (kJ mol^{-1}):** -382.327176695013
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.293510 1.195388 0.644156 6 0.602622 -0.015200 0.027727 6 -0.462424 -0.624090 0.994698 6 1.585534 -1.040703 -0.519289 1 -0.294166 -1.679424 1.202030 1 -0.512860 -0.056636 1.926309 1 2.199791 -0.598452 -1.303423 1 1.055890 -1.896432 -0.935451 1 2.249191 -1.386277 0.273928 1 1.831727 0.911070 1.550333 1 2.007626 1.624466 -0.058060 1 0.559666 1.956642 0.905660 8 -1.692465 -0.541174 0.287162 8 -1.492573 0.654548 -0.497622 8 -0.216502 0.390709 -1.095174	80.0602, 222.7854, 258.4457, 285.5419, 335.1301, 379.6914, 404.4257, 489.6463, 606.3722, 701.6879, 745.0957, 806.7591, 880.0871, 924.237, 934.6973, 962.0069, 981.4057, 1010.6615, 1042.6659, 1184.2543, 1209.9053, 1243.3396, 1290.8022, 1354.3792, 1404.1802, 1421.3895, 1480.4039, 1488.7181, 1497.9931, 1504.6803, 1512.8664, 3030.0927, 3033.6991, 3039.9606, 3094.5957, 3103.0264, 3106.5376, 3113.4511, 3114.5155

Compound: $(CH_3)_2CCH_2$ + O_3 TS_{DMFO}	**Energy (kJ mol^{-1}):** -382.297810552684
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.930711 0.436070 -0.595089 6 -0.646102 -0.052458 0.015149 6 0.621471 1.316250 0.071448 6 -0.694106 -0.578627 1.427775 1 0.215141 1.778140 0.983666 1 0.401271 1.870563 -0.851894 1 -1.313597 0.073392 2.040732 1 0.298352 -0.656845 1.858313 1 -1.146215 -1.573775 1.414010 1 -2.261384 1.341634 -0.088006 1 -1.800566 0.652787 -1.653481 1 -2.716400 -0.313618 -0.482312 8 1.746576 0.722655 0.172754 8 1.220571 -1.175188 -0.384344 8 0.060364 -0.784928 -0.880502	-451.3844, 161.9753, 177.7789, 194.0767, 244.9575, 301.2076, 326.3375, 377.7665, 397.314, 527.9858, 565.0285, 641.4867, 787.8394, 880.9253, 959.7992, 990.7402, 997.4451, 1031.5578, 1139.43, 1178.3834, 1222.2873, 1285.0709, 1292.5411, 1367.7344, 1404.2913, 1419.738, 1469.6832, 1480.3633, 1492.504, 1502.8754, 1534.2718, 2921.1346, 2983.4244, 3032.4621, 3037.4782, 3097.404, 3105.2941, 3126.0785, 3157.7927

IRC

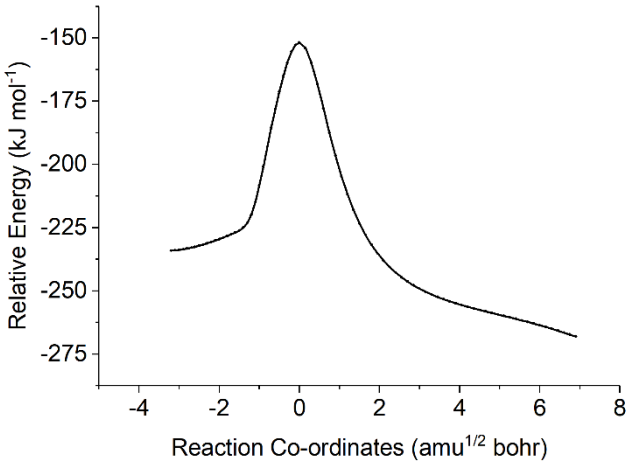


Compound: $(CH_3)_2CCH_2$ + O3 C_{DMFO}	**Energy (kJ mol^{-1}):** -382.341486411877
Reaction Coordinates: 6 -2.043458 -0.874161 -0.631204 6 -1.072495 0.054887 -0.001042 6 -0.962731 0.253805 1.455502 1 -1.771821 -0.247035 1.980591 1 -0.946788 1.325195 1.665337 1 -0.000909 -0.136396 1.793214 8 -0.346508 0.708157 -0.802479 8 0.619741 1.545799 -0.254407 1 -1.966081 -0.844589 -1.714628 1 -3.059965 -0.618029 -0.324049 1 -1.846212 -1.889599 -0.280290 6 2.284541 -0.339339 -0.107437 1 2.754133 0.306828 0.649986 1 2.513721 -0.091917 -1.154964 8 1.612865 -1.300908 0.193122	**Frequencies (cm^{-1}):** 61.1756, 85.7419, 95.0671, 124.8024, 156.5813, 163.4536, 233.0177, 305.5814, 313.9084, 368.3302, 388.7124, 481.4006, 594.9426, 812.1856, 913.2456, 932.1036, 987.7618, 1073.9019, 1098.2539, 1165.9873, 1258.6409, 1306.1315, 1386.4409, 1405.6594, 1445.758, 1457.9145, 1469.8317, 1481.8062, 1526.0821, 1571.4298, 1760.5409, 2933.9772, 2994.1048, 3028.9861, 3037.1841, 3077.8226, 3088.8812, 3138.2306, 3141.3182

Compound: $(CH_3)_2CCH_2$ + O_3 TS_{FO}	**Energy (kJ mol^{-1}):** -382.292467755139
Reaction Coordinates: 6 1.186010 1.459163 0.013213 6 0.730152 0.008980 0.203404 6 -0.582798 -0.257857 -1.111567 6 1.754319 -1.054703 -0.230514 1 -0.622491 -1.339814 -1.096221 1 -0.297127 0.240825 -2.030129 1 2.043274 -0.951734 -1.277036 1 1.359786 -2.052457 -0.051484 1 2.650458 -0.927795 0.379048 1 1.601803 1.638325 -0.978985 1 0.356888 2.141148 0.189547 1 1.962247 1.675933 0.749201 8 -1.600834 0.353308 -0.515223 8 -1.909782 -0.273767 0.606306	**Frequencies (cm^{-1}):** -448.4063, 105.6065, 197.3812, 223.1851, 256.7873, 295.2322, 297.1893, 406.6525, 487.1599, 493.27, 552.0641, 606.1783, 769.8578, 888.663, 914.2972, 981.6376, 1000.5277, 1056.9223, 1066.2426, 1160.2609, 1182.0942, 1222.9942, 1267.5665, 1379.3347, 1397.6846, 1412.6804, 1473.0153, 1481.7119, 1486.9202, 1493.1104, 1504.0795, 3028.8231, 3033.7111, 3088.3762, 3093.6254, 3104.4006, 3122.7197, 3124.3114, 3221.8747

8 0.062999 -0.249282 1.267522	

IRC



Compound: $(CH_3)_2CCH_2$ + O3 C_{FO}	**Energy (kJ mol^{-1}):** -382.334939529468
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.027434 -0.206214 -0.032585 6 -1.523681 -0.059575 0.009154 6 -0.973876 1.342228 -0.040487 1 -1.506913 1.984490 0.663305 1 0.096331 1.364295 0.160651 1 -1.156900 1.756174 -1.036238 8 -0.806720 -1.040626 0.077180 1 -3.455815 0.202623 0.885706 1 -3.447739 0.369470 -0.858970 1 -3.304803 -1.252663 -0.125160 6 1.868621 -1.133264 0.148599 1 1.808896 -2.040853 -0.434867 1 1.576975 -1.054498 1.186321 8 2.330170 -0.136076 -0.443598 8 2.392574 1.053191 0.247814	31.9742, 54.7165, 81.1514, 84.3169, 99.2779, 112.666, 155.0764, 205.748, 395.907, 498.6377, 518.5888, 547.041, 680.6712, 791.9739, 860.1657, 890.2118, 906.0155, 994.0329, 1092.057, 1124.4266, 1234.7156, 1246.5682, 1388.5228, 1401.6351, 1414.0699, 1462.2137, 1465.6447, 1477.1367, 1495.2706, 1568.4278, 1752.3072, 3015.2894, 3031.9002, 3073.2498, 3085.3958, 3110.8754, 3134.6449, 3139.0544, 3278.2398

7.0 Cartesian Coordinates for Chapter 4: Criegee Intermediate–Alcohol Reactions

7.1 sCI 1 + Alcohol Reactions

7.1.1 sCI 1 + MeOH Reactions

MeOH

```
C    0.00000000  0.00000000  0.00000000
O    1.41624500  0.14257700  0.00000000
H    1.81886800 -0.72978900 -0.00002400
H   -0.35919900 -0.52416200 -0.89057100
H   -0.35934200 -0.52335600  0.89097500
H   -0.41607300  1.00533100 -0.00052400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -115.607114913569

Frequencies (cm^{-1}): 297.0572, 1039.0836, 1076.1933, 1170.4398, 1365.9554, 1477.1085, 1498.2639, 1508.9046, 2995.0446, 3040.4839, 3109.1615, 3828.974

CH_2OO (CI1)

```
C    0.00000000  0.00000000  0.00000000
O   -1.06987500  0.65393400  0.00000000
O   -2.24787900 -0.00864800  0.00000000
H   -0.03946100 -1.08236700  0.00000000
H    0.90449400  0.59146700  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -189.400847103496

Frequencies (cm^{-1}): 527.7246, 674.2281, 912.6314, 951.0264, 1242.0203, 1401.9254, 1543.4142, 3118.0445, 3267.4287

CH_2OO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2)

```
C    0.00000000  0.00000000  0.00000000
O    2.95160400 -0.59761700 -0.00042000
C    4.29806900 -1.04512300  0.00022800
H    4.52809900 -1.63979100  0.88944700
H    4.93763300 -0.16376200  0.00108100
H    4.52923200 -1.63890600 -0.88929600
O   -0.31370400 -1.21237700  0.00017400
O    0.66271900 -2.16922400 -0.00016400
H    2.33453100 -1.35459000 -0.00031000
H    1.04371100  0.30178900 -0.00037800
H   -0.84482200  0.67609900  0.00031900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.020987896971

Frequencies (cm^{-1}): 19.7054, 80.9009, 105.299, 110.7152, 135.7651, 259.741, 549.9878, 664.5084, 696.053, 879.2877, 1019.6283, 1061.1237, 1138.5179, 1172.6095, 1273.2345, 1421.2527, 1449.7641, 1477.2118, 1497.4926, 1511.8731, 1560.5798, 2992.9731, 3037.736, 3082.7637, 3095.3056, 3244.2556, 3518.8918

CH_2OO + MeOH TS-AAAH 1

```
C    0.00000000  0.00000000  0.00000000
O    1.63613800 -1.01061900 -0.51440300
C    2.56561900 -1.22277800  0.55109800
H    2.05546200 -1.27749200  1.51531900
H    3.27309400 -0.39630600  0.55145500
H    3.10206300 -2.15775000  0.38446700
O   -0.49810200 -0.88369000  0.76322000
O   -0.55929500 -2.12124200  0.00861400
H    0.91994200 -1.75332000 -0.47169000
H   -0.23462000 -0.00917500 -1.05618800
H    0.32576400  0.91215100  0.49053100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.012537386425

Frequencies (cm^{-1}): -304.0447, 135.2585, 152.1383, 189.4437, 331.8347, 453.8557, 543.758, 800.4178, 866.8398, 1006.8807, 1113.3556, 1166.2474, 1182.2002, 1211.2361, 1252.7362, 1381.3901, 1465.1548, 1490.5141, 1494.4322, 1518.3036, 1546.3545, 2565.4312, 3022.158, 3082.7073, 3101.6811, 3117.2132, 3225.5418

$MeOCH_2OOH$ (TS-AAAH 1 conformer)

```
C     0.00000000  0.00000000  0.00000000
O     0.97684800 -0.83211100 -0.54740700
C     1.92297700 -1.32704700  0.39576900
H     1.44354000 -1.93321500  1.16735200
H     2.46169100 -0.50231000  0.87300900
H     2.62796300 -1.94084900 -0.15913500
O    -0.94781700 -0.68552200  0.78901900
O    -1.82402300 -1.42033900 -0.10166700
H    -1.30761600 -2.22148400 -0.27269700
H    -0.49670700  0.49467900 -0.83269200
H     0.42832600  0.72435200  0.70287200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.089756012820

Frequencies (cm^{-1}): 107.063, 139.5145, 198.2164, 256.5252, 337.928, 479.6946, 625.7444, 876.011, 931.6294, 997.0373, 1090.2579, 1166.9358, 1175.9712, 1228.5458, 1319.5406, 1378.6071, 1404.2061, 1465.4227, 1483.4622, 1491.9143, 1509.5191, 2998.8963, 3004.8504, 3060.7731, 3106.2569, 3124.7939, 3733.5712

IRC:

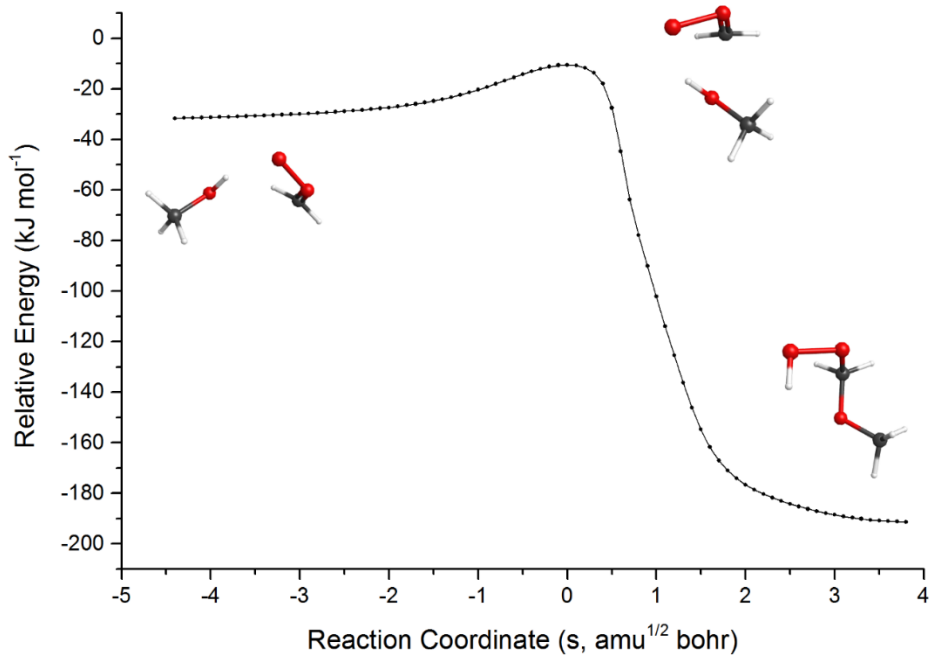


Figure S29: CI1 + MeOH TS1 IRC

CH_2OO + MeOH TS-AAAH 2

```
C     0.00000000  0.00000000  0.00000000
O     1.51316500 -0.97623500 -0.83125600
C     2.70308200 -1.12816300 -0.06403000
H     3.21801700 -2.04237500 -0.36352900
H     3.34859300 -0.27429100 -0.26030900
H     2.48970300 -1.18473300  1.00759300
O    -0.90019700 -0.75919600 -0.46981600
O    -0.57412200 -2.11709700 -0.06988000
H     0.85427900 -1.74828400 -0.61331300
H     0.42033100 -0.21181500  0.97622800
H     0.02771700  1.00235400 -0.41462200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.010696838391

Frequencies (cm^{-1}): -314.0631, 108.0485, 162.098, 201.1445, 340.2037, 430.9942, 528.5951, 805.8632, 868.3201, 1023.6243, 1085.2333, 1163.6515, 1178.5415, 1213.3036, 1229.4267, 1382.3248, 1466.0463, 1495.1125, 1496.4904, 1518.162, 1588.6707, 2479.8, 3006.7795, 3069.2072, 3093.6827, 3111.2056, 3215.0493

$MeOCH_2OOH$ (TS-AAAH 2- conformer)

```
C     0.00000000  0.00000000  0.00000000
O     0.85819200 -0.88261500 -0.68186500
C     2.14503000 -0.98007600 -0.09578700
H     2.70262300 -1.71268000 -0.67371100
```

```
H     2.67644400 -0.02276300 -0.13002400
H     2.08430000 -1.31383600  0.94583100
O    -1.29634300 -0.14992500 -0.48070500
O    -1.81011100 -1.41552500  0.00699900
H    -1.47182000 -2.02603200 -0.66476700
H     0.03856200 -0.18801700  1.07978200
H     0.24400800  1.04652300 -0.22100200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.086311352255

Frequencies (cm^{-1}): 65.4552, 149.8986, 212.3498, 293.673, 338.5774, 404.0039, 593.085, 884.6145, 980.6794, 1062.9644, 1112.8846, 1150.2276, 1182.3539, 1223.7494, 1285.9793, 1379.9794, 1420.3924, 1473.8978, 1493.344, 1495.0447, 1510.5595, 2974.1783, 2986.7853, 3021.754, 3029.6421, 3122.1827, 3732.2853

IRC:

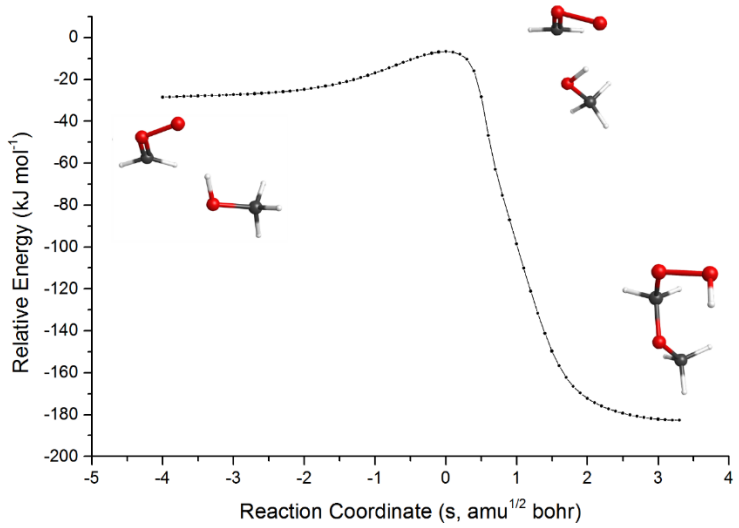


Figure S30: CI1 + MeOH TS2 IRC

7.1.2 sCI 1 + EtOH Reactions

EtOH

```
C    0.00000000  0.00000000  0.00000000
C   -1.29275100  0.79694500  0.06803400
O   -2.45713100 -0.01435600 -0.08782100
H   -2.48887000 -0.65366100  0.63022800
H   -1.33831900  1.51829600 -0.74772400
H   -1.34470200  1.36140700  1.00590300
H    0.06802800 -0.54407300 -0.94219300
H    0.86366500  0.66316300  0.08031000
H    0.05982700 -0.72255100  0.81735300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -154.868522279987

Frequencies (cm^{-1}): 255.8377, 266.0191, 420.0526, 805.1083, 881.3913, 1057.0411, 1066.4055, 1131.6148, 1279.2047, 1368.3146, 1402.6096, 1415.6213, 1488.0281, 1492.9965, 1516.8863, 2990.3833, 3020.1257, 3064.6811, 3085.1337, 3099.1308, 3810.9009

EtOH (conformer 2- unused):

```
C    0.00000000  0.00000000  0.00000000
C    1.18725800  0.96509800  0.00000000
O    2.39445400  0.19298900 -0.00000000
H    3.14773500  0.79078500 -0.00000000
H    1.16080200  1.61114600  0.88290700
H    1.16080200  1.61114600 -0.88290700
H    0.37455500 -1.02297100 -0.00000000
H   -0.62718200  0.12639300  0.88152000
H   -0.62718200  0.12639300 -0.88152000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -154.865295342549

Frequencies (cm^{-1}): 232.0393, 276.7567, 416.5451, 820.5593, 894.1636, 1028.6088, 1096.0585, 1177.865, 1265.0334, 1298.7948, 1404.6379, 1445.8158, 1482.8381, 1500.0914, 1526.0788, 2981.833, 3005.3878, 3034.5674, 3098.7534, 3103.1493, 3825.9958

CH_2OO + EtOH PRC (For TS-AAAH 1.1 and TS-AAAH 1.3):

```
C    0.00000000  0.00000000  0.00000000
C   -0.71103700 -0.99171100 -0.90837100
O   -2.07120500 -1.19915700 -0.54179300
H   -2.59209400 -0.38250500 -0.66764400
H   -0.23235400 -1.97004900 -0.84836600
H   -0.64768800 -0.66230600 -1.95153500
H   -0.03748700 -0.33341200  1.03748900
H    1.04713400  0.10343900 -0.29242600
H   -0.46459500  0.98585900 -0.05839400
C   -5.05823000 -1.39104700 -0.18112300
O   -5.24210500 -0.18039300 -0.44334300
O   -4.17379800  0.62531500 -0.72358700
H   -4.05574400 -1.81017400 -0.17797400
H   -5.96600400 -1.94217300  0.02653800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.282343872339

Frequencies (cm^{-1}): 20.7138, 50.2805, 81.5897, 98.5166, 126.8539, 222.6442, 281.0594, 431.2829, 548.9501, 659.8925, 695.5439, 809.1907, 878.9596, 886.8034, 1019.8855, 1062.3046, 1112.7366, 1148.3084, 1271.8796, 1302.9503, 1394.2504, 1410.4393, 1422.797, 1448.2678, 1489.6911, 1494.4892, 1517.0064, 1559.2397, 2991.0048, 3023.3678, 3056.0963, 3080.9753, 3085.2874, 3096.9711, 3243.4395, 3520.5309

CH_2OO + EtOH TS-AAAH 1.1:

```
C    0.00000000  0.00000000  0.00000000
C   -1.12886600 -0.96967000 -0.29593800
O   -2.11896200 -0.93643400  0.74729700
H   -2.56244600 -0.00806600  0.73959600
H   -0.76584400 -1.99656900 -0.33825100
H   -1.60077000 -0.72696400 -1.25204700
H    0.47991900 -0.23954900  0.94845600
H    0.75056700 -0.05217200 -0.79039000
H   -0.37140300  1.02426500  0.04477800
C   -3.97099100 -1.36580200  0.16506800
O   -4.15763000 -0.34014100 -0.55933800
O   -3.86340800  0.82503000  0.25320500
H   -4.22127300 -1.33173100  1.21719700
H   -3.92631500 -2.31167200 -0.36593200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.275187505775

Frequencies (cm^{-1}): -281.6395, 51.0931, 131.6999, 142.9005, 256.2777, 299.1085, 438.3074, 456.5293, 547.3438, 797.7403, 817.7987, 849.5611, 899.0463, 1029.1117, 1094.2533, 1135.7088, 1172.6258, 1210.8923, 1225.3792, 1317.3897, 1378.0621, 1402.0084, 1416.8369, 1476.3916, 1497.286, 1502.4528, 1514.7496, 1545.1694, 2627.1072, 3021.1702, 3033.2862, 3072.9858, 3097.2602, 3101.5599, 3109.7871, 3224.782

$EtOCH_2OOH$ (for TS-AAAH 1.1):

```
C     0.00000000  0.00000000  0.00000000
C    -1.23235900 -0.71562100 -0.50829900
O    -2.20298700 -0.75478600  0.54551800
H    -4.11957700  1.05924600  0.07448000
H    -0.99199000 -1.74265500 -0.80749000
H    -1.65062400 -0.20388300 -1.37941500
H     0.41665600 -0.51406200  0.86587300
H     0.76084100  0.03477500 -0.78054700
H    -0.23850100  1.02293300  0.29123600
C    -3.38594900 -1.41818200  0.22280100
O    -4.21900800 -0.69315600 -0.65669500
O    -4.82175200  0.39247500  0.09098400
H    -3.90982200 -1.60706200  1.15826700
H    -3.19625700 -2.34714100 -0.32747400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.351408139350

Frequencies (cm^{-1}): 53.8672, 96.6264, 155.3799, 230.078, 250.1839, 311.3889, 361.3551, 492.9387, 645.6419, 822.0966, 852.3331, 875.8386, 995.1752, 1027.0848, 1095.2143, 1124.4453, 1180.5958, 1190.5691, 1300.6076, 1311.96, 1376.5943, 1397.2713, 1409.7032, 1427.9559, 1476.2434, 1484.503, 1500.1008, 1526.5953, 2986.8598, 3005.1758, 3031.2596, 3037.0852, 3101.1157, 3103.6048, 3106.129, 3732.171

IRC:

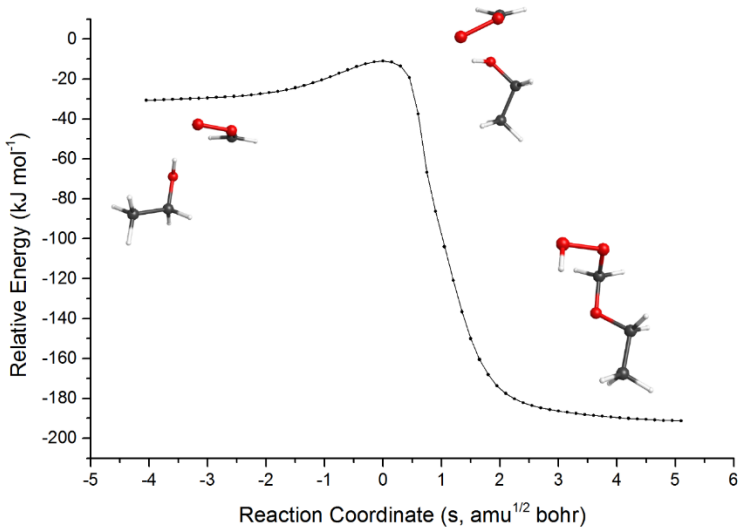


Figure S31: CI1 + EtOH TS-AAAH1.1 IRC

CH_2OO + EtOH PRC (For TS-AAAH 1.2 and TS-AAAH 2.2):

```
C     0.00000000  0.00000000  0.00000000
C     1.08963300 -1.05282400  0.00118700
O     2.35814900 -0.40420100  0.00021700
H     3.08382200 -1.05764300 -0.00000100
H     0.99446700 -1.69446900 -0.88189400
H     0.99466200 -1.69225000  0.88590400
H     0.07782300  0.63296700 -0.88472600
H    -0.98460100 -0.46976800  0.00076400
H     0.07810100  0.63523700  0.88307600
C     5.18792500  0.63920200  0.00077600
O     5.68647500 -0.50968900  0.00030700
O     4.87060400 -1.60629100  0.00016300
H     4.10996900  0.77458400  0.00103200
H     5.91728700  1.43847400  0.00087300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.282413508506

Frequencies (cm^{-1}): 20.2337, 33.1537, 77.6425, 84.112, 123.8886, 225.079, 252.6623, 450.3035, 550.0023, 662.9519, 696.4462, 815.8774, 879.9489, 897.5145, 1018.4765, 1060.0837, 1115.4359, 1178.7833, 1270.8178,

1299.8575, 1341.0482, 1403.7494, 1431.535, 1475.0879, 1484.2978, 1499.1157, 1525.3566, 1560.2636, 2981.7368, 3004.2782, 3030.2359, 3083.1644, 3094.712, 3095.7903, 3244.7037, 3523.1766

CH_2OO + EtOH TS-AAAH 1.2:

```
C     0.00000000  0.00000000  0.00000000
C     1.23451700 -0.85997000 -0.16088300
O     2.18378900 -0.54348300  0.87113100
H     3.02354900 -1.12602800  0.72880900
H     1.69978100 -0.71526100 -1.14025400
H     0.98878600 -1.92057300 -0.06899700
H     0.23970100  1.05921300 -0.10486200
H    -0.73517400 -0.25468900 -0.76423700
H    -0.45344200 -0.15274700  0.97902700
C     3.55699400  0.80354600  0.37224800
O     4.16744600  0.09932400 -0.49047000
O     4.51560300 -1.15734400  0.14553200
H     3.85725000  0.75896400  1.41075500
H     3.03447800  1.67128200 -0.01807800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.275108274620

Frequencies (cm^{-1}): -297.061, 63.9315, 118.3462, 161.5557, 254.6812, 290.8063, 428.0371, 457.9171, 554.1986, 798.6483, 812.8783, 850.6272, 896.9701, 1042.6814, 1092.3482, 1158.9454, 1180.587, 1210.6549, 1226.4056, 1305.6221, 1373.9398, 1381.2893, 1413.4412, 1486.5915, 1497.5217, 1505.4673, 1519.4635, 1545.5612, 2577.5231, 3016.4062, 3033.5297, 3047.578, 3095.2319, 3102.7345, 3106.3132, 3225.6326

$EtOCH_2OOH$ (TS-AAAH 1.2 -Conformer):

```
C     0.00000000  0.00000000  0.00000000
C     1.25871300 -0.84653000 -0.09165600
O     2.25939600 -0.43349600  0.85297500
H     4.59842700 -1.48031100  0.26080100
H     1.67642800 -0.83081000 -1.10157100
H     1.03763100 -1.88400700  0.15744300
H     0.19529800  1.04372800 -0.24946000
H    -0.75160300 -0.37222400 -0.69838700
H    -0.41541600 -0.03953900  1.00670600
C     3.09631700  0.59685900  0.42125200
O     4.06502400  0.17169100 -0.51286400
O     5.04805600 -0.62487900  0.19392300
H     3.58435300  1.00001100  1.30705900
H     2.55673400  1.37700100 -0.12538700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.349995267820

Frequencies (cm^{-1}): 59.598, 90.5537, 152.6431, 215.4354, 262.5319, 301.4853, 432.1765, 479.516, 627.3702, 807.8834, 845.0502, 876.0967, 993.1523, 996.0843, 1070.8177, 1106.9121, 1163.1847, 1212.2933, 1303.3289, 1338.0405, 1380.0367, 1386.9966, 1409.7816, 1414.6296, 1476.1872, 1489.7978, 1497.1329, 1517.2466, 3016.6321, 3028.6215, 3032.5126, 3074.0536, 3093.3351, 3103.7802, 3106.7085, 3728.2016

IRC:

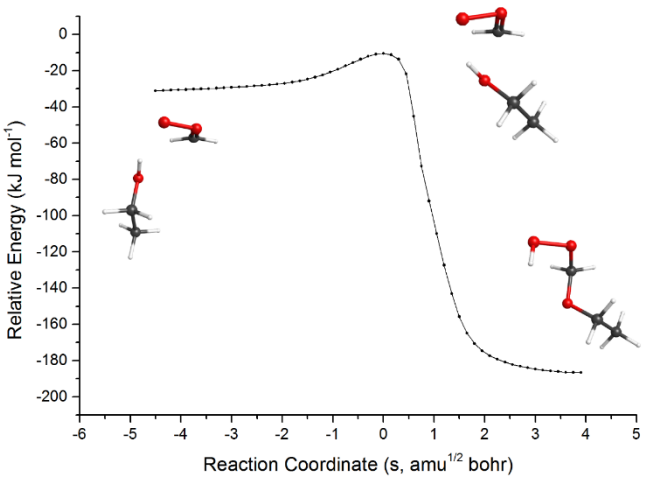


Figure S32: CI1 + EtOH TS-AAAH1.2 IRC

CH_2OO + EtOH TS-AAAH 1.3:

C 0.00000000 0.00000000 0.00000000
C 0.07852600 -1.44128000 -0.47438800
O 1.40936900 -1.98318900 -0.55812700
H 2.01292400 -1.41982500 -1.18849300
H -0.47311200 -2.10366000 0.19278200
H -0.35929300 -1.53470000 -1.47180600
H 0.35628100 0.11081300 1.02420200
H -1.04097500 0.32616700 -0.02674100
H 0.58408700 0.66027100 -0.63955700
C 2.87481600 -1.50559900 0.64124000
O 3.15623900 -0.36022000 0.16367800
O 3.30439700 -0.52270400 -1.27471200
H 3.36044100 -2.38565600 0.23994800
H 2.49345400 -1.50583600 1.65774000

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.271494347953

Frequencies (cm-1): -329.5458, 43.2573, 124.9624, 166.4141, 262.8935, 341.0563, 385.7123, 482.4567, 547.1835, 798.7612, 805.0031, 845.6539, 902.0559, 1028.6151, 1100.669, 1141.2947, 1189.1453, 1212.2413, 1235.6191, 1318.1122, 1365.2224, 1399.5142, 1420.3138, 1449.6727, 1491.5551, 1493.9697, 1512.6777, 1546.485, 2490.8771, 3022.4271, 3035.6068, 3071.2198, 3094.8505, 3100.7606, 3115.3086, 3219.6969

$EtOCH_2OOH$ (TS-AAAH 1.3-conformer):

C 0.00000000 0.00000000 0.00000000
C 0.18896400 -1.50537000 -0.09770300
O 1.40677800 -1.87937200 -0.75614600
H 3.06537100 0.22912400 -0.94773000
H 0.15936900 -1.96514200 0.89564300
H -0.60952000 -1.94794700 -0.69375100
H 0.76079100 0.45582900 0.63200400
H -0.97943700 0.22423900 0.42694000
H 0.04480900 0.45418700 -0.99078600
C 2.51448800 -2.09263700 0.06071300
O 3.09697600 -0.91117000 0.57266400
O 3.78919200 -0.24464600 -0.51168800
H 3.24635000 -2.63302300 -0.53761700
H 2.24959100 -2.64442400 0.97003900

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.349852883241

Frequencies (cm-1): 50.1372, 82.4027, 159.3515, 224.5384, 266.5944, 339.603, 405.6147, 491.0129, 622.8563, 806.5041, 838.6792, 873.9283, 988.5258, 1001.9815, 1089.2672, 1109.6236, 1166.6057, 1212.0665, 1306.5162, 1341.4314, 1377.2428, 1397.0816, 1409.6723, 1415.4231, 1472.1845, 1488.3447, 1497.4318, 1515.7213, 3001.7506, 3006.968, 3030.525, 3067.4123, 3089.3186, 3101.7869, 3112.5287, 3724.7686

IRC:

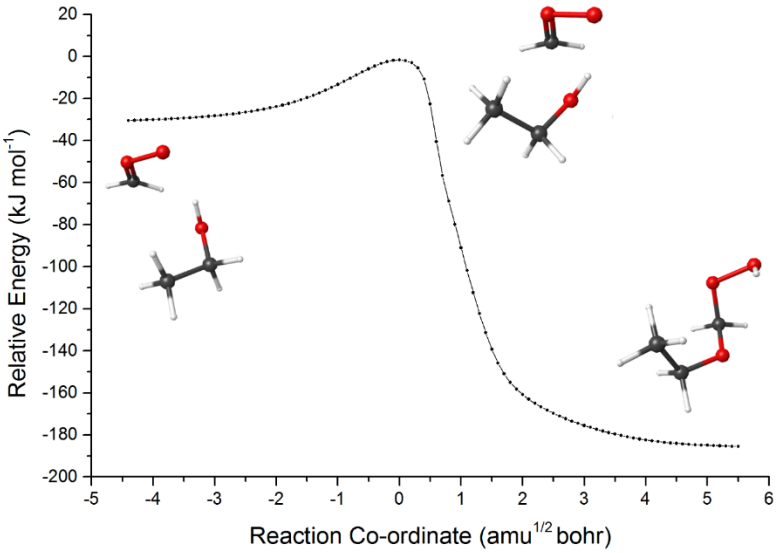


Figure S33: CI1 + EtOH TS-AAAH1.3 IRC

CH_2OO + EtOH PRC (For TS-AAAH 2.1):

```
C     0.00000000  0.00000000  0.00000000
C    -1.03905900 -1.07985900  0.26040500
O    -2.17061700 -0.97738300 -0.59706500
H    -2.66505200 -0.16672400 -0.37249300
H    -1.35038200 -1.05132500  1.31254000
H    -0.61243900 -2.06705100  0.07555400
H    -0.41131200  0.99225300  0.19379100
H     0.86679400 -0.13813400  0.65004200
H     0.33551100 -0.03388700 -1.03673000
C    -4.99174700 -1.37110900  0.20244100
O    -5.12665800 -0.20530700 -0.22396200
O    -4.22416200  0.74564700  0.18451600
H    -4.18472600 -1.60934000  0.88184000
H    -5.71736700 -2.08303700 -0.16828000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.281080234002

Frequencies (cm^{-1}): 24.0894, 43.7872, 61.8646, 91.6667, 145.3184, 193.4831, 266.0622, 428.461, 523.9116, 649.5576, 693.9732, 808.7346, 868.1654, 886.4768, 990.0846, 1062.2234, 1108.7781, 1141.9003, 1243.6863, 1303.6244, 1395.5725, 1410.8875, 1417.3759, 1444.6625, 1489.4345, 1494.2215, 1513.7725, 1568.0592, 2969.1734, 3023.1237, 3051.6788, 3084.363, 3098.2526, 3126.0935, 3271.3843, 3536.9333

CH_2OO + EtOH TS-AAAH 2.1:

```
C     0.00000000  0.00000000  0.00000000
C    -1.07729700 -1.00994100  0.35304400
O    -2.24219600 -0.81893800 -0.45870000
H    -2.68225100  0.08705800 -0.22335200
H    -1.34404000 -0.92630100  1.41222300
H    -0.73398700 -2.02818500  0.16860900
H    -0.34459300  1.01772800  0.18581300
H     0.88768100 -0.17378400  0.61033300
H     0.27937800 -0.08484700 -1.04955900
C    -3.98973900 -1.40433900  0.26394900
O    -4.64530600 -0.41717100 -0.18781800
O    -4.00733100  0.79033800  0.30790800
H    -3.57917900 -1.35685700  1.26560000
H    -4.19838500 -2.35826600 -0.20924000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.272715044989

Frequencies (cm^{-1}): -289.4819, 44.515, 129.1496, 150.0217, 255.8448, 319.8719, 423.3451, 445.0657, 531.1481, 805.8297, 816.6428, 868.516, 892.401, 1036.3701, 1072.6586, 1125.3238, 1165.4918, 1204.5605, 1217.2411, 1321.2196, 1381.2253, 1401.9647, 1416.5699, 1482.933, 1496.6234, 1506.6066, 1518.2887, 1580.9453, 2537.3837, 2997.9389, 3033.9378, 3067.2582, 3094.839, 3097.932, 3110.3919, 3215.6403

$EtOCH_2OOH$ (TS-AAAH 2.1-conformer):

```
C     0.00000000  0.00000000  0.00000000
C    -1.07988800 -0.93672100  0.49793500
O    -2.30009900 -0.62008600 -0.16546200
H    -4.31158000  0.99927100 -0.02581700
H    -1.21372200 -0.83515400  1.58212100
H    -0.80654700 -1.97973800  0.29482200
H    -0.26071100  1.03653600  0.21322300
H     0.94707900 -0.22478800  0.49166000
H     0.13634800 -0.10643300 -1.07584100
C    -3.39192100 -1.40113100  0.25403400
O    -4.57077200 -0.86217000 -0.25329700
O    -4.84936100  0.36385400  0.46964600
H    -3.42894200 -1.45212700  1.34878000
H    -3.35597100 -2.40783200 -0.18031100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.348003582367

Frequencies (cm^{-1}): 49.132, 72.6248, 157.5468, 222.5771, 244.2151, 294.3726, 387.8434, 445.3789, 585.9528, 825.6513, 883.6656, 910.8047, 1031.6302, 1058.5677, 1114.4635, 1137.6496, 1158.8532, 1187.2528, 1284.464, 1306.0136, 1380.0425, 1389.5993, 1412.7583, 1445.0621, 1484.9407, 1491.087, 1500.1898, 1527.1874, 2967.5997, 2979.768, 2994.3897, 3022.651, 3037.9908, 3102.1928, 3107.1542, 3732.0544

IRC:

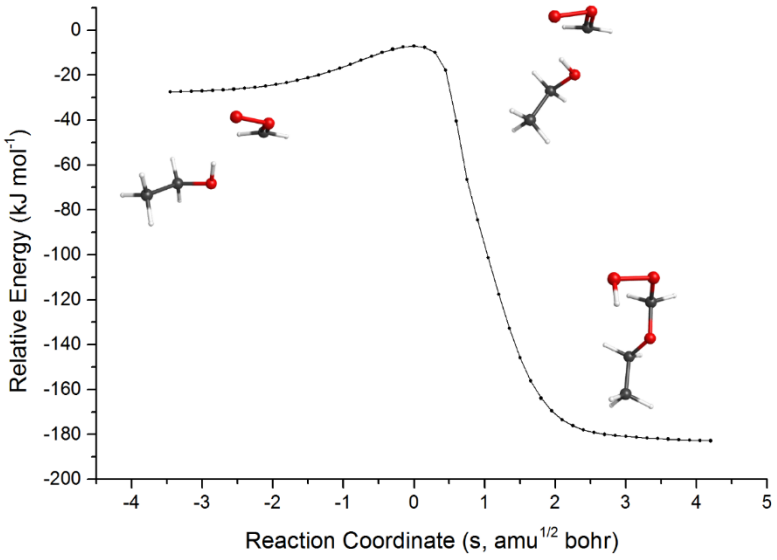


Figure S34: CI1 + EtOH TS-AAAH2.1 IRC

CH_2OO + EtOH TS-AAAH 2.2

```
C     0.00000000  0.00000000  0.00000000
C     1.16715200 -0.92221300  0.28244900
O     2.29785800 -0.52756600 -0.50160000
H     3.09265900 -1.16901500 -0.32025900
H     0.92203100 -1.95453000  0.02021300
H     1.42834300 -0.91174400  1.34686800
H    -0.25842100 -0.02067400 -1.05827200
H    -0.87276000 -0.31119500  0.57516200
H     0.23585000  1.02905900  0.27473900
C     3.62211300  0.69153700  0.32242900
O     4.63760500  0.12639100 -0.18572600
O     4.58300600 -1.27747000  0.18276600
H     3.27473300  0.38238000  1.30152000
H     3.40062400  1.68168500 -0.06191100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.272515495281

Frequencies (cm^{-1}): -307.2176, 47.9089, 118.4288, 169.045, 265.7815, 299.2502, 393.2583, 465.3214, 538.7845, 805.8823, 809.5774, 868.7802, 890.9306, 1047.627, 1088.5625, 1151.224, 1174.8055, 1179.3059, 1215.8541, 1305.7523, 1378.4345, 1389.3696, 1415.8226, 1486.5692, 1496.9401, 1509.4043, 1521.6071, 1587.71, 2492.3465, 2991.4816, 3033.7047, 3038.5849, 3092.0385, 3096.3052, 3107.4122, 3213.6559

$EtOCH_2OOH$ (TS-AAAH 2.2-Conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -1.27475500  0.61102700 -0.55718700
O    -2.18616000 -0.38777400 -1.03479900
H    -4.53118500  1.31517400 -0.93416000
H    -1.04997300  1.23704300 -1.42114900
H    -1.77159000  1.23641000  0.18827600
H     0.48457800 -0.62418200 -0.75073300
H     0.69634000  0.78678900  0.29639600
H    -0.20427800 -0.61555400  0.87729700
C    -3.10525400 -0.89015800 -0.11535600
O    -4.42973000 -0.48947900 -0.38201100
O    -4.54504600  0.92074900 -0.05094700
H    -2.83752500 -0.61486800  0.90891200
H    -3.16892100 -1.97525400 -0.22402400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.347453460265

Frequencies (cm^{-1}): 51.888, 65.0625, 141.5279, 240.6659, 271.3902, 345.7229, 383.6587, 467.5552, 589.0721, 806.1233, 858.6474, 878.4643, 995.3696, 1001.4562, 1085.2472, 1109.7358, 1157.0402, 1212.0066, 1307.3968, 1333.2349, 1366.4172, 1391.7719, 1411.0374, 1421.2392, 1476.3372, 1487.3914, 1496.9778, 1517.3532, 3009.9403, 3028.1995, 3030.2192, 3069.6676, 3074.922, 3091.2009, 3104.3052, 3750.1972

IRC:

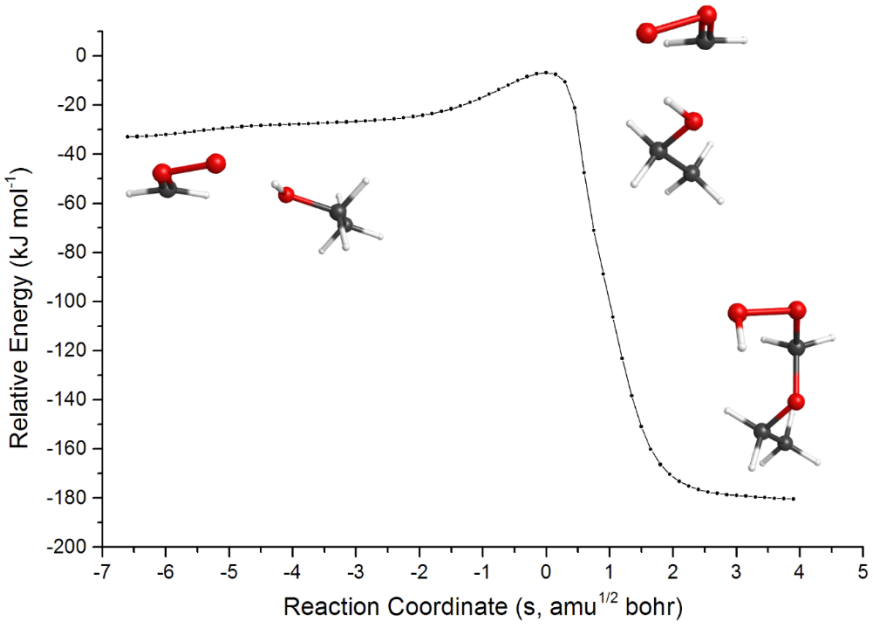


Figure S35: CI1 + EtOH TS-AAAH2.2 IRC

7.1.3 sCI 1 + iPrOH Reactions

iPrOH:

```
C    0.00000000  0.00000000  0.00000000
C   -1.32664200 -0.58449100 -0.45163800
H   -1.46179000 -1.58847500 -0.04797100
H   -2.15290800  0.03929200 -0.11221900
H   -1.36461300 -0.63997500 -1.54068500
C    1.19499100 -0.82340500 -0.46531100
H    2.13432000 -0.37108800 -0.13912400
H    1.15477700 -1.83369200 -0.05416400
H    1.20872100 -0.89206300 -1.55413300
O    0.05439800  1.33515000 -0.52531500
H    0.88883500  1.73780800 -0.26710800
H    0.00827400  0.05055400  1.09625500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -194.131538784597

Frequencies (cm^{-1}): 216.86, 258.4018, 282.5817, 363.0657, 414.1135, 482.5204, 817.873, 931.6449, 948.5742, 956.1892, 1082.9134, 1152.8117, 1185.8809, 1274.8545, 1373.3866, 1393.9545, 1411.3776, 1424.4328, 1483.1536, 1487.134, 1497.0007, 1508.081, 2966.9649, 3018.8632, 3033.209, 3077.5134, 3090.3621, 3098.8253, 3105.1855, 3813.4792

iPrOH (conformer 2 unused):

```
C    0.00000000  0.00000000  0.00000000
C    1.26898500 -0.70320000  0.46828100
H    1.31334700 -1.72567900  0.08931300
H    2.15180000 -0.16730600  0.12114200
H    1.30374900 -0.75124100  1.56019700
C   -1.26891400 -0.70336800  0.46826900
H   -2.15180000 -0.16780200  0.12080900
H   -1.31291700 -1.72596900  0.08959800
H   -1.30384400 -0.75107200  1.56019200
O   -0.00010600  1.37937200  0.39031700
H   -0.00024500  1.42732300  1.35227600
H   -0.00000500  0.04058500 -1.09113700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 220.2753, 257.1485, 264.1908, 361.2771, 424.5654, 471.2292, 812.4588, 923.7547, 939.5624, 958.1787, 1080.8803, 1145.2499, 1181.7394, 1296.2797, 1366.3578, 1398.5936, 1409.4512, 1415.5297, 1482.9007, 1484.411, 1497.2864, 1506.1659, 3014.2302, 3017.8539, 3039.093, 3072.3763, 3084.5685, 3101.1503, 3103.0004, 3792.2761

CH_2OO + iPrOH PRC (For TS-AAAH 1.1, TS-AAAH 1.2, TS-AAAH 2.1 and TS-AAAH 2.2):

```
C    0.00000000  0.00000000  0.00000000
C   -0.91928800 -1.18364600  0.25052800
H   -1.94628400 -0.93955100 -0.02317500
H   -0.60184300 -2.04579900 -0.33596600
H   -0.90037800 -1.46092100  1.30609300
C   -0.40157600  1.23327500  0.80243600
H    0.28804900  2.05840400  0.61791100
H   -1.40457400  1.56542000  0.52795300
H   -0.38976600  1.01127900  1.87087300
O    1.32683100 -0.41849500  0.33342800
C    4.25558600 -1.06846900  0.68369500
O    4.62972700  0.07472000  0.33477600
O    3.70186300  1.02387900  0.00886300
H    1.97103100  0.29171000  0.14883500
H    5.06495300 -1.74626100  0.92111300
H    3.19822600 -1.31482800  0.72626100
H   -0.03186000  0.24928200 -1.06821600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.545293537029

Frequencies (cm^{-1}): 15.5863, 38.1454, 70.47, 80.3346, 113.7197, 210.1828, 219.3469, 258.0776, 365.2464, 444.8779, 489.486, 549.101, 656.7137, 695.0949, 821.0992, 879.9427, 931.2706, 947.2468, 965.2624, 1018.7345, 1125.8117, 1156.9684, 1187.4224, 1270.982, 1328.8375, 1375.3864, 1397.5388, 1413.1467, 1427.6466, 1448.2735, 1483.6589, 1488.7668, 1499.8458, 1507.7996, 1559.2808, 2968.0655, 3021.9329, 3029.6712, 3081.6385, 3085.3385, 3088.5641, 3094.6546, 3099.8882, 3244.0761, 3527.0235

CH_2OO + iPrOH TS-AAAH 1.1:

```
C     0.00000000  0.00000000  0.00000000
C     0.94892700 -1.17790800  0.12512900
H     1.72625700 -1.11930300 -0.63695300
H     0.42286600 -2.12454300 -0.00327200
H     1.42545200 -1.18192100  1.10609100
C     0.68200200  1.34719800  0.19012200
H    -0.04131900  2.15964000  0.11835500
H     1.16968700  1.39675200  1.16443400
H     1.43654200  1.49887600 -0.58281700
O    -1.02833200 -0.15232400  1.00712300
C    -2.67663500 -1.08473200  0.42346200
O    -3.08962700 -0.20239200 -0.39164100
O    -3.13927900  1.05917800  0.32349300
H    -1.69229800  0.62703900  0.90953700
H    -2.37222600 -2.02632900 -0.02263500
H    -2.97583200 -1.03639200  1.46219100
H    -0.48551400 -0.01520000 -0.98140100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.537016353136

Frequencies (cm^{-1}): -276.892, 49.3144, 102.8041, 134.9488, 215.185, 251.2029, 276.2465, 352.3125, 430.4505, 463.5267, 479.7975, 563.9639, 785.3104, 814.9051, 880.9576, 930.8549, 942.5483, 951.5578, 1119.847, 1128.1384, 1176.0813, 1192.5188, 1210.6285, 1220.5692, 1358.2081, 1375.6539, 1386.0675, 1406.5828, 1420.6943, 1472.329, 1485.6681, 1492.5771, 1508.4903, 1515.5751, 1543.8047, 2632.7808, 3004.1105, 3030.2591, 3034.6798, 3095.2892, 3096.348, 3102.2328, 3102.7181, 3105.474, 3224.6205

iPrOCH_2OOH (TS-AAAH 1.1-conformer):

```
C     0.00000000  0.00000000  0.00000000
C    -1.02371300 -1.11833700  0.15244100
H    -1.82479000 -1.00326600 -0.57909900
H    -0.57332300 -2.09926300 -0.00201900
H    -1.46081500 -1.09677200  1.15145300
C    -0.59716800  1.37342000  0.25256600
H     0.14979300  2.15423000  0.11147500
H    -0.97453800  1.44061300  1.27380500
H    -1.42391600  1.56189000 -0.43285600
O     1.07302100 -0.17287100  0.95430700
C     2.10614900 -1.02029700  0.55509200
O     2.98650600 -0.42253300 -0.37338300
O     3.77427400  0.56794900  0.33280900
H     3.14922800  1.30494300  0.40158300
H     1.74529300 -1.90221500  0.01628600
H     2.65152700 -1.30299000  1.45424500
H     0.42924300 -0.02512600 -1.00601200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.612894029409

Frequencies (cm^{-1}): 50.5824, 77.9494, 145.658, 211.6163, 213.9686, 252.832, 293.2683, 355.8415, 414.1311, 446.3564, 497.4393, 648.1382, 795.9267, 875.8096, 910.0418, 934.4337, 948.2675, 993.8386, 1081.0035, 1125.5085, 1147.8146, 1179.0451, 1210.1448, 1308.6658, 1372.0942, 1379.8354, 1384.91, 1403.8382, 1407.9279, 1421.3467, 1476.3515, 1482.5817, 1486.5887, 1497.628, 1508.2417, 3011.5512, 3021.8837, 3030.4147, 3035.4963, 3093.0116, 3096.3215, 3101.5071, 3102.4614, 3103.6281, 3726.3506

IRC:

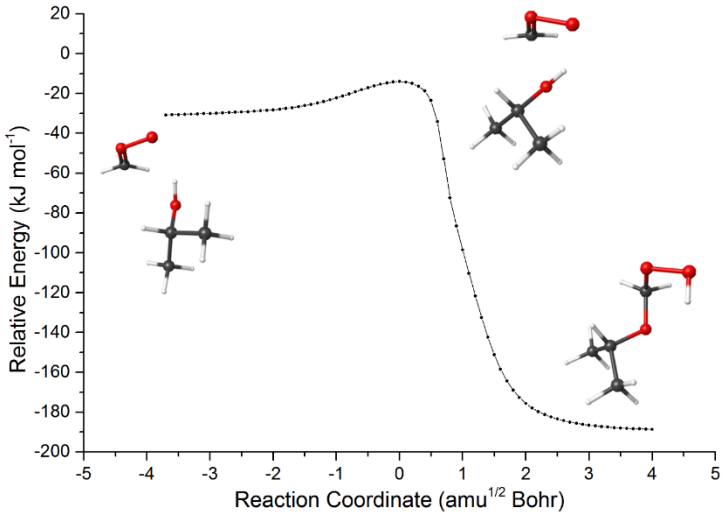


Figure S36: CI1 + iPrOH TS-AAAH1.1 IRC

CH_2OO + iPrOH TS-AAAH 1.2:

```
C     0.00000000  0.00000000  0.00000000
C    -1.11650000 -0.87821900  0.53498100
H    -2.04750700 -0.31376600  0.59299900
H    -1.27357900 -1.73978500 -0.11257100
H    -0.87838100 -1.23836900  1.53789800
C     0.26500200  1.22547600  0.86481200
H     1.10855900  1.80120200  0.48762100
H    -0.61748500  1.86651600  0.86507700
H     0.47310200  0.94495200  1.89849400
O     1.17037400 -0.83749400 -0.16764500
C     2.56563300 -1.09833800  1.16486300
O     3.17849700  0.01050200  1.03545500
O     3.43080000  0.19432000 -0.38607300
H     1.96058800 -0.31204300 -0.59390800
H     2.09341900 -1.25818900  2.12916400
H     2.85686900 -1.94338400  0.55449700
H    -0.25662800  0.33287200 -1.01108900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.534307354431

Frequencies (cm^{-1}): -327.6792, 36.0852, 117.4419, 147.6804, 226.9734, 276.5298, 302.3397, 357.905, 370.422, 469.0671, 515.1221, 556.5198, 780.4369, 811.569, 885.3165, 934.5129, 937.3561, 948.9653, 1128.6574, 1143.9835, 1165.6285, 1203.7688, 1212.235, 1225.5964, 1342.9997, 1360.5371, 1378.8129, 1405.7808, 1423.5361, 1456.9363, 1486.5523, 1488.0288, 1504.0623, 1507.4273, 1544.8955, 2467.8275, 3002.5431, 3029.171, 3034.7351, 3088.207, 3096.1801, 3100.7442, 3109.3093, 3114.8133, 3218.6921

iPrOCH$_2$OOH (TS-AAAH 1.2-Conformer):

```
C     0.00000000  0.00000000  0.00000000
C    -1.02718000 -0.87533400  0.71113200
H    -1.99579300 -0.37397500  0.72502400
H    -1.14126500 -1.82740700  0.19383000
H    -0.74994600 -1.07366900  1.74767600
C     0.20712100  1.34635000  0.68520700
H     0.93768000  1.95020200  0.14856700
H    -0.73763300  1.89183400  0.70659700
H     0.55183800  1.23380000  1.71321600
O     1.23365700 -0.72192400 -0.23060500
C     2.04197500 -1.02953600  0.86501900
O     2.96820100 -0.01047700  1.18212900
O     3.97818200  0.00940500  0.14374900
H     3.52115900  0.48707700 -0.56464200
H     1.47893800 -1.15186900  1.79354000
H     2.58263900 -1.94147300  0.61384800
H    -0.35087200  0.18068100 -1.01687100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.609410883506

Frequencies (cm^{-1}): 42.2567, 83.9949, 137.0537, 224.7392, 232.1582, 255.904, 288.71, 364.0328, 380.7054, 445.3988, 544.9087, 625.6305, 774.6008, 876.2616, 907.2428, 925.625, 939.6481, 994.6704, 1044.9277, 1144.6632, 1154.6058, 1167.1942, 1205.3114, 1316.812, 1370.8411, 1375.8464, 1393.5568, 1402.7, 1404.5419, 1421.2246, 1476.9341, 1483.1008, 1488.2459, 1501.9853, 1506.1846, 3028.5762, 3033.5652, 3039.2234, 3047.6587, 3088.6029, 3095.7958, 3099.5911, 3105.3413, 3108.8873, 3722.6506

IRC:

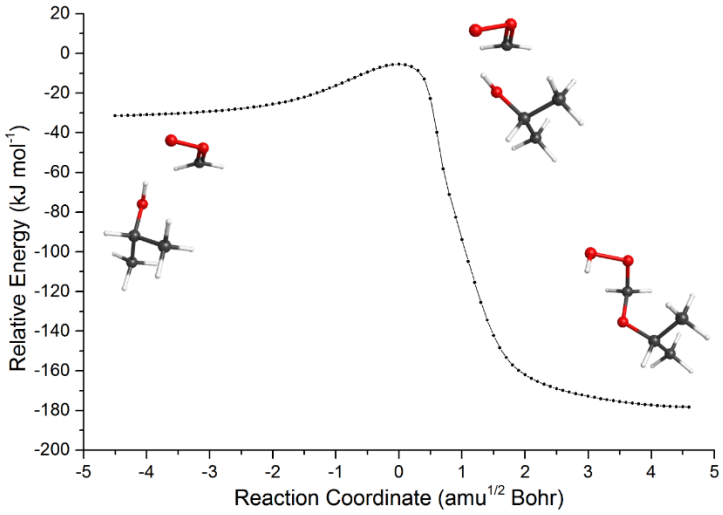


Figure S37: CI1 + iPrOH TS-AAAH1.2 IRC

CH$_2$OO + iPrOH PRC (For TS-AAAH 1.3):

```
C     0.00000000  0.00000000  0.00000000
C    -0.43480300 -1.26905000  0.72631000
H    -1.52033000 -1.30420600  0.83480900
H    -0.11440000 -2.15285500  0.17497400
H     0.00562200 -1.31111200  1.72513100
C    -0.42702200  1.26754500  0.73355300
H    -0.10160200  2.15253400  0.18709000
H    -1.51228200  1.30852100  0.84267300
H     0.01408000  1.30120700  1.73238400
O     1.41043200 -0.00362800 -0.23739600
C     4.42239000  0.00138800 -0.42461500
O     4.58218000 -0.00286100  0.81767500
O     3.49277100 -0.00823400  1.64260000
H     1.90330400 -0.00627300  0.60629700
H     5.34508700  0.00520900 -0.98983400
H     3.42378300  0.00084600 -0.85296500
H    -0.44434900  0.00416000 -0.99816000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.544554740165

Frequencies (cm^{-1}): 21.6943, 32.0121, 70.8173, 81.2645, 120.2768, 214.3786, 227.9568, 276.6565, 367.8817, 421.5769, 497.2875, 548.5462, 644.5088, 693.2865, 816.0877, 880.7047, 924.901, 939.124, 964.1775,

1018.4411, 1133.3917, 1146.2545, 1184.267, 1271.9322, 1348.1034, 1367.3487, 1398.3495, 1414.9679, 1420.7124, 1442.5002, 1482.887, 1485.679, 1499.4114, 1507.9875, 1558.3092, 3019.4674, 3022.1826, 3028.1313, 3078.0041, 3080.3574, 3088.3658, 3097.1681, 3099.271, 3243.4182, 3520.9533

CH_2OO + iPrOH TS-AAAH 1.3:

```
C     0.00000000  0.00000000  0.00000000
C     0.25439200  1.22038500 -0.87532800
H    -0.68537400  1.74608300 -1.04862900
H     0.94405000  1.91922100 -0.40352400
H     0.67120800  0.92950400 -1.83970300
C    -1.02449400 -0.95044800 -0.60523300
H    -1.17870500 -1.81296400  0.04150800
H    -1.97962500 -0.44033900 -0.73753100
H    -0.69055700 -1.30348800 -1.58252200
O     1.20478700 -0.76041000  0.26975000
C     2.98462600 -0.00722600  0.52925500
O     3.27157000  0.26001800 -0.68114200
O     3.01450200 -0.94336000 -1.45734500
H     1.67174500 -1.05842400 -0.60462800
H     2.89004200  0.85192700  1.18637100
H     3.23291900 -0.97981800  0.93403800
H    -0.34442700  0.32208000  0.98473100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.534979603122

Frequencies (cm^{-1}): -300.5573, 33.2201, 114.2525, 140.7928, 222.3545, 264.9798, 306.7074, 362.7433, 394.7586, 475.8884, 503.4613, 550.498, 779.5901, 813.4778, 886.9799, 925.0916, 933.8696, 947.1311, 1098.086, 1144.5551, 1172.3673, 1196.5643, 1212.0205, 1216.7708, 1356.8413, 1369.2969, 1385.7697, 1406.2487, 1424.6772, 1440.3485, 1484.8258, 1485.7647, 1501.1843, 1509.3951, 1543.6743, 2549.2681, 3029.9839, 3037.1106, 3038.3292, 3092.4239, 3099.393, 3100.7883, 3108.8797, 3110.8371, 3218.4665

$iPrOCH_2OOH$ (TS-AAAH 1.3-Conformer):

```
C     0.00000000  0.00000000  0.00000000
C     0.15286000  1.51400300 -0.09554600
H    -0.66863900  2.01177100  0.42215000
H     1.08798600  1.84361700  0.35394900
H     0.13179300  1.82814100 -1.14083700
C    -1.30879600 -0.49058100 -0.59738700
H    -1.39929300 -1.57145000 -0.49606800
H    -2.15675800 -0.02205400 -0.09665500
H    -1.35656200 -0.24156500 -1.65831100
O     1.06212500 -0.67417500 -0.70873500
C     2.19402200 -1.01574700  0.02514200
O     3.05318500  0.06963800  0.31382900
O     3.72286800  0.45049600 -0.91320100
H     3.05102400  1.00022800 -1.34341300
H     1.93767700 -1.39112200  1.02241100
H     2.73263900 -1.76240600 -0.55669400
H     0.05480800 -0.30159500  1.05249400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.612611451963

Frequencies (cm^{-1}): 42.427, 80.1353, 150.2292, 218.4168, 232.8519, 271.4762, 310.6455, 359.3967, 369.6282, 447.2725, 518.0033, 647.7612, 794.6932, 873.1453, 916.5747, 934.5294, 944.6865, 989.6664, 1100.612, 1127.6378, 1147.0814, 1175.7877, 1212.2267, 1310.71, 1363.3851, 1380.2755, 1385.6637, 1401.7191, 1410.4654, 1419.7753, 1472.2585, 1482.2777, 1490.4932, 1497.1562, 1514.6679, 2987.1191, 3005.6089, 3027.8886, 3035.2767, 3086.9742, 3098.2272, 3099.9278, 3105.8424, 3112.8727, 3725.0743

IRC:

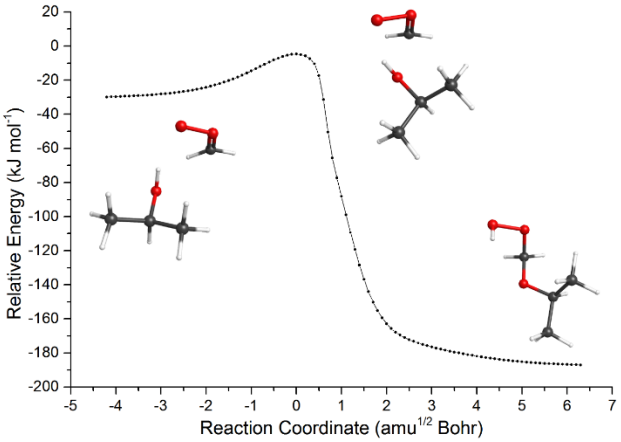


Figure S38: CI1 + iPrOH TS-AAAH1.3 IRC

CH_2OO + iPrOH TS-AAAH 2.1

```
C     0.00000000  0.00000000  0.00000000
C     0.85885900 -1.22099500 -0.27778600
H     1.76738000 -1.19212800  0.32407900
H     0.32482200 -2.14116100 -0.03804500
H     1.14169800 -1.25430800 -1.33046500
C     0.69999400  1.31353400 -0.32035700
H     0.04199900  2.16168200 -0.13002100
H     1.58823400  1.42851100  0.30216800
H     1.00377800  1.33846700 -1.36730300
O    -1.19206100 -0.10539700 -0.80316700
C    -2.75626000 -1.04872000 -0.05440000
O    -3.62175500 -0.24913000 -0.52464100
O    -3.27761100  1.08473200 -0.06309400
H    -1.82232900  0.68436500 -0.59000000
H    -2.74535700 -2.03709300 -0.50164700
H    -2.36748100 -0.88414600  0.94380100
H    -0.29553900  0.00724200  1.05656200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.536107797350

Frequencies (cm^{-1}): -280.0286, 44.1046, 105.5784, 137.5081, 215.0456, 254.8159, 291.6288, 332.2799, 417.6225, 471.6062, 477.9893, 540.634, 806.8564, 824.0616, 872.989, 935.2938, 942.5914, 951.9572, 1090.9609, 1136.91, 1164.8813, 1177.0021, 1199.9007, 1217.9126, 1363.1068, 1380.8846, 1381.4249, 1406.383, 1420.7659, 1479.3124, 1485.6581, 1492.9343, 1507.9376, 1516.1746, 1583.7733, 2564.7405, 2976.3492, 3030.6999, 3034.916, 3092.7742, 3095.9922, 3097.3663, 3102.3792, 3106.0519, 3214.3274

iPrOCH_2OOH (TS-AAAH 2.1 -conformer)

```
C     0.00000000  0.00000000  0.00000000
C     0.97086200 -1.14370800  0.26920400
H     1.72139500 -0.84381100  1.00219800
H     0.45354000 -2.02002900  0.66133700
H     1.48086000 -1.43147700 -0.65125500
C     0.69064900  1.22540500 -0.57271700
H    -0.02395900  2.03096100 -0.73917400
H     1.46176100  1.58305500  0.11028900
H     1.16076400  0.98419600 -1.52688800
O    -0.99635100 -0.40323700 -0.96412000
C    -2.10060800 -1.09961800 -0.47973100
O    -3.29560900 -0.35238100 -0.53533000
O    -3.22778500  0.67515600  0.49026300
H    -3.04790700  1.45668500 -0.05042100
H    -2.32391800 -1.93478400 -1.14775100
H    -1.93793000 -1.45191700  0.54263900
H    -0.51292700  0.27209000  0.92702400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.610436067045

Frequencies (cm^{-1}): 39.3775, 57.2794, 135.1836, 216.117, 233.0296, 253.1635, 310.2216, 328.1687, 379.4315, 444.2469, 483.4726, 607.8863, 816.1247, 873.4163, 918.1895, 932.8976, 946.8476, 999.0556, 1094.0041, 1125.4278, 1142.7123, 1176.3168, 1209.0651, 1310.9088, 1365.8368, 1368.7195, 1377.4957, 1404.632,

1417.4423, 1420.246, 1481.1086, 1481.7163, 1486.8226, 1496.0354, 1508.4298, 3009.7648, 3018.5382, 3027.5265, 3035.3663, 3073.9415, 3091.4332, 3094.2998, 3102.4389, 3103.2869, 3751.6659

IRC:

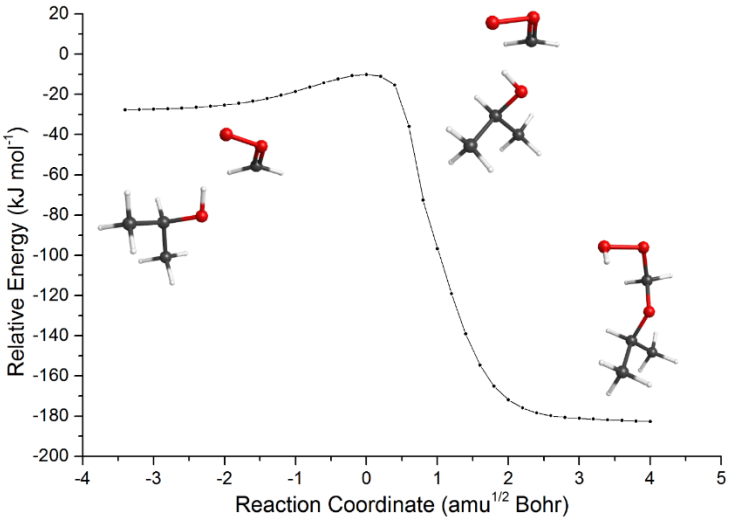


Figure S39: CI1 + iPrOH TS-AAAH2.1 IRC

CH_2OO + iPrOH TS-AAAH 2.2

```
C     0.00000000  0.00000000  0.00000000
C     0.94846400 -1.13036100  0.35796900
H     1.97549000 -0.76639700  0.39625100
H     0.89157400 -1.92783700 -0.38161700
H     0.70259900 -1.54765600  1.33659400
C     0.03528100  1.15144300  0.99862900
H    -0.71965900  1.90158300  0.76505900
H     1.01378200  1.63193900  0.96641600
H    -0.12495300  0.80293900  2.02043500
O    -1.31938700 -0.56583700 -0.16286300
C    -2.62274100 -0.90918500  1.22250000
O    -3.63338200 -0.67073100  0.48563300
O    -3.46147300  0.68373300 -0.03170900
H    -2.03049200  0.16384400 -0.38517000
H    -2.47720100 -1.95174300  1.48505700
H    -2.23718800 -0.12167000  1.85538900
H     0.26510300  0.38859900 -0.98882800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.533171904719

Frequencies (cm^{-1}): -335.9506, 29.8142, 106.3165, 161.13, 236.9516, 263.1573, 306.7262, 336.2653, 403.2478, 442.8767, 502.2221, 556.9605, 802.2767, 811.3736, 881.7513, 933.5489, 939.0312, 946.3207, 1097.0098, 1138.3216, 1157.6428, 1178.0026, 1200.2751, 1216.6615, 1354.4197, 1365.5182, 1375.8239, 1404.782, 1421.4439, 1477.7972, 1486.2291, 1490.5478, 1502.2546, 1512.6262, 1577.2131, 2440.4226, 3001.1843, 3028.2557, 3033.0381, 3087.8418, 3095.7258, 3106.4568, 3109.9472, 3110.493, 3229.6218

iPrOCH$_2$OOH (TS-AAAH 2.2-Conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -0.90151600 -1.01908600 -0.69096100
H    -1.92201200 -0.63841100 -0.74915900
H    -0.91870200 -1.95560600 -0.13364500
H    -0.57022400 -1.22777900 -1.70988800
C     0.06410000  1.33657900 -0.73385200
H     0.72839500  2.02682400 -0.21532200
H    -0.93113900  1.78195600 -0.76998500
H     0.41427600  1.23252000 -1.76114400
O     1.30769800 -0.54059800  0.27900000
C     2.08632400 -0.97882900 -0.80418900
O     3.44380300 -0.80843100 -0.50933400
O     3.73743600  0.61105100 -0.54404500
H     3.52612900  0.86507400  0.36628100
H     2.00464100 -2.06227200 -0.94285600
H     1.83220100 -0.45232500 -1.72681000
H    -0.39276300  0.18057600  1.00149200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.606617721668

Frequencies (cm^{-1}): 27.7398, 70.4475, 161.4776, 215.7011, 230.4114, 257.0562, 304.2863, 341.3376, 386.6578, 423.1794, 514.1675, 596.2994, 813.093, 882.3387, 922.7925, 936.4569, 943.5758, 1029.6363, 1042.012, 1142.1779, 1154.4799, 1167.7173, 1201.2283, 1293.9154, 1371.2249, 1373.1922, 1394.287, 1402.8869, 1414.726, 1425.472, 1482.6521, 1485.0197, 1496.0205, 1503.466, 1509.096, 3004.7497, 3027.9261, 3035.9848, 3046.5706, 3058.7664, 3087.2956, 3097.7452, 3101.2751, 3107.7379, 3733.8586

IRC:

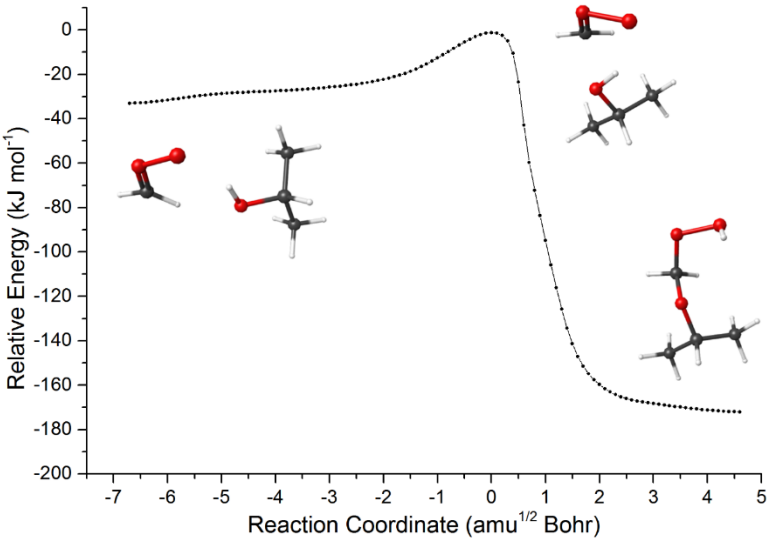


Figure S40: CI1 + iPrOH TS-AAAH2.2 IRC

7.2 sCI 2 + MeOH Reactions

***Syn*-MeCHOO (CI2)**

```
C     0.00000000  0.00000000  0.00000000
C    -0.88282300  1.16994600 -0.00000100
O    -2.13933700  1.06098000  0.00000000
O    -2.66024200 -0.20369400  0.00000000
H    -0.54826500  2.20039200  0.00000100
H     1.04634000  0.29177100 -0.00000900
H    -0.23373500 -0.62566100  0.86707600
H    -0.23374100 -0.62568100 -0.86705900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -228.674140712195

Frequencies (cm^{-1}): 185.6842, 296.0948, 461.2445, 674.9886, 757.5707, 901.4083, 982.8526, 1047.1334, 1110.689, 1349.4956, 1399.8709, 1438.0596, 1460.7204, 1559.8328, 3016.4993, 3051.0462, 3140.3408, 3178.4935

***Syn*-MeCHOO unimolecular TS to VHP:**

```
C     0.00000000  0.00000000  0.00000000
C    -0.67457500  1.22416000  0.05167200
O    -1.96969500  1.18508000  0.04408600
O    -2.39028100 -0.15894900 -0.01072400
H    -0.28185900  2.22423900 -0.09118300
H     1.02162500  0.02630600 -0.35582600
H    -0.14758800 -0.67352500  0.84412500
H    -1.14530200 -0.51704200 -0.45867900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): -1612.8168, 489.796, 531.863, 720.6846, 743.4295, 863.4252, 897.882, 973.0349, 1036.0964, 1211.5778, 1277.9136, 1330.9908, 1488.4542, 1541.8986, 1830.4853, 3078.5518, 3172.2501, 3187.4244

H_2C=CH(OOH) - VHP

```
C     0.00000000  0.00000000  0.00000000
C     0.71221400  1.11616400  0.00268900
O     2.06916700  1.27071400 -0.02686800
O     2.73136100 -0.01252900 -0.10647200
H     0.28161400  2.11000200  0.02150900
H    -1.07564600  0.07582100  0.02330000
H     0.45360900 -0.97642200 -0.03533100
H     3.20821800 -0.01177300  0.73560500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -228.706016537877

Frequencies (cm^{-1}): 157.884, 242.3481, 321.3908, 621.3538, 710.2925, 865.9, 892.088, 968.7988, 970.9419, 1151.0315, 1324.1731, 1380.0399, 1430.679, 1696.5894, 3172.2762, 3186.6558, 3271.3623, 3751.8409

IRC:

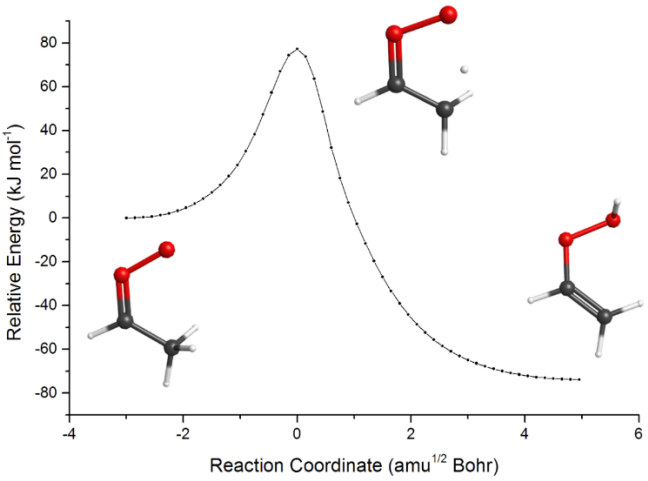


Figure S41:CI2 TS unimolecular IRC

CI2 to CI3 TS:

```
C     0.00000000  0.00000000  0.00000000
C     0.00000000  0.00000000  1.47806900
O     1.01634400  0.00000000  2.24856400
O     1.51132200  1.27380800  1.64579200
H    -0.95815000 -0.17391700  1.98236300
H    -0.57067100 -0.87431800 -0.33604100
H    -0.52915000  0.87858200 -0.37651200
H     1.01037100  0.00384600 -0.39385200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -228.633600557624

Frequencies (cm^{-1}): -656.1328, 254.7726, 364.8092, 490.7743, 744.1668, 875.8109, 908.1133, 1083.8987, 1141.803, 1354.9558, 1397.4696, 1434.5604, 1459.0306, 1568.8739, 2995.8184, 3028.4703, 3060.3705, 3165.384

Note: This is the highest barrier in a multi barrier process between CI2 and CI3 via a dioxirane channel discussed in other literature.

***Syn*-MeCHOO + MeOH PRC (for all TS-AAAH 1, TS-AAAH 2, TS-VHP 1 and TS-VHP 2):**

```
C     0.00000000  0.00000000  0.00000000
C     0.30422000  1.11923500 -0.89224000
H     0.18981500  0.79195500 -1.92871400
H    -0.32388700  1.97676800 -0.66819900
H     1.36346800  1.38504400 -0.78328700
O     0.45054600 -1.16432700 -0.15752600
O     1.29345500 -1.38552100 -1.23372100
H     2.77520500 -0.41361400 -0.84359000
O     3.35394100  0.30781700 -0.52490600
C     4.68027500 -0.16644000 -0.36773000
H     4.73760200 -0.99235000  0.34861800
H     5.11107400 -0.49889500 -1.31774000
H     5.28295200  0.65829100  0.01121500
H    -0.64194100  0.07508300  0.87138700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.294569443117

Frequencies (cm^{-1}): 33.8286, 68.9308, 87.8043, 112.9201, 122.9514, 217.6984, 228.9642, 307.7844, 462.2212, 666.7554, 736.6675, 777.4673, 872.1268, 981.8739, 1062.3217, 1069.9872, 1117.3385, 1137.1121, 1173.1658, 1356.9011, 1399.1593, 1431.7251, 1445.7564, 1475.1483, 1477.7088, 1496.5686, 1512.2108, 1575.9193, 2986.0825, 2994.4945, 3028.6867, 3056.603, 3088.0863, 3139.7364, 3165.761, 3477.6795

***Syn*-MeCHOO + MeOH TS-AAAH 1:**

```
C     0.00000000  0.00000000  0.00000000
C    -0.91612300  0.72835400 -0.91834000
H    -1.88372600  0.79152100 -0.40934900
H    -0.55457900  1.73945200 -1.08766900
H    -1.04087300  0.20174500 -1.85702500
O     0.07220900 -1.28116900  0.09339600
O     0.16516100 -1.83600500 -1.25194700
H     1.17601900 -0.72773300 -1.48948100
O     1.59721700  0.17762100 -1.14645800
C     2.82503100 -0.12742900 -0.48554600
H     2.68027400 -0.88923400  0.28398700
H     3.54660100 -0.50028100 -1.21413100
H     3.20992000  0.78599500 -0.03532300
H     0.26786500  0.48886100  0.93577600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.279406528527

Frequencies (cm^{-1}): -397.1958, 131.6307, 150.0609, 167.6721, 189.1059, 273.5897, 306.2364, 384.0684, 501.6987, 622.7617, 803.4262, 890.536, 961.1349, 1018.0323, 1095.279, 1129.9263, 1162.4976, 1180.6471, 1279.1974, 1331.1838, 1394.942, 1445.1954, 1466.6335, 1481.7969, 1492.1, 1494.3413, 1514.5557, 1546.5267, 2239.7408, 3018.3546, 3023.911, 3078.031, 3107.2483, 3108.9157, 3114.9856, 3179.2014

MeOCMeH(OOH) (syn-TS-AAAH 1- conformer):

```
C     0.00000000  0.00000000  0.00000000
C    -0.98023900  1.01671600 -0.54052500
H    -1.84106700  1.08931700  0.12171400
H    -1.31899200  0.72756800 -1.53186400
H    -0.49436400  1.98906200 -0.60370900
O    -0.58959600 -1.25813600  0.32171200
O    -1.31811500 -1.76315200 -0.82570100
H    -0.61274000 -2.18738900 -1.33503300
O     1.05435800 -0.13747100 -0.91344000
C     2.20931000 -0.78554100 -0.39182900
H     1.98864900 -1.80372000 -0.06391800
H     2.94205200 -0.81461100 -1.19446900
```

```
H     2.62315000 -0.22395700  0.45192600
H     0.38275300  0.29290900  0.98675900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.353514591133

Frequencies (cm^{-1}): 104.443, 119.9967, 179.107, 200.6491, 224.7602, 287.1186, 298.4192, 408.1047, 543.7423, 677.0747, 811.0196, 879.9263, 918.5731, 1044.7376, 1102.9028, 1116.7671, 1158.7282, 1177.0854, 1228.3618, 1363.4196, 1367.0968, 1378.9297, 1416.6599, 1472.78, 1485.2333, 1490.3867, 1492.3036, 1510.5043, 2986.4766, 2999.6127, 3057.2325, 3057.4133, 3122.3806, 3123.2293, 3141.1224, 3736.0719

IRC:

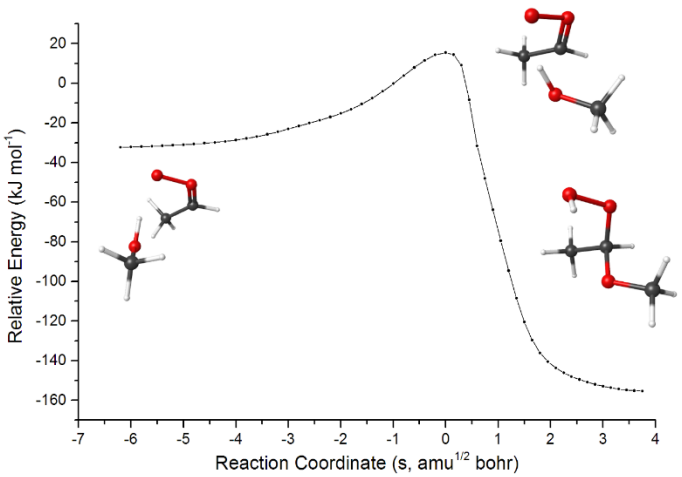


Figure S42: CI2 + MeOH TS-AAAH1 IRC

***Syn*-MeCHOO + MeOH TS-AAAH 2:**

```
C     0.00000000  0.00000000  0.00000000
C    -0.21625100  1.01915200  1.06184800
H     0.63509000  1.70557400  1.00494900
H    -1.11551900  1.60061500  0.87022600
H    -0.24174300  0.56795900  2.04697500
O     0.74049300 -1.04245900  0.14693300
O     0.34168300 -1.71144600  1.38577000
H    -1.00734100 -1.57642100  0.81067800
O    -1.64097400 -1.05679100  0.12197600
C    -2.83883400 -0.62516600  0.75149600
H    -3.50315500 -1.48311600  0.87621600
H    -2.65412900 -0.18293600  1.73301400
H    -3.33222400  0.10710100  0.11288700
H    -0.01943500  0.33797200 -1.03409000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.275604420859

Frequencies (cm^{-1}): -446.1592, 103.8828, 163.1521, 193.1136, 220.5592, 292.1517, 340.1672, 383.661, 463.0537, 611.913, 803.9935, 889.2708, 949.3244, 1016.5869, 1088.107, 1115.1724, 1154.5596, 1176.214, 1234.2944, 1321.9098, 1390.5893, 1429.6039, 1454.0909, 1482.9457, 1487.3505, 1497.2426, 1507.0099, 1586.809, 2115.1408, 3013.34, 3024.7526, 3069.0802, 3093.7878, 3104.4872, 3121.1195, 3173.9841

MeOCMeH(OOH) (syn-TS-AAAH 2-conformer):

```
C     0.00000000  0.00000000  0.00000000
C    -0.20555400  1.32671800 -0.70744900
H    -0.85534300  1.96841500 -0.11348400
H     0.75045200  1.83317600 -0.84015900
H    -0.65721900  1.16510800 -1.68275900
O    -1.20080100 -0.68186500  0.28177200
O    -1.91460100 -0.92640500 -0.95653600
H    -1.47877300 -1.73581200 -1.26184700
O     0.83616800 -0.87593000 -0.73375500
C     2.22430800 -0.70350700 -0.51407200
H     2.73277100 -1.48704500 -1.07097100
H     2.57964800  0.26780100 -0.87245100
H     2.47313400 -0.80271600  0.54838600
H     0.40843200  0.14550900  1.00847100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.348485320129

Frequencies (cm^{-1}): 29.3133, 118.3578, 175.9247, 209.5919, 260.0598, 310.5526, 357.1934, 411.8952, 479.2721, 659.3282, 824.7269, 889.994, 933.7988, 1065.7409, 1102.5152, 1119.7562, 1149.3943, 1174.5695, 1222.7065, 1356.1056, 1372.6921, 1383.4161, 1406.1285, 1473.8874, 1485.6111, 1490.8902, 1496.3555, 1507.0807, 2983.5378, 2991.3478, 3031.4191, 3048.6354, 3108.099, 3116.1468, 3139.2105, 3730.4572

IRC:

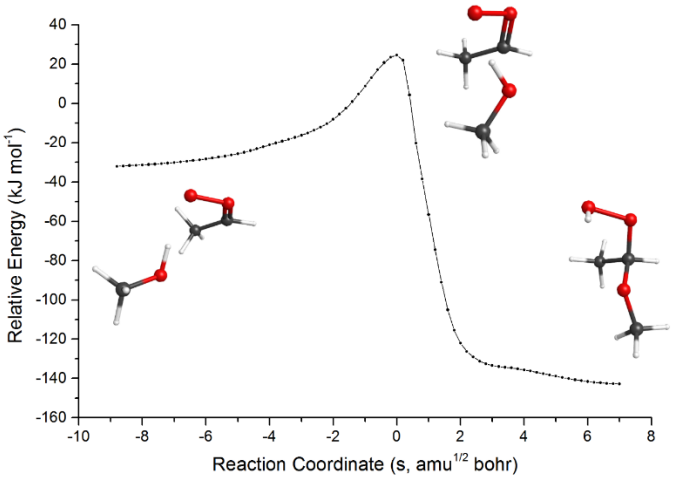


Figure S43: CI2 + MeOH TS-AAAH2 IRC

***Syn*-MeCHOO + MeOH TS-VHP 1:**

```
C     0.00000000  0.00000000  0.00000000
C    -0.90878400 -0.85314300 -0.62917200
H    -1.24929600 -0.51520500 -1.60585600
H    -0.67930300 -1.90711000 -0.55131400
H    -2.02628200 -0.41422900 -0.02226800
O    -0.03627100  1.28704500  0.00255100
O    -1.12287600  1.87122500 -0.72684200
H    -2.16567400  1.28280200 -0.14443800
O    -2.85851400  0.53040800  0.32392900
C    -4.13087900  0.49066300 -0.31566700
H    -4.63508600  1.44875100 -0.18657000
H    -4.03633400  0.28482300 -1.38634500
H    -4.73662800 -0.28842700  0.14552600
H     0.78490500 -0.35449500  0.66269900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.266640210157

Frequencies (cm^{-1}): -1530.7382, 87.3068, 102.6275, 168.9847, 203.9693, 299.8036, 416.9415, 510.5014, 533.9398, 630.9529, 740.5212, 855.9951, 882.6891, 1001.1029, 1022.6338, 1062.5289, 1071.2723, 1168.4684, 1188.7897, 1226.6186, 1331.4791, 1343.7663, 1391.201, 1450.2197, 1497.5103, 1501.4886, 1520.2661, 1567.6408, 1609.1575, 1854.5331, 3004.5386, 3070.7592, 3090.8088, 3099.3488, 3142.6128, 3199.2117

H_2C=CH(OOH) - VHP + MeOH complex 1:

```
C     0.00000000  0.00000000  0.00000000
C    -0.33985900  0.93638800  0.88021600
H    -0.92698800  0.71728500  1.75723300
H     0.03577200  1.93771400  0.73927800
H    -2.93967100  0.41347000 -0.07209300
```

```
O    -0.33936600 -1.31338000 -0.02864300
O    -1.16628700 -1.67922700  1.09451200
H    -2.05456300 -1.42307200  0.75871400
O    -3.39928600 -0.43032900  0.00828500
C    -4.73412000 -0.21479900  0.47004200
H    -5.20269600 -1.19294100  0.54537800
H    -4.74957200  0.26169900  1.45303500
H    -5.30240500  0.39314100 -0.23669800
H     0.62605300  0.19390900 -0.86328100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.325392828367

Frequencies (cm^{-1}): 31.7819, 40.0738, 79.7338, 95.3892, 117.9366, 204.5889, 297.7216, 323.9278, 395.4797, 623.0355, 663.2986, 731.3899, 852.148, 897.1172, 981.2267, 985.4758, 1039.8809, 1087.2077, 1166.9172, 1174.3809, 1322.9567, 1368.6711, 1425.8772, 1477.995, 1499.1126, 1510.1241, 1523.5455, 1680.1363, 3013.7517, 3068.3937, 3122.6849, 3165.9197, 3179.5639, 3264.4978, 3451.8589, 3774.0356

IRC:

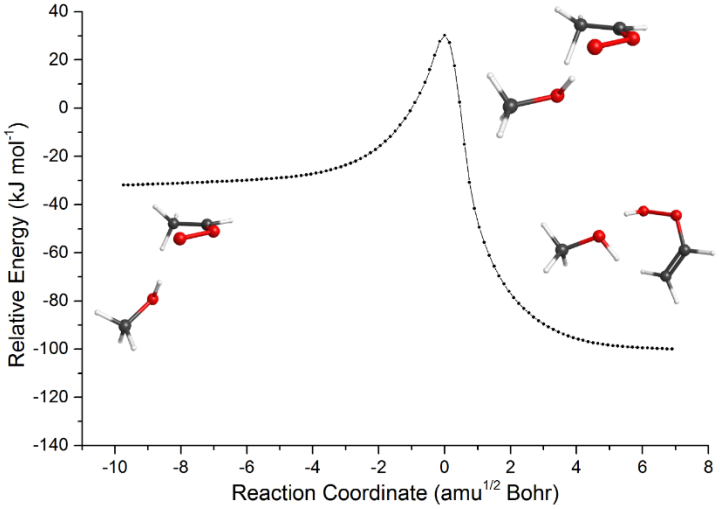


Figure S44: CI2 + MeOH TS-VHP1 IRC

***Syn*-MeCHOO + MeOH TS-VHP 2:**

```
C     0.00000000  0.00000000  0.00000000
C     0.44839500  0.89603200 -0.97284600
H     0.34185000  0.55099100 -1.99946700
H     0.19562100  1.93276700 -0.79776800
H     1.74179100  0.56272800 -0.96415700
O     0.14337300 -1.27943900 -0.01764100
O     0.80219600 -1.80918800 -1.17649800
H     1.94312600 -1.12700100 -1.16229400
O     2.71182800 -0.31037800 -1.12763600
C     3.61710100 -0.41780900 -0.03398200
H     3.94944700 -1.45070400  0.07129200
H     4.48359300  0.21530200 -0.22206300
H     3.14803400 -0.10661800  0.90591200
H    -0.42180700  0.31783800  0.95001500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.267273733505,

Frequencies (cm^{-1}): -1512.6012, 60.7508, 99.6999, 162.3849, 217.0393, 307.1675, 425.9458, 500.4219, 527.4264, 633.7485, 754.0229, 850.0857, 875.9974, 1005.4435, 1020.6123, 1068.8079, 1132.5827, 1164.7838, 1182.8747, 1228.8595, 1324.3611, 1340.3225, 1435.3473, 1469.4813, 1490.121, 1501.7385, 1515.3217, 1578.035, 1607.5096, 1755.4713, 2993.4577, 3066.3841, 3091.4508, 3099.1109, 3139.4463, 3200.5616

H_2C=CH(OOH) - VHP + MeOH complex 2:

```
C     0.00000000  0.00000000  0.00000000
C    -0.06927700  0.87007700 -1.00238800
H     0.25643700  0.62785100 -2.00102000
H    -0.52033400  1.83278600 -0.81957800
H     2.70489400  0.71119900 -0.84332200
O     0.51266600 -1.25729400  0.00904400
O     0.98945100 -1.65230000 -1.29328600
H     1.88917500 -1.25184200 -1.28694900
O     3.23541900 -0.05230700 -1.10035600
C     4.33770800 -0.19921500 -0.20088700
H     4.90352000 -1.06466500 -0.53661300
H     4.98721400  0.67780700 -0.22829000
H     4.00027200 -0.37208800  0.82320300
H    -0.36244500  0.21253800  0.99921200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.326400120091

Frequencies (cm^{-1}): 32.6476, 38.3289, 75.0564, 106.3568, 122.6463, 203.2842, 292.9931, 325.3109, 442.5272, 625.1624, 700.5628, 742.9204, 854.9108, 896.669, 980.5174, 984.7182, 1036.4971, 1089.545, 1165.9722, 1174.8168, 1323.4698, 1368.7856, 1427.7273, 1477.4537, 1499.0609, 1506.5522, 1511.0693, 1680.5952, 3016.7566, 3072.6337, 3123.8852, 3164.9465, 3179.0679, 3264.4967, 3425.1115, 3767.2729

IRC:

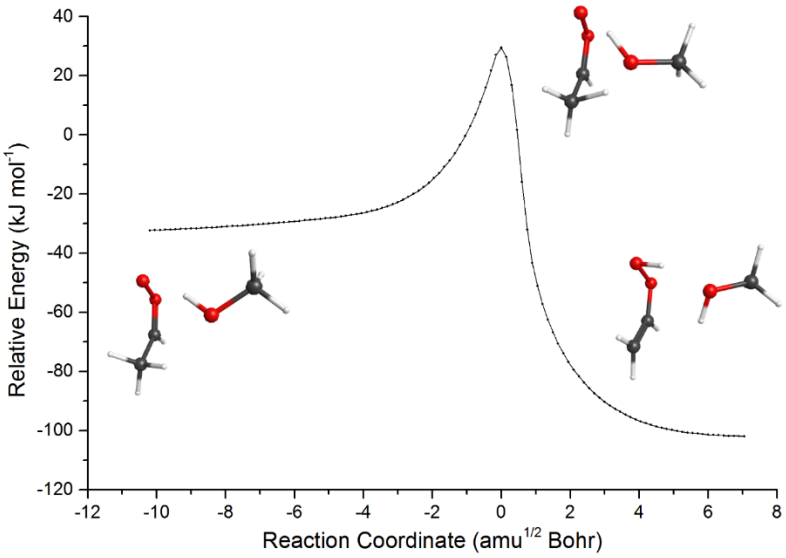


Figure S45: CI2 + MeOH TS-VHP2 IRC

7.3 sCI 3 + MeOH Reactions

***Anti*-CH_3CHOO (sCI3):**

```
C    0.00000000  0.00000000  0.00000000
C   -1.38803600  0.50558200 -0.00000400
O   -2.34008600 -0.31152000 -0.00000400
O   -3.62306400  0.17147900  0.00000200
H   -1.64849900  1.56040000 -0.00000300
H    0.53486200  0.37351800  0.87740600
H    0.01869600 -1.08709800 -0.00007200
H    0.53491300  0.37364100 -0.87732100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -228.668479728521

Frequencies (cm^{-1}): 160.7712, 257.9322, 323.9454, 553.463, 868.0016, 892.5804, 968.0414, 1067.4143, 1157.1835, 1344.0387, 1414.6149, 1458.7683, 1462.9479, 1577.5039, 3020.0875, 3061.4456, 3132.2104, 3146.0088

***Anti*-CH_3CHOO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2):**

```
C    0.00000000  0.00000000  0.00000000
C    1.11334700 -0.86845900  0.42606800
H    1.77621900 -1.06164600 -0.42127400
H    1.67574800 -0.42154200  1.24172700
H    0.71366200 -1.83689700  0.73873400
O   -0.18000500  1.08891100  0.59154600
O   -1.25217500  1.88161900  0.19382300
H   -2.54110500  0.64583400  0.00376600
O   -2.94017200 -0.24538800 -0.09260000
C   -4.19246400 -0.28299700  0.57020500
H   -4.59251100 -1.29118800  0.46662200
H   -4.90813200  0.41765700  0.12808600
H   -4.09906200 -0.05670200  1.63739700
H   -0.68810700 -0.26291400 -0.79710300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.291194821865

Frequencies (cm^{-1}): 24.1277, 58.5239, 94.5458, 109.9884, 142.1899, 176.1324, 222.6489, 278.1331, 342.8755, 550.5453, 763.9483, 865.1221, 875.434, 963.6916, 1063.5511, 1077.1458, 1140.6275, 1167.2565, 1172.982, 1367.0671, 1413.6171, 1456.5842, 1460.1495, 1461.609, 1477.7834, 1496.6622, 1514.0436, 1593.768, 2986.0785, 3024.4888, 3028.2979, 3068.7618, 3086.6158, 3138.8693, 3163.4716, 3420.8118

***Anti*-CH_3CHOO + MeOH TS-AAAH 1:**

```
C    0.00000000  0.00000000  0.00000000
C   -0.61097900 -1.28818400 -0.40941900
H   -0.41419700 -1.50900500 -1.45561000
H   -0.23222100 -2.08912000  0.22297000
H   -1.69165600 -1.22810300 -0.25710900
O    0.11755000  0.91711800 -0.88794900
O    0.99621300  1.93869400 -0.33291800
H    1.83183200  0.83317500  0.14939300
O    1.93630200 -0.21545600  0.33533000
C    2.67728100 -0.79000100 -0.73711400
H    3.70249600 -0.41614700 -0.71280900
H    2.69130300 -1.87197700 -0.61322600
H    2.24036000 -0.53487200 -1.70624300
H   -0.04189800  0.31385400  1.03653200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.284400718806

Frequencies (cm^{-1}): -393.3306, 122.7671, 134.4411, 153.7728, 168.2617, 276.953, 298.1085, 390.8011, 530.3497, 547.1394, 834.7784, 947.205, 972.9554, 1006.7118, 1112.87, 1147.7291, 1174.8048, 1182.8873, 1266.4063, 1344.3021, 1406.9368, 1447.1639, 1463.7634, 1477.5304, 1493.1988, 1496.3787, 1514.7178, 1545.678, 2092.9072, 3011.7606, 3038.1481, 3069.6983, 3099.8287, 3103.567, 3139.1644, 3156.4855

MeOCMeH(OOH) (TS-AAAH 1 - conformer):

```
C     0.00000000  0.00000000  0.00000000
C     0.86314200  1.13998900  0.51304400
H     0.28950300  2.06443800  0.49677300
H     1.19705500  0.96343800  1.53421100
H     1.73358100  1.25387500 -0.13150400
O    -1.01839000 -0.17412700  0.97165300
O    -2.06167600 -0.99474900  0.39444600
H    -1.64089500 -1.86780300  0.37349500
O     0.68077500 -1.21069400 -0.24737600
C     1.51381400 -1.70236800  0.79993300
H     0.98720400 -1.73066600  1.75628100
H     1.79313700 -2.71425400  0.51618200
H     2.42160700 -1.10401100  0.90572200
H    -0.46529800  0.24426300 -0.95480300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.352771418775

Frequencies (cm^{-1}): 109.0938, 145.1609, 188.2537, 223.7424, 252.1432, 295.0359, 326.63, 393.6881, 550.8546, 642.2534, 825.5391, 861.3783, 949.9567, 999.3459, 1089.9956, 1134.9783, 1167.2628, 1174.1278, 1220.7307, 1350.3371, 1388.4468, 1400.7708, 1415.6577, 1468.6003, 1485.4159, 1495.3909, 1502.6202, 1513.5496, 3012.9142, 3052.0661, 3069.0697, 3073.7671, 3117.9549, 3123.0287, 3126.3706, 3717.0227

IRC:

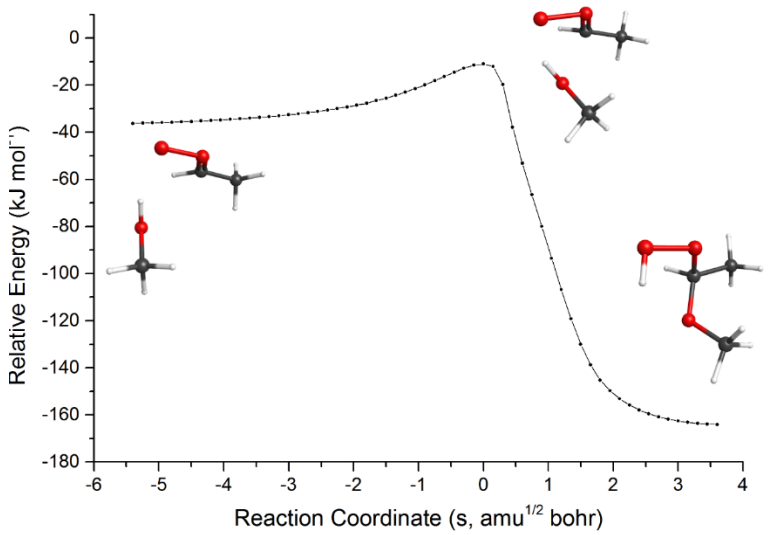


Figure S46: CI3 + MeOH TS-AAAH1 IRC

***Anti*-CH_3CHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C     0.66337100 -1.26545300  0.39696200
H    -0.03996300 -2.09170500  0.31199000
H     1.49323100 -1.46121900 -0.28705800
H     1.04174800 -1.20385500  1.41383700
O     0.44159000  1.08799900  0.50700400
O    -0.54232600  2.12718800  0.23078300
H    -1.51609800  1.15041300  0.71521800
O    -1.75390400  0.12406000  0.90882600
C    -2.90152400 -0.25754800  0.16603800
H    -3.08003200 -1.32210500  0.31420800
H    -3.77251800  0.29829200  0.51919100
H    -2.77991600 -0.05838200 -0.90414300
H    -0.52186200  0.07164900 -0.94949800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.282545043808

Frequencies (cm^{-1}): -394.9855, 80.4244, 116.505, 145.2087, 202.4621, 262.8528, 294.3244, 391.2047, 501.6111, 533.7763, 837.5701, 945.0333, 987.6606, 1021.5677, 1091.9192, 1132.6488, 1175.4093, 1180.1427, 1244.0182, 1328.6498, 1403.3432, 1438.9491, 1456.3302, 1475.7515, 1494.4683, 1496.9772, 1505.9988, 1586.9451, 2094.5908, 2994.0729, 3037.4152, 3056.2325, 3093.3918, 3105.3984, 3122.6524, 3149.3408

MeOCMeH(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -0.35125000  1.45787000 -0.23016500
H     0.27351000  2.10457300  0.38379000
H    -0.20973100  1.70955100 -1.28012900
H    -1.39462300  1.62770100  0.03297100
O     1.32638200 -0.14786600 -0.43393600
O     1.78447200 -1.46614500 -0.05041900
H     1.40306500 -2.00743900 -0.75801100
O    -0.80856400 -0.87590300 -0.76615800
C    -1.96094700 -1.35896100 -0.09657900
H    -2.67297500 -0.55688300  0.12271400
H    -2.43738700 -2.07327100 -0.76397500
H    -1.69545200 -1.86268000  0.83870200
H    -0.06849000 -0.28238200  1.05735700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -344.352166027901

Frequencies (cm^{-1}): 65.672, 144.7937, 179.9866, 207.1258, 255.0937, 294.1767, 368.3543, 389.6626, 533.1852, 573.93, 845.0489, 890.7359, 955.6489, 1056.8447, 1110.572, 1121.4475, 1172.6028, 1176.3062, 1227.7075, 1354.8775, 1386.4962, 1393.2652, 1410.1388, 1474.1542, 1485.3854, 1489.9677, 1496.4658, 1508.1268, 2985.7972, 2995.0324, 3035.1603, 3047.7784, 3115.9663, 3116.9699, 3124.868, 3724.7087

IRC:

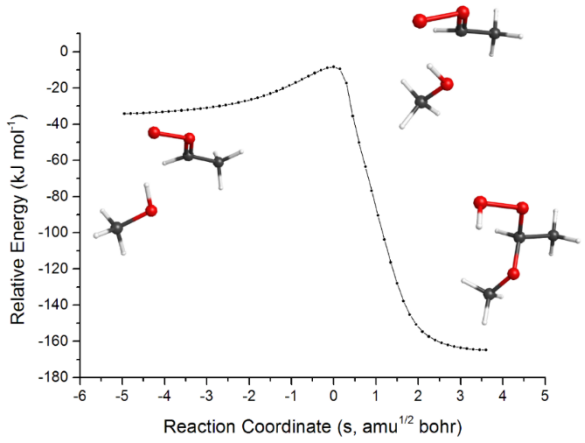


Figure S47: CI3 + MeOH TS-AAAH1 IRC

7.4 sCI 4 + MeOH Reactions

$(CH_3)_2COO$ (sCI 4):

```
C    0.00000000  0.00000000  0.00000000
C   -0.30578400 -1.44069700 -0.00004900
O    0.63931300 -2.28149100 -0.00006200
O    1.93004900 -1.79139200  0.00006000
C   -1.67952100 -2.00628600  0.00001900
H   -2.22979800 -1.65674400 -0.87712800
H   -1.65054000 -3.09294000 -0.00074000
H   -2.22914600 -1.65810600  0.87815100
H   -0.90400600  0.60295400 -0.00000100
H    0.62828600  0.22944300  0.86521800
H    0.62830100  0.22943600 -0.86521500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -267.942548424148

Frequencies (cm^{-1}): 154.4006, 175.2362, 276.7598, 307.3227, 362.2999, 482.7868, 597.6461, 812.1378, 923.5456, 934.001, 985.0296, 1069.8677, 1093.6544, 1305.1965, 1393.1797, 1408.4507, 1437.8517, 1457.7152, 1469.1474, 1476.0494, 1560.1656, 3020.7584, 3025.473, 3060.802, 3066.4683, 3135.3854, 3137.3671

$(CH_3)_2COO$ (sCI 4) unimolecular TS to VHP:

```
C    0.00000000  0.00000000  0.00000000
C    0.53755300 -1.29688400 -0.08508400
O   -0.33316300 -2.26651200 -0.07391500
O   -1.63959300 -1.73747100  0.04568700
C    1.95437800 -1.73148600  0.01732700
H    2.45048200 -1.16616000  0.80741400
H    2.02407800 -2.79577100  0.23219700
H    2.48153700 -1.51533900 -0.91370100
H    0.66937200  0.77546400  0.34991800
H   -0.62150100  0.31474100 -0.83776700
H   -1.11770000 -0.57024400  0.47282200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -267.913397296005

Frequencies (cm^{-1}): -1584.8495, 111.7224, 272.4485, 362.2987, 516.9334, 544.7828, 662.8644, 741.519, 858.314, 922.5496, 954.2223, 988.4561, 1035.0763, 1083.4103, 1325.5424, 1357.0368, 1404.5, 1456.5571, 1470.8431, 1504.5593, 1531.3424, 1843.6945, 3037.2371, 3080.9141, 3090.9011, 3128.3112, 3177.6281

H_2C=CMe(OOH) - VHP:

```
C    0.00000000  0.00000000  0.00000000
C   -0.14486200 -1.31972500  0.00603800
O    0.87877900 -2.24322000  0.03204200
O    2.17426800 -1.61037900  0.09820800
C   -1.43650300 -2.07652900 -0.00593200
H   -1.49480000 -2.73423600 -0.87478900
H   -1.52632900 -2.69903400  0.88564300
H   -2.27140200 -1.38094300 -0.03506900
H   -0.88071200  0.62200800 -0.01988600
H    0.96736900  0.47167000  0.02978700
H    2.50385200 -1.78635200 -0.79468700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -267.970969822090

Frequencies (cm^{-1}): 144.318, 154.2998, 168.4195, 317.6569, 400.862, 507.8903, 550.6466, 739.3176, 850.8333, 864.0816, 928.1528, 974.1543, 1025.2415, 1075.3812, 1265.3971, 1381.6336, 1405.8651, 1433.9865, 1472.7973, 1490.7223, 1718.1838, 3035.5108, 3084.4467, 3130.7106, 3180.8733, 3271.5462, 3745.0049

IRC

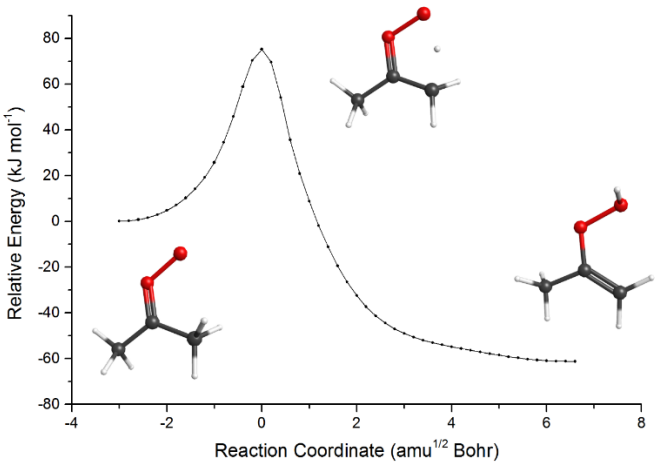


Figure S48: SCI 4 + MeOH TS-AAAH1 IRC

$(CH_3)_2COO$ + MeOH PRC (for all TS-AAAH 1, TS-AAAH 2, TS-VHP 1 and TS-VHP 2):

```
C     0.00000000  0.00000000  0.00000000
O    -1.28736900 -0.27840200  0.51958800
H    -3.25510100 -0.94680500  1.52696600
H    -0.04847600  0.56953300 -0.93423600
H     0.48884500 -0.95223300 -0.20512400
H     0.61843400  0.55606800  0.71257400
C    -4.64570700  0.21254800  0.46498300
C    -4.26312200 -0.54135600  1.66970300
H    -4.96584800 -1.34594700  1.86869700
H    -4.18577300  0.14889600  2.51199000
O    -4.07651900  1.29947800  0.16451300
O    -3.05585300  1.75172300  1.00467200
H    -1.76600200  0.56019300  0.69551900
C    -5.70507500 -0.23021300 -0.47711600
H    -5.81611100  0.47092600 -1.29982100
H    -5.45357400 -1.21866600 -0.86887300
H    -6.65452900 -0.33052500  0.05374900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 29.2301, 50.293, 83.0903, 104.8733, 126.475, 152.2589, 202.663, 234.0962, 305.7377, 322.6976, 370.7865, 493.0567, 589.8817, 782.5501, 813.4058, 906.9631, 929.7052, 989.0856, 1065.9963, 1074.6435, 1101.1533, 1139.6531, 1173.1989, 1305.7738, 1391.1632, 1407.0417, 1439.5073, 1457.6824, 1458.9983, 1470.9003, 1476.8964, 1488.4994, 1495.8741, 1513.5426, 1571.4374, 2982.1615, 3010.7591, 3022.8432, 3029.4251, 3069.7265, 3075.8566, 3082.7413, 3138.8025, 3141.748, 3412.8051

$(CH_3)_2COO$ + MeOH TS-AAAH 1:

```
C     0.00000000  0.00000000  0.00000000
O    -1.11295900 -0.52599300  0.71068900
H    -3.43504900 -1.71010100  1.33597300
H    -0.13814600 -0.08491800 -1.08157500
H     0.13460000  1.04726600  0.27027300
H     0.90119700 -0.55307300  0.27364400
C    -2.87517500 -0.30540600 -0.18064600
C    -3.64997300 -0.69049600  1.04021400
H    -3.44214800 -0.00581900  1.85763400
H    -4.71045800 -0.61037000  0.78192200
O    -2.60612300 -1.16620200 -1.11585000
O    -2.08334000 -2.38099200 -0.50467600
H    -1.32259200 -1.52781200  0.31970300
C    -2.98851600  1.09962700 -0.67672300
H    -2.35171000  1.26306800 -1.54174900
H    -2.72613400  1.79482100  0.11833000
H    -4.02526200  1.29385900 -0.96037800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): -542.1058, 105.2947, 140.8329, 145.6405, 164.2125, 170.4625, 253.6007, 309.9624, 315.1715, 375.4308, 413.2895, 528.4149, 562.7184, 789.0468, 877.509, 933.241, 982.7668, 991.8185, 1053.8371, 1075.6199, 1139.0335, 1175.4217, 1224.9417, 1293.6019, 1400.7749, 1405.0681, 1422.2621, 1455.6239, 1467.6699, 1477.5918, 1490.4867, 1493.9917, 1499.9618, 1512.1355, 1536.8006, 1894.3654, 3006.1197, 3028.563, 3043.8559, 3061.5936, 3089.1853, 3107.2207, 3121.1314, 3146.4292, 3179.5415

$MeOCMe_2(OOH)$ (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
O    -1.11784900  0.58322700  0.66105000
H    -3.41419400  1.24041700  1.50895200
H    -0.29764100 -0.53698500 -0.90339200
H     0.75157800  0.74897600 -0.26037200
H     0.43788600 -0.70237300  0.70582800
C    -2.02044600  1.33699300 -0.13094900
C    -2.98933500  1.98587100  0.84326100
H    -2.46165000  2.72847800  1.43966400
H    -3.79514600  2.47216800  0.29669300
O    -2.68153200  0.47400300 -1.06876100
O    -3.52544400 -0.47269500 -0.37275100
H    -2.87492000 -1.09563500 -0.01617600
C    -1.33707200  2.35606700 -1.04022700
H    -0.75870900  1.86962100 -1.82320600
H    -0.67448500  2.98330200 -0.44540800
H    -2.08634700  2.98671700 -1.51374200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 108.6153, 131.8909, 181.6035, 188.4754, 221.4317, 240.4669, 266.2507, 305.599, 358.8687, 395.6225, 419.6752, 561.7407, 592.8478, 752.2496, 817.923, 927.8505, 935.0723, 947.6452, 1018.1094, 1081.1583, 1172.3246, 1175.2916, 1200.6824, 1224.5345, 1284.536, 1381.7463, 1401.6313, 1417.7927, 1467.0273, 1477.8099, 1483.9939, 1493.2019, 1499.8278, 1507.4927, 1516.0929, 3011.1758, 3052.8434, 3058.5851, 3066.0529, 3113.4003, 3120.5911, 3125.3895, 3129.3025, 3145.079, 3722.9154

IRC:

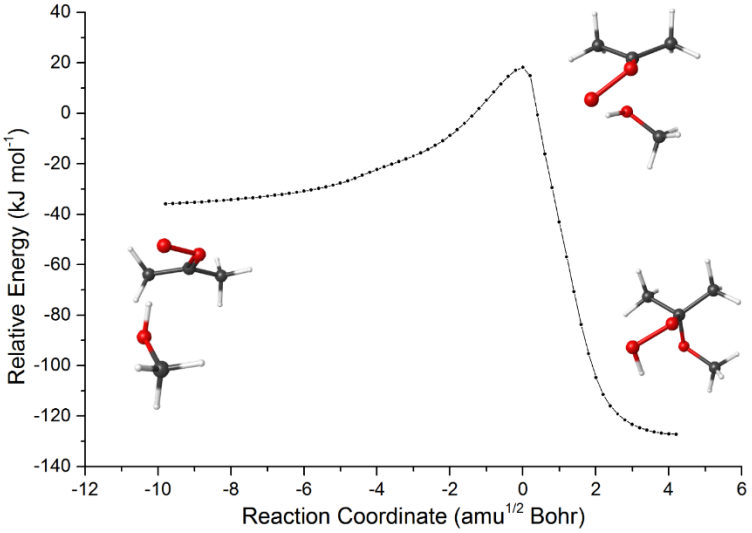


Figure S49: SCI 4 + MeOH TS-AAAH2 IRC

$(CH_3)_2COO$ + MeOH TS-AAAH 2

```
C     0.00000000  0.00000000  0.00000000
O     1.16748900  0.45758600 -0.65678300
H     2.21448300  1.06170900  1.93213600
H    -0.87938500  0.33011100 -0.55910200
H    -0.00190200 -1.09114100  0.02641500
H    -0.07893500  0.38078600  1.02197900
C     3.00159900  0.32881900  0.08306900
C     2.69036700  0.17173800  1.53727300
H     2.08064000 -0.70955000  1.72059700
H     3.64698700  0.02391900  2.04797700
O     3.30371400  1.48817300 -0.41592000
O     2.30745600  2.46468600  0.01636600
H     1.38913100  1.50869300 -0.40716500
C     3.63066400 -0.81356300 -0.64483300
H     3.68178200 -0.60328600 -1.70901700
H     3.06144500 -1.72489600 -0.47441500
H     4.64116200 -0.96977200 -0.25965800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): -584.6247, 93.485, 99.7219, 138.3562, 194.5328, 205.7747, 242.7864, 294.4172, 337.3609, 373.5505, 416.6378, 492.5093, 548.4031, 785.2219, 872.894, 925.8863, 953.6621, 984.2998, 1054.9711, 1083.6158, 1121.2347, 1173.9684, 1213.6066, 1282.3549, 1368.0143, 1396.3183, 1407.7932, 1430.0297, 1458.3665, 1476.5658, 1482.4862, 1493.6838, 1495.5358, 1504.6778, 1537.0986, 1943.1351, 3000.0751, 3028.0434, 3041.9028, 3054.0903, 3070.4794, 3106.6607, 3112.4802, 3152.281, 3173.0231

$MeOCMe_2(OOH)$ (TS-AAAH 2- conformer)

```
C     0.00000000  0.00000000  0.00000000
O     1.30336700  0.26162500 -0.48977400
H     2.34729100  0.30412100  1.98193500
H    -0.42146600 -0.76392800 -0.64983800
H    -0.64258700  0.88456700 -0.04499600
H     0.01181800 -0.37905800  1.02494600
C     2.04564300  1.33118400  0.10092500
C     2.04563600  1.28560300  1.62517000
H     1.06169900  1.52588500  2.02566500
H     2.75403700  2.02260100  1.99938700
O     3.35529800  1.18703600 -0.42801500
O     3.93884400 -0.05644500  0.02789500
H     3.47693000 -0.69192400 -0.53976900
C     1.59588500  2.67846400 -0.45547200
H     1.67798600  2.67150700 -1.54044500
H     0.55933700  2.86844200 -0.17993400
H     2.21042400  3.48215900 -0.05376100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 108.6153, 131.8909, 181.6035, 188.4754, 221.4317, 240.4669, 266.2507, 305.599, 358.8687, 395.6225, 419.6752, 561.7407, 592.8478, 752.2496, 817.923, 927.8505, 935.0723, 947.6452, 1018.1094, 1081.1583, 1172.3246, 1175.2916, 1200.6824, 1224.5345, 1284.536, 1381.7463, 1401.6313, 1417.7927, 1467.0273, 1477.8099, 1483.9939, 1493.2019, 1499.8278, 1507.4927, 1516.0929, 3011.1758, 3052.8434, 3058.5851, 3066.0529, 3113.4003, 3120.5911, 3125.3895, 3129.3025, 3145.079, 3722.9154

IRC:

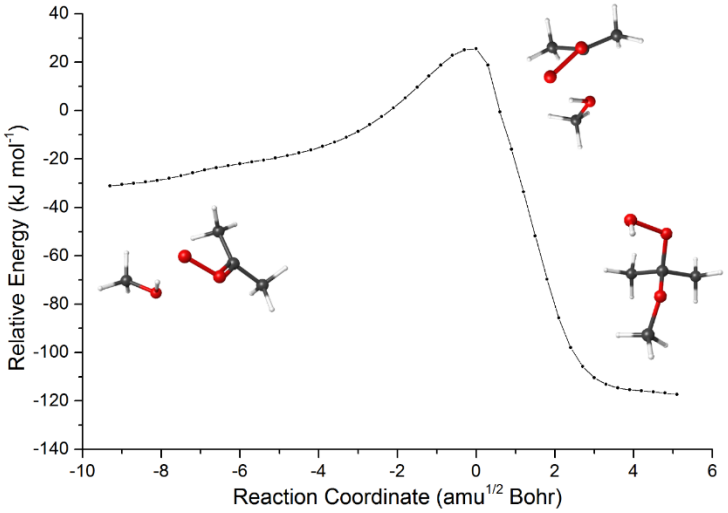


Figure S50: SCI 4 + MeOH TS-AAAH2 IRC

$(CH_3)_2COO$ + MeOH VHP-TS1

```
C     0.00000000  0.00000000  0.00000000
O    -1.32517500  0.18582600 -0.47385600
H    -2.24766400 -0.50245800  0.16011900
H     0.63817600  0.81127900 -0.35485800
H     0.39575600 -0.94211500 -0.38149100
H     0.04126900 -0.01830200  1.09494500
C    -4.17157700  0.26836500  0.27362800
C    -3.31156800 -0.60398300  0.95800100
H    -3.70599900 -1.59719900  1.12863200
H    -2.80085100 -0.15438500  1.80656300
O    -3.88995300  1.51190900  0.03427700
O    -2.61758400  1.97118300  0.51437600
H    -1.83573500  1.15397600 -0.04385200
C    -5.45142600 -0.15369800 -0.37116900
H    -5.84480200  0.63165500 -1.01116600
H    -5.28463400 -1.05549800 -0.96090500
H    -6.18584500 -0.39661600  0.39847000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.535424640651

Frequencies (cm^{-1}): -1594.6705, 69.3128, 74.8652, 88.9827, 143.3423, 170.7932, 266.8212, 305.316, 372.0185, 472.7133, 552.6919, 601.5793, 618.4108, 708.9615, 858.8442, 871.9535, 923.0351, 979.3887, 1010.4476, 1054.5491, 1072.8212, 1087.1724, 1169.4178, 1185.5864, 1274.4606, 1348.7056, 1389.0911, 1406.9266, 1446.1006, 1473.8413, 1482.6185, 1497.1474, 1498.5275, 1503.5348, 1560.2298, 1596.7206, 1832.1122, 2988.745, 3042.3362, 3052.1461, 3079.4098, 3091.9264, 3097.44, 3140.0195, 3189.4064

H_2C=CMe(OOH) - VHP + MeOH (TS-VHP 1 complex):

```
C     0.00000000  0.00000000  0.00000000
O    -1.35761900  0.26667100 -0.35291100
H    -1.93194200 -0.42072900  0.00827700
H     0.59928000  0.80469200 -0.41917200
H     0.33980500 -0.94731300 -0.42383400
H     0.14069200 -0.01765300  1.08352400
C    -4.66646600  0.28302800  0.27665900
C    -4.16500900 -0.29998700  1.36673500
H    -4.56396000 -1.25112400  1.68182200
H    -3.42770800  0.18497200  1.98490800
O    -4.27717000  1.48658400 -0.24239500
O    -3.23979100  2.12036800  0.52982400
H    -2.44293600  1.66961400  0.17191000
C    -5.75003200 -0.27136900 -0.59618900
H    -5.40243100 -0.37852000 -1.62463200
H    -6.06968900 -1.24217400 -0.22595300
H    -6.60796900  0.40251100 -0.60806900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.590545229659

Frequencies (cm^{-1}): 34.4524, 46.6981, 79.4594, 91.0047, 122.1561, 147.3463, 163.76, 246.4209, 322.4014, 402.4579, 420.7433, 527.0608, 557.187, 675.6031, 756.032, 839.8422, 869.6658, 931.8412, 989.3061, 1027.416, 1041.6763, 1074.174, 1093.1976, 1174.3548, 1281.5583, 1373.7908, 1403.3782, 1430.9277, 1472.2756, 1477.1221, 1490.4161, 1499.0017, 1510.0379, 1522.8883, 1695.4424, 3011.242, 3038.3394, 3064.7692, 3088.6797, 3120.1439, 3131.2497, 3175.0858, 3264.6745, 3460.2036, 3741.2533

IRC:

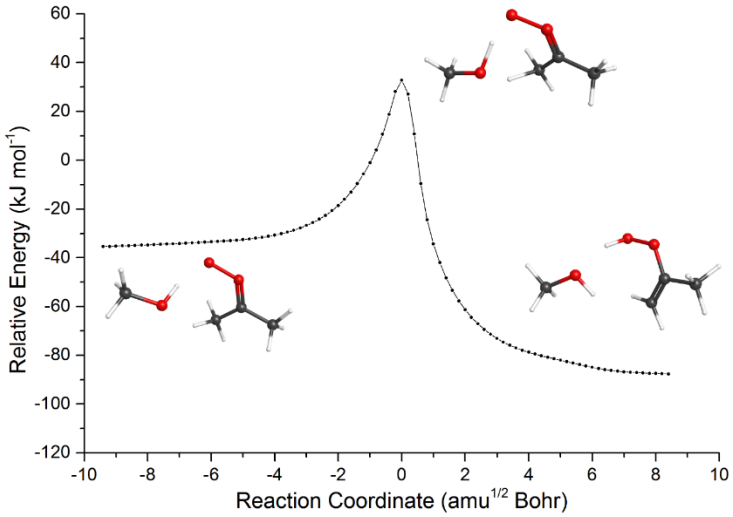


Figure S51: SCI 4 + MeOH TS-VHP1 IRC

$(CH_3)_2COO$ + MeOH TS-VHP 2

```
C     0.00000000  0.00000000  0.00000000
O    -0.54721100  0.72128700  1.09204600
H    -1.67248900  0.24051400  1.58836600
H    -0.76323900 -0.59705200 -0.51391600
H     0.78176800 -0.67172900  0.35731900
H     0.43698400  0.68946400 -0.72457100
C    -3.50853700  0.76929200  0.76409500
C    -2.93119300  0.38479700  1.98390100
H    -3.39871800 -0.46092000  2.47066300
H    -2.66769100  1.21238800  2.63880300
O    -3.10973100  1.79255500  0.07403200
O    -2.03916400  2.56155800  0.64651600
H    -1.14800400  1.67981300  0.79711200
C    -4.56885800 -0.01009800  0.05555600
H    -4.63065900  0.27152800 -0.99261200
H    -4.36982100 -1.07748700  0.14231700
H    -5.53251700  0.18325000  0.53145800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.535800181699

Frequencies (cm^{-1}): -1565.4743, 47.9277, 76.7446, 100.9373, 157.7549, 165.4775, 278.6508, 312.2948, 367.0841, 472.7308, 555.039, 584.9121, 614.3866, 740.0767, 867.131, 869.698, 918.2927, 984.5426, 1012.9337, 1055.5033, 1071.6305, 1096.6679, 1168.0784, 1179.3929, 1341.5511, 1349.1594, 1405.7055, 1432.7597, 1462.1, 1475.8943, 1483.9598, 1491.0947, 1501.4776, 1526.4916, 1553.4961, 1576.0403, 1715.9907, 2978.3014, 3040.7055, 3047.7921, 3079.1283, 3093.3993, 3099.4994, 3138.6948, 3192.5381

H_2C=CMe(OOH) - VHP + MeOH (TS-VHP 2 complex)

```
C     0.00000000  0.00000000  0.00000000
O    -0.86513500  0.79849200  0.80985500
H    -1.52309200  0.23784900  1.23993000
H    -0.55019300 -0.51614800 -0.78993900
H     0.54158300 -0.73114200  0.60359300
H     0.71795400  0.67710200 -0.45631200
C    -4.25491300  0.67486400  0.47448400
C    -4.06161800  0.77295400  1.79023900
H    -4.56458900  0.08051800  2.44655300
H    -3.47625200  1.56671200  2.22429700
O    -3.69772600  1.48031400 -0.48129800
O    -2.89181700  2.53539000  0.07703900
H    -2.04282300  2.06090300  0.22630100
C    -5.11640100 -0.33871400 -0.21433000
H    -4.54037000 -0.91099500 -0.94313500
H    -5.54611200 -1.02249000  0.51336100
H    -5.92502500  0.15687000 -0.75372800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -383.591348152262

Frequencies (cm^{-1}): 31.6634, 42.8335, 80.133, 88.3117, 118.3903, 153.91, 161.857, 233.7713, 321.6895, 400.3668, 456.8527, 524.5145, 556.2369, 706.3067, 758.2925, 843.3365, 870.1948, 930.7342, 988.3076, 1027.5599, 1039.4795, 1073.6798, 1094.2156, 1174.2588, 1279.8218, 1370.7828, 1403.9255, 1430.9187, 1471.5176, 1477.0989, 1489.5772, 1499.1179, 1503.6343, 1510.0766, 1696.9922, 3014.1736, 3036.5534, 3068.9324, 3085.941, 3121.8008, 3129.6944, 3175.3935, 3264.8588, 3440.5522, 3748.2505

IRC:

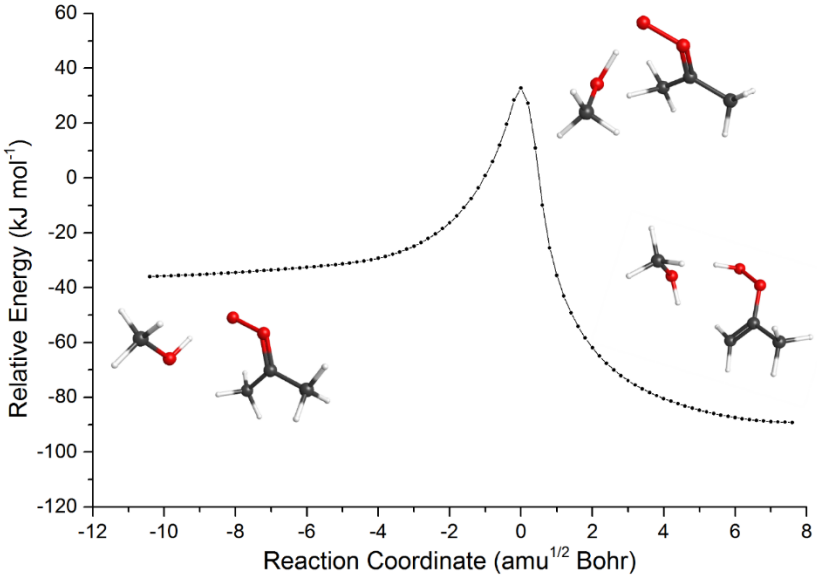


Figure S52: SCI 4 + MeOH TS-VHP2 IRC

7.5 sCI 5 + MeOH Reactions

***Syn*-FCHOO (SCI 5)**

```
C    0.00000000  0.00000000  0.00000000
F    1.26206600 -0.28955700 -0.00000000
H   -0.28198500  1.04286300  0.00000000
O   -0.87888600 -0.87633300  0.00000000
O   -0.50569100 -2.20595700  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -288.580110102018

Frequencies (cm^{-1}): 290.0998, 484.4623, 767.8081, 783.282, 845.1624, 1205.1578, 1343.4876, 1593.6522, 3233.1781

***Syn*-FCHOO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2):**

```
C    0.00000000  0.00000000  0.00000000
O   -1.26400800 -0.46837100  0.44400600
H   -1.76819700  0.27791900  0.81308800
H   -0.09487800  0.78466600 -0.75762100
H    0.60414900  0.38569100  0.82703700
H    0.52509800 -0.84539200 -0.44260800
C   -4.14481300 -0.39146200 -0.34132700
O   -3.83708300  0.80853500 -0.34757300
O   -3.35044700  1.37347900  0.83624500
H   -4.48713500 -0.85548600 -1.25613900
F   -4.10620000 -1.11541400  0.72125900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.200995269936

Frequencies (cm^{-1}): 40.0578, 63.7428, 96.8831, 105.0978, 132.4428, 185.3574, 301.423, 467.2318, 686.9161, 762.6129, 827.2996, 850.9734, 1059.221, 1123.5203, 1174.2018, 1228.5582, 1349.9282, 1427.7322, 1477.1241, 1496.8311, 1512.4489, 1618.221, 2988.8996, 3031.9336, 3092.7475, 3225.642, 3583.6681

***Syn*-FCHOO + MeOH TS-AAAH 1**

```
C    0.00000000  0.00000000  0.00000000
O    1.15800300 -0.44728000 -0.70939900
H    1.64126500  0.36558500 -1.07138100
H    0.26484000  0.71996000  0.77743900
H   -0.69586700  0.47152400 -0.69474800
H   -0.47494600 -0.87074500  0.44680800
C    2.87112200 -0.51304100  0.38860400
O    2.96897800  0.72856200  0.54905000
O    2.93821100  1.40311700 -0.74621000
H    2.62241700 -1.12305900  1.24915900
F    3.49393100 -1.14322500 -0.56824200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.194848468159

Frequencies (cm^{-1}): -263.332, 120.3279, 135.5756, 170.513, 260.7143, 287.4416, 368.9789, 485.9757, 725.7462, 777.8646, 970.5243, 1043.8343, 1068.8496, 1168.8742, 1179.9512, 1208.0177, 1336.4609, 1463.9607, 1475.8856, 1494.5081, 1512.3513, 1551.6255, 2897.2012, 3024.4443, 3084.7801, 3119.0527, 3188.3411

MeOCFH(OOH) (TS-AAAH 1- conformer):

```
C    0.00000000  0.00000000  0.00000000
O    1.13591100  0.64024000 -0.58441700
H    2.86034500 -1.16421200 -0.88760800
H    0.26805000 -0.95439000  0.45756400
H   -0.70290000 -0.16927200 -0.81024000
H   -0.46367700  0.64376400  0.75199200
C    2.12496300  0.96887300  0.31619900
O    2.91862900 -0.11419700  0.69850300
O    3.57597200 -0.66358400 -0.46721300
H    1.73102700  1.33755900  1.27033100
F    2.87194200  1.93667200 -0.27169100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.277939256858

Frequencies (cm^{-1}): 86.1439, 112.2983, 161.7705, 177.3801, 285.6537, 311.1955, 490.0165, 556.6396, 764.1943, 878.1197, 1020.9953, 1037.1157, 1110.1341, 1118.8177, 1177.3717, 1229.3443, 1357.8454, 1375.2246, 1397.6425, 1480.8773, 1493.8184, 1509.9108, 3011.93, 3028.1721, 3070.3836, 3139.499, 3723.3756

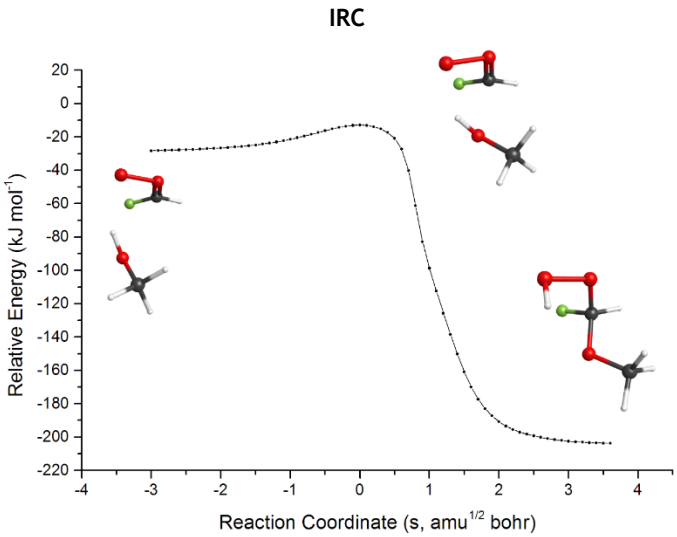


Figure S53: SCI 5 + MeOH TS-AAAH 1 IRC

***Syn*-FCHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
O     1.18144500 -0.35077000 -0.72238000
H     1.77734300 -0.92920100 -0.14122000
H    -0.58379200 -0.90066200  0.19665300
H     0.23921600  0.48613900  0.94660000
H    -0.58488100  0.67520400 -0.62072200
C     2.82626600  0.82665900 -0.65451400
O     3.62177500 -0.14074100 -0.63109700
O     3.32181700 -1.01578000  0.50361000
H     2.74736000  1.40395000 -1.56741500
F     2.47296800  1.47191000  0.43024700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.195639339832

Frequencies (cm^{-1}): -267.3433, 105.7844, 144.9997, 180.6944, 272.9473, 316.0373, 376.1674, 459.0338, 717.5807, 777.1712, 955.4165, 1009.5497, 1058.8367, 1167.5957, 1178.5024, 1197.3012, 1343.6229, 1463.5892, 1485.1075, 1496.6795, 1513.1337, 1581.8697, 2874.2911, 3028.877, 3088.744, 3119.6511, 3198.3964

MeOCFH(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
O    -1.39637500 -0.27982900  0.12381700
H    -3.64867400 -1.08108300 -0.43205000
H     0.47550700 -0.93932100 -0.26575500
H     0.18161900  0.73986900 -0.77862200
H     0.40790700  0.35686300  0.94989900
C    -2.15791900  0.76697000  0.57213200
O    -3.45743300  0.36051300  0.78191100
O    -4.00313200 -0.17889000 -0.44521500
H    -1.83202000  1.16105100  1.54128000
F    -2.09833300  1.81187300 -0.33268400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.280265083401

Frequencies (cm^{-1}): 101.093, 134.6776, 174.4823, 217.9943, 267.6596, 340.673, 491.2346, 564.3975, 746.1368, 888.9413, 1000.5809, 1040.9133, 1082.265, 1141.8236, 1177.4698, 1233.3165, 1345.0245, 1387.2297, 1402.9887, 1482.0593, 1491.18, 1509.9153, 3015.0941, 3031.8565, 3090.9127, 3142.2306, 3725.5424

IRC:

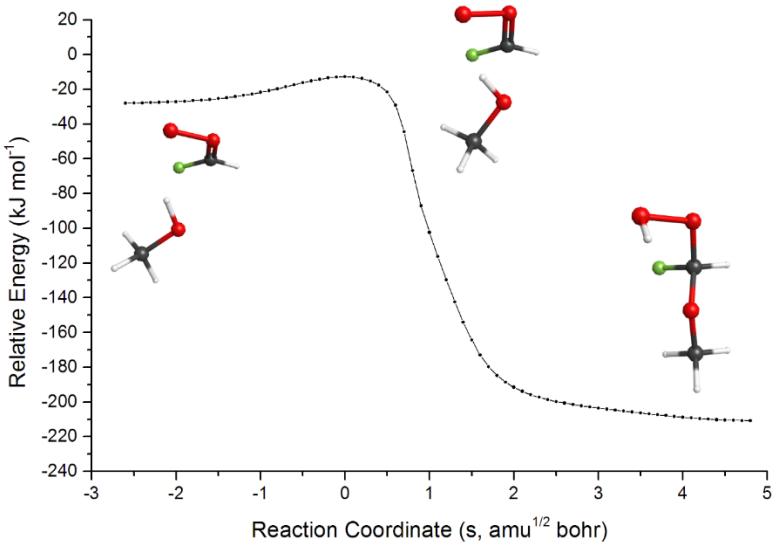


Figure S54: SCI 5 + MeOH TS-AAAH 2 IRC

7.6 sCI 6 + MeOH Reactions

***Anti*-FCHOO (SCI 6):**

```
C    0.00000000  0.00000000  0.00000000
F   -1.13941500  0.63740300  0.00000000
H    0.91413500  0.57992600  0.00000000
O   -0.03415800 -1.23311900  0.00000000
O    1.20173400 -1.89294200  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -288.578109102783

Frequencies (cm^{-1}): 267.9837, 334.8286, 574.4392, 882.3564, 899.2189, 1214.6688, 1317.7697, 1591.1732, 3211.5083

***Anti*-FCHOO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2):**

```
C    0.00000000  0.00000000  0.00000000
F   -1.09431000 -0.70885600  0.00034000
O   -0.14600100  1.22663400  0.00004300
O    1.02168100  2.02757700  0.00017500
H    2.46302800  0.88975300 -0.00023100
O    2.85887700 -0.00667300 -0.00099900
C    4.27787400  0.05471200  0.00066500
H    4.65954600  0.56731300 -0.88659800
H    4.65156400 -0.96776200 -0.00294100
H    4.65777900  0.56044800  0.89263200
H    0.96198600 -0.51352700 -0.00021600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.202192105245

Frequencies (cm^{-1}): 26.4063, 88.3458, 101.0701, 109.8576, 145.5052, 244.4525, 276.9925, 375.3826, 567.4434, 694.1145, 882.6065, 976.0247, 1060.3462, 1140.2837, 1173.6022, 1230.2064, 1378.5206, 1450.1886, 1478.1213, 1497.8099, 1512.3852, 1586.3511, 3000.1352, 3048.1528, 3100.1938, 3101.3876, 3463.3138

***Anti*-FCHOO + MeOH TS-AAAH 1**

```
C    0.00000000  0.00000000  0.00000000
F    0.04815100 -1.24436500 -0.39497100
O   -0.27027500  0.84833400 -0.88480700
O    0.04093700  2.16250500 -0.30601000
H    1.46172400  1.49169200  0.18981300
O    1.92914300  0.60541400  0.35218700
C    2.83027600  0.34899100 -0.72794900
H    2.30754300  0.33831100 -1.68733000
H    3.29451600 -0.61847900 -0.55264000
H    3.60029600  1.12088800 -0.75614900
H   -0.15232800  0.16489100  1.05642800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.200846412495

Frequencies (cm^{-1}): -152.1009, 112.9894, 130.3728, 157.9917, 263.9198, 310.3225, 395.8801, 532.476, 580.1978, 857.5821, 971.1062, 1078.3639, 1095.6537, 1171.7687, 1185.2556, 1225.0602, 1312.2072, 1458.4508, 1473.2803, 1494.7729, 1509.4848, 1550.9206, 2852.4137, 3021.8701, 3080.6841, 3123.683, 3224.9832

MeOCFH(OOH) (TS-AAAH 1 - conformer)

```
C    0.00000000  0.00000000  0.00000000
F    0.68243800 -1.04821600 -0.56230500
O   -0.96950600  0.30034500 -0.98704000
O   -1.96760700  1.11508100 -0.33786500
H   -1.62843700  2.00959600 -0.48919000
O    0.83472000  1.03881400  0.29239400
C    1.66489900  1.50974300 -0.78330100
H    1.07474100  1.71456300 -1.67644600
H    2.43849100  0.77984300 -1.01610200
H    2.12074900  2.42672600 -0.42259300
H   -0.48048900 -0.31515800  0.92326200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.280077281596

Frequencies (cm^{-1}): 103.4568, 118.7288, 176.0386, 228.7812, 286.1516, 328.5719, 470.1384, 563.7806, 714.1108, 924.615, 970.3367, 1014.0186, 1084.3553, 1160.5433, 1181.0725, 1218.2319, 1333.2577, 1390.0189, 1402.62, 1474.8317, 1494.2049, 1512.297, 3042.8549, 3110.07, 3123.9829, 3144.423, 3731.0727

IRC:

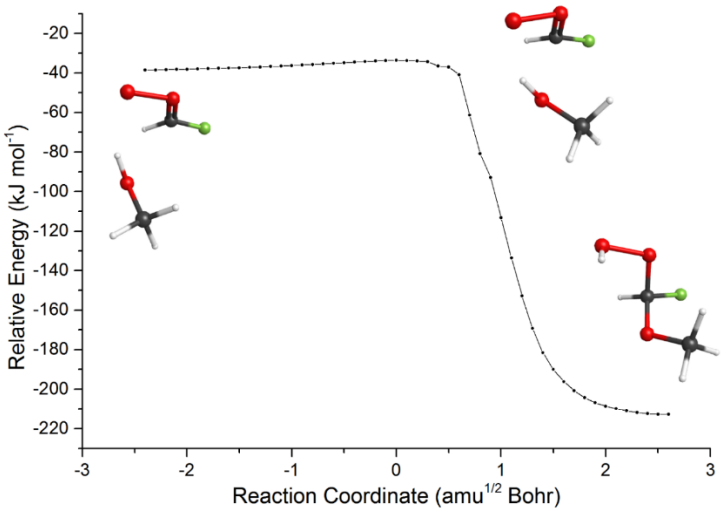


Figure S55: SCI 6 + MeOH TS-AAAH 1 IRC

***Anti*-FCHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
F    -0.31376700 -1.20487200 -0.38853600
O    -0.64156700  0.94056200 -0.52843800
O     0.08305100  2.17343200 -0.18570200
H     1.38400800  1.38286800 -0.73949400
O     1.76324500  0.44831500 -0.89497700
C     2.95987200  0.27342500 -0.14163900
H     3.72529000  0.96597400 -0.49452500
H     3.30587100 -0.74725700 -0.28951300
H     2.79724200  0.45160700  0.92603000
H     0.48031900  0.08062700  0.96609300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.199590330737

Frequencies (cm^{-1}): -173.0932, 106.7732, 132.2575, 176.9343, 283.8099, 291.1718, 401.2925, 516.1443, 577.4177, 862.9568, 1000.391, 1039.0523, 1082.2909, 1176.6058, 1191.9389, 1225.8631, 1309.4609, 1465.1748, 1483.1521, 1496.4957, 1510.001, 1585.6524, 2764.8939, 3004.7541, 3070.2131, 3117.3126, 3194.8602

MeOCFH(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
F    -0.41168600  1.28552500 -0.24948600
O     1.30710700 -0.03258500 -0.49109900
O     1.89079700 -1.26439100 -0.01845700
H     1.65543500 -1.87171300 -0.73606000
O    -0.76536300 -0.90010400 -0.68923400
C    -2.05635700 -1.14698400 -0.12591800
H    -2.69182100 -0.26460900 -0.20719000
H    -1.97167700 -1.44512000  0.92242600
H    -2.48970400 -1.96123200 -0.69888300
H    -0.02650300 -0.16581100  1.08146500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -404.279520926944

Frequencies (cm^{-1}): 91.8858, 126.2437, 160.867, 266.49, 291.8129, 356.8781, 473.1423, 574.2874, 619.9383, 969.376, 1018.9427, 1050.6549, 1118.275, 1138.3869, 1177.4066, 1233.9581, 1348.6972, 1393.5695, 1399.3016, 1482.1636, 1492.6547, 1509.0239, 3016.3377, 3037.5558, 3083.3891, 3140.5352, 3727.4957

IRC:

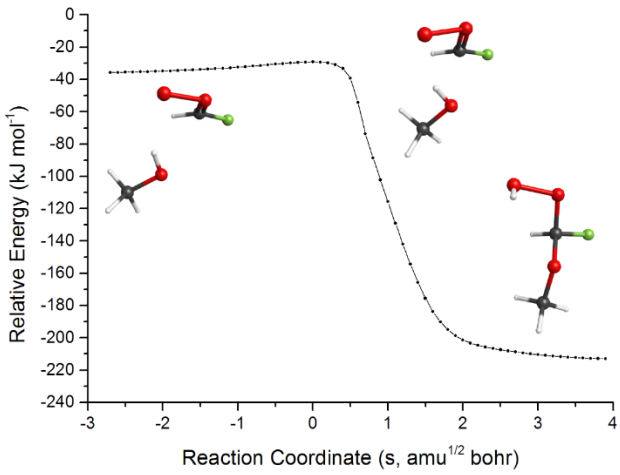


Figure S56: SCI 6 + MeOH TS-AAAH 2 IRC

7.7 sCI 7 + MeOH Reactions

CF_2OO (sCI 7):

```
C     0.00000000  0.00000000  0.00000000
F     1.27754000 -0.04809900  0.00000000
F    -0.48764000  1.19884600  0.00000000
O    -0.75082000 -0.96966200  0.00000000
O    -0.13781700 -2.25916300  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -387.753628872559

Frequencies (cm^{-1}): 237.8686, 270.0697, 493.9733, 614.641, 622.7752, 820.459, 986.5498, 1434.0629, 1705.7711

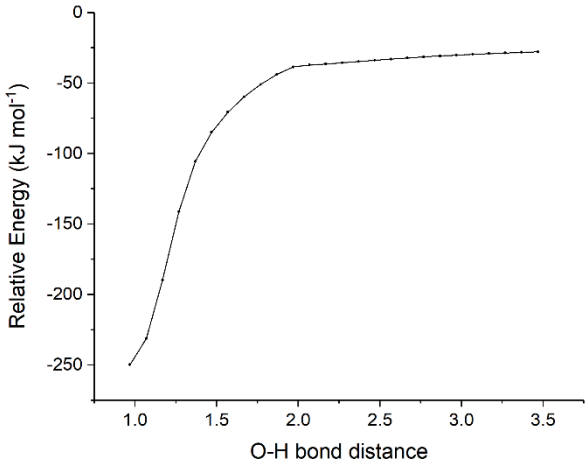
CF_2OO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2):

```
C     0.00000000  0.00000000  0.00000000
O    -1.17605800  0.32559700 -0.73461900
H    -1.45805400  1.23558700 -0.51042400
H     0.82284400  0.66842100 -0.26344000
H    -0.16836900  0.05330100  1.07907100
H     0.27913900 -1.01780600 -0.26468700
C    -3.43331200 -0.07605500 -0.05352200
O    -3.70142300  1.00400600 -0.58033000
O    -3.07765200  2.14227000  0.07445500
F    -3.77824600 -1.16839400 -0.64373000
F    -3.02599100 -0.24523800  1.14776100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -503.379028134458

Frequencies (cm^{-1}): 30.4621, 85.3119, 103.7716, 127.7917, 196.3578, 211.5099, 275.1387, 316.27, 505.6116, 599.4734, 617.4756, 746.2108, 817.5431, 990.2471, 1053.714, 1138.9548, 1175.338, 1431.166, 1439.2265, 1476.8112, 1497.5496, 1511.5689, 1693.7919, 3006.8053, 3059.4665, 3110.057, 3501.5954

CF_2OO + MeOH TS-AAAH 1 (barrierless) IRC:



CF_2OO + MeOH TS-AAAH 2

```
C     0.00000000  0.00000000  0.00000000
O    -1.17664800  0.31020500 -0.74231400
C    -3.33085900 -0.13941100 -0.05084500
H    -1.47077300  1.22109400 -0.52362300
H     0.81488800  0.67574900 -0.26806000
H    -0.17362600  0.06252700  1.07730300
H     0.28972900 -1.01695900 -0.25568000
O    -3.67816400  0.92617600 -0.56602800
O    -3.06578800  2.08715900  0.06947800
F    -3.63287700 -1.24728400 -0.63707100
F    -2.92929000 -0.29223500  1.15715900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -503.378983026328

Frequencies (cm^{-1}): -42.8744, 96.4442, 108.3599, 127.8816, 206.7172, 229.5227, 277.7835, 328.6989, 506.9839, 593.9359, 614.6318, 785.7546, 816.7653, 985.913, 1052.3673, 1144.6162, 1176.4289, 1421.4184, 1443.878, 1476.9287, 1497.6289, 1511.8214, 1682.3283, 3011.132, 3065.577, 3113.0872, 3442.1508

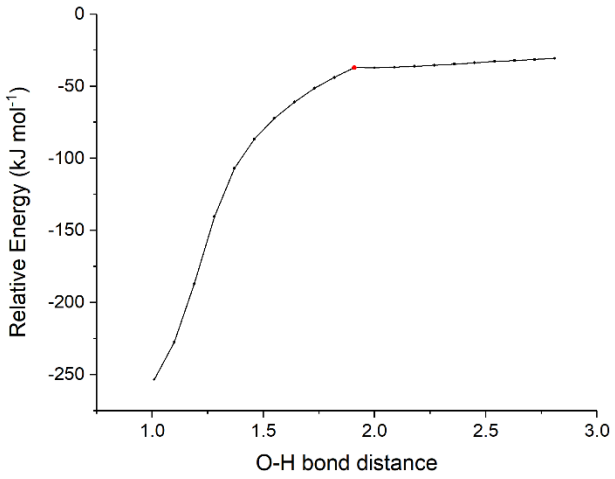
$MeOCF_2OOH$ (TS-AAAH 2 conformer)

```
C     0.00000000  0.00000000  0.00000000
O     1.36532800  0.10340000 -0.44585200
H     3.78672900 -0.74569300 -0.56421100
H    -0.40781600 -0.86032000 -0.52036900
H    -0.03882000 -0.15989500  1.07549600
H    -0.55866700  0.89471900 -0.27112000
C     2.07030700  1.16209300  0.00211800
O     3.38575200  1.09178300 -0.41984800
O     3.97839900 -0.09944100  0.13262000
F     1.62626600  2.33420200 -0.51343600
F     1.98820200  1.28316900  1.35253200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -503.474274432831

Frequencies (cm^{-1}): 83.1774, 127.7469, 155.6582, 225.1112, 283.479, 296.3756, 439.6299, 443.1667, 575.6752, 592.7255, 686.3175, 820.8494, 980.5464, 1061.2113, 1119.6282, 1148.6842, 1176.8338, 1231.3156, 1234.0542, 1413.9183, 1483.9589, 1496.0636, 1506.9405, 3050.8106, 3124.0014, 3155.5771, 3724.8455

IRC:



7.8 sCI 8 + MeOH Reactions

***Syn*-ClCHOO (sCI 8):**

```
C    0.00000000  0.00000000  0.00000000
Cl  -1.27950800 -1.09418400  0.00000000
H   -0.19577400  1.06192200  0.00000000
O    1.20494800 -0.35173900  0.00000000
O    1.53847800 -1.66851400  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -648.572175406265

Frequencies (cm^{-1}): 242.0771, 471.8954, 657.6577, 752.7142, 870.3526, 902.6469, 1331.3986, 1461.1123, 3221.0274

***Syn*-ClCHOO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2):**

```
C    0.00000000  0.00000000  0.00000000
O    1.36324000 -0.36848300 -0.12926600
H    1.84001400  0.33111500 -0.60791700
H   -0.12173700  0.94810200  0.53422500
H   -0.49622800  0.08256600 -0.97251700
H   -0.49728900 -0.78238100  0.57210000
C    4.53645500  0.61048600  0.54786700
O    3.85934600  1.60120700  0.18750900
O    3.20493500  1.58082100 -1.02094200
H    5.01690800  0.68618000  1.51313200
Cl   4.73377800 -0.77544100 -0.37305900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.190542251436

Frequencies (cm^{-1}): 32.8449, 43.0564, 58.4719, 103.7087, 120.951, 183.0564, 252.9164, 466.0725, 653.6628, 663.741, 802.0973, 857.3971, 896.5315, 1059.4892, 1121.7566, 1172.6879, 1335.7014, 1426.1873, 1476.0879, 1480.6587, 1496.4562, 1511.8383, 2985.1427, 3026.2512, 3089.7736, 3211.123, 3589.7286

***Syn*-ClCHOO + MeOH TS-AAAH 1**

```
C    0.00000000  0.00000000  0.00000000
O    1.31462100 -0.07000500 -0.55987900
H    1.52129400  0.83552400 -1.00556900
H   -0.72925600  0.09325400 -0.80555600
H   -0.18271600 -0.92201900  0.54748300
H   -0.10009700  0.85911400  0.66647100
C    2.74104600  0.63336700  0.65051100
O    2.36224000  1.84157200  0.59004200
O    2.24487300  2.25658200 -0.79742300
H    2.56891300  0.12773700  1.59320800
Cl   4.06807000  0.00740500 -0.25718300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.176633553068

Frequencies (cm^{-1}): -348.2547, 127.0406, 136.2523, 174.4943, 229.9097, 251.7858, 346.5018, 479.4452, 601.9576, 782.6756, 821.8901, 970.5812, 1029.24, 1102.044, 1175.4088, 1233.8462, 1312.4064, 1435.1029, 1463.1859, 1488.8062, 1493.832, 1514.7664, 2605.2947, 3024.7544, 3086.6492, 3120.2584, 3172.4966

MeOCClH(OOH) (TS-AAAH 1- conformer)

```
C    0.00000000  0.00000000  0.00000000
O    1.34375100  0.08171000 -0.49477900
H    1.83455300  2.34775000 -1.02107000
H   -0.61580700 -0.28439400 -0.84804800
H   -0.07563700 -0.76464900  0.77673900
H   -0.33786500  0.95877700  0.39678200
C    2.26994200  0.43207500  0.46799900
O    2.28066400  1.79585200  0.74520200
O    2.59112100  2.54928800 -0.44711100
H    2.07025200 -0.01892300  1.44171700
Cl   3.87507800 -0.18004000 -0.08518300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.257522986589

Frequencies (cm^{-1}): 80.5194, 122.3894, 167.4756, 205.114, 266.4656, 284.2099, 376.9412, 443.2722, 693.3815, 824.5211, 877.4591, 987.862, 1019.4654, 1094.2639, 1172.8917, 1205.5837, 1285.1522, 1360.679, 1408.4917, 1476.0466, 1492.9912, 1507.7097, 3017.353, 3065.1247, 3079.1688, 3140.8871, 3701.3218

IRC:

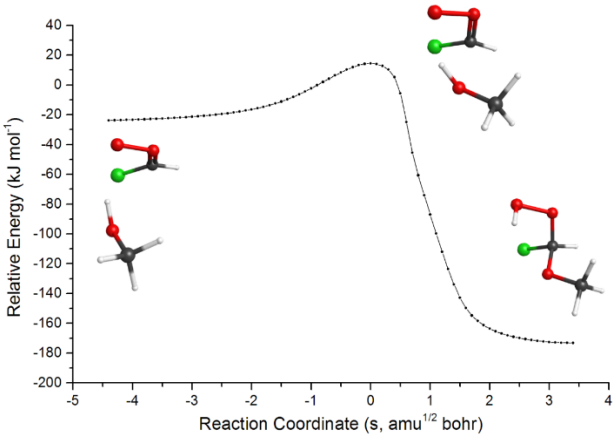


Figure S57: sSCI 8 + MeOH TS-AAAH 1 IRC

***Syn*-ClCHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
O    -0.99065700 -0.86272500  0.55097100
H    -1.47664300 -1.38814600 -0.19634300
H    -0.43812600  0.74044600 -0.67128600
H     0.50515000  0.50431100  0.82079000
H     0.72245200 -0.59933100 -0.55694100
C    -2.86705900 -0.33658400  0.92175100
O    -3.31336200 -1.47301800  0.59220600
O    -2.89202500 -1.80104100 -0.76466800
H    -2.83558700 -0.12398500  1.98274400
Cl   -3.04144400  1.07308600 -0.07215200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.175749305248

Frequencies (cm^{-1}): -353.8487, 91.6863, 147.7673, 178.9175, 240.8538, 311.6581, 364.4052, 446.3336, 586.6757, 771.5206, 802.2082, 964.323, 1051.4927, 1067.9276, 1172.6697, 1210.6479, 1316.8809, 1405.8615, 1464.7215, 1491.4625, 1500.5508, 1566.5038, 2532.1397, 3023.3912, 3082.2434, 3118.9907, 3185.1745

MeOCClH(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
O     1.41108800 -0.22303600 -0.02527200
H     3.62937300 -0.85899200 -0.74648500
H    -0.36904300  0.01693600  1.02868500
H    -0.44615800 -0.83372600 -0.53349500
H    -0.24883000  0.93758700 -0.49599000
C     2.16710600  0.64170800  0.71331600
O     3.45407100  0.17677100  0.82958700
O     4.03788000 -0.02165400 -0.47672200
H     1.82118900  0.76951800  1.74034300
Cl    2.11695700  2.35679800 -0.00430600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.259589321571

Frequencies (cm^{-1}): 107.1782, 127.464, 175.7936, 200.8447, 250.3923, 330.3517, 403.224, 424.1022, 615.9568, 757.8752, 887.8738, 1019.419, 1073.4363, 1136.6164, 1173.63, 1215.2333, 1272.9941, 1367.6711, 1404.9472, 1478.0091, 1489.5835, 1505.4492, 3019.5768, 3067.6316, 3093.3759, 3144.7277, 3718.6568

IRC:

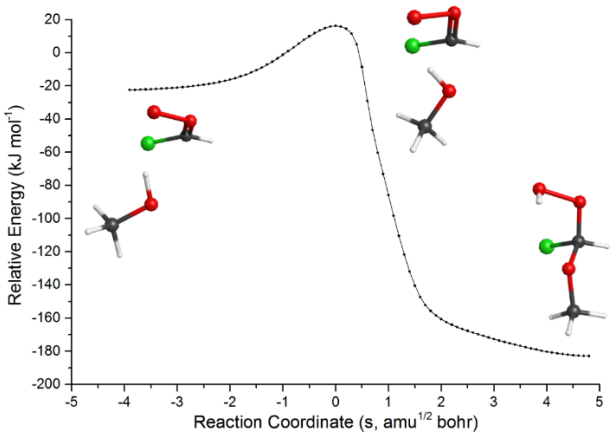


Figure S58: SCI 8 + MeOH TS-AAAH 2 IRC

7.9 sCI 9 + MeOH Reactions

***Anti*-ClCHOO (sSCI 9)**

```
C     0.00000000  0.00000000  0.00000000
Cl   -1.53484300 -0.72205100  0.00000000
H     0.09377100  1.07891100  0.00000000
O     1.01281800 -0.72974000 -0.00000000
O     2.23700200 -0.09715600 -0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -648.567488736211

Frequencies (cm^{-1}): 229.5711, 303.8529, 458.7496, 867.3814, 891.3292, 914.86, 1292.069, 1476.934, 3187.4996

***Anti*-ClCHOO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2):**

```
C     0.00000000  0.00000000  0.00000000
Cl    1.55141600 -0.68746200 -0.00013500
O    -0.08239400  1.24511600 -0.00012200
O    -1.35430500  1.81655300 -0.00011100
H    -2.62079800  0.46094900 -0.00015300
O    -2.87873400 -0.48219400 -0.00010700
C    -4.29096200 -0.62913300 -0.00012200
H    -4.74355600 -0.18241500  0.88974500
H    -4.74363300 -0.18150300 -0.88948600
H    -4.51040200 -1.69551000 -0.00066700
H    -0.88099500 -0.63988200  0.00021100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.189491562894

Frequencies (cm^{-1}): 23.2019, 81.8012, 83.1605, 107.4304, 136.443, 220.5861, 237.2611, 340.2739, 459.0398, 675.1347, 876.5837, 914.1134, 931.8279, 1060.3992, 1141.0721, 1173.2406, 1358.4094, 1442.9625, 1477.3345, 1483.4236, 1497.9862, 1511.8143, 2997.6511, 3044.5248, 3099.2613, 3103.3532, 3501.1113

***Anti*-ClCHOO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
Cl    1.47637600  0.77115000 -0.42366700
O    -0.57693300 -0.65908800 -0.92185700
O    -1.91523000 -0.95889000 -0.41094800
H    -1.96595800  0.48920300  0.08028700
O    -1.40867600  1.34689300  0.29173100
C    -1.56645100  2.28094100 -0.77841800
H    -1.31549000  1.82798900 -1.74004500
H    -2.60359800  2.61714400 -0.80783200
H    -0.91513100  3.13066000 -0.58854000
H    -0.12278400 -0.26208400  1.04118500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.185108692488

Frequencies (cm^{-1}): -298.7981, 106.2218, 132.1978, 162.7594, 254.0232, 282.3497, 383.4048, 438.8199, 552.4748, 830.8279, 844.0466, 981.8199, 1099.9084, 1123.8317, 1177.1268, 1243.8985, 1284.5087, 1432.3659, 1459.8664, 1488.4896, 1496.1063, 1510.6564, 2405.0483, 3023.5458, 3084.5875, 3123.8918, 3194.9261

MeOCClH(OOH) (TS-AAAH 1 - conformer)

```
C     0.00000000  0.00000000  0.00000000
Cl    1.67191300 -0.47363300 -0.56439800
O    -0.82395300 -0.51990000 -1.01920300
```

```
O    -2.16459100 -0.57502800 -0.46373100
H    -2.52370600  0.28744700 -0.71922500
O    -0.14095400  1.33745200  0.21416500
C     0.11704200  2.21955500 -0.88836500
H    -0.43680100  1.91697200 -1.77670200
H    -0.21178500  3.20077900 -0.56000600
H     1.18248700  2.24069600 -1.11330900
H    -0.18133700 -0.50756400  0.94104000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.261110927024

Frequencies (cm^{-1}): 100.8967, 118.9221, 180.9691, 216.8952, 267.26, 290.2233, 372.2304, 422.3535, 667.1879, 773.0908, 914.87, 920.0542, 1024.034, 1130.0266, 1174.9217, 1214.4596, 1265.0151, 1372.912, 1390.9411, 1471.8118, 1490.1759, 1510.3764, 3042.2795, 3109.05, 3144.823, 3146.1942, 3733.5913

IRC:

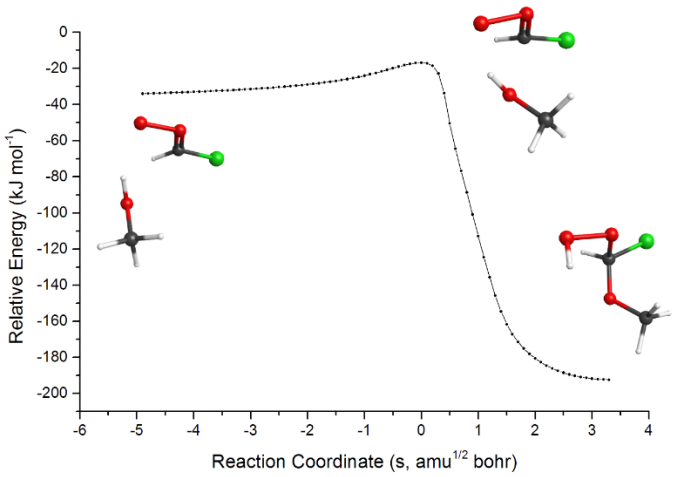


Figure S59: sSCI 9 + MeOH TS-AAAH 1 IRC

***Anti*-ClCHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
Cl   -1.41619600 -0.88009400 -0.40447100
O     0.12284900  1.15178300 -0.51949900
O     1.50706600  1.55474100 -0.26434000
H     1.87670100  0.17486800 -0.77496100
O     1.53595500 -0.80409000 -0.93092500
C     2.31651800 -1.72725900 -0.17888400
H     3.32400200 -1.77342700 -0.59485400
H     2.38925800 -1.43396600  0.87283600
H     1.85404800 -2.70962900 -0.25196800
H     0.45110500 -0.23070300  0.95660800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.182317726145

Frequencies (cm^{-1}): -312.2062, 77.5869, 123.0062, 194.5969, 246.4849, 269.8278, 387.2977, 439.8996, 511.8339, 839.9662, 846.085, 1013.0668, 1083.1288, 1100.6083, 1176.4881, 1226.2047, 1282.6901, 1406.5903, 1465.6766, 1494.5247, 1499.9037, 1560.6326, 2360.3482, 3006.09, 3071.1901, 3112.5209, 3166.3612

MeOCClH(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
Cl    1.43084800 -1.10978800 -0.25915400
O    -1.07438500 -0.74421000 -0.47970000
O    -2.27398100 -0.05193500 -0.04146600
H    -2.42463200  0.54881200 -0.78687100
O     0.10943500  1.16250500 -0.70677000
C     0.97447400  2.14556700 -0.13512000
H     2.01305700  1.81466700 -0.17679100
H     0.85168900  3.04360700 -0.73281800
H     0.69450400  2.35295200  0.90078400
H    -0.06835200  0.16381600  1.07660700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -764.260672584363

Frequencies (cm^{-1}): 98.3811, 133.2314, 163.0832, 229.991, 270.5765, 339.9726, 383.5521, 421.9018, 585.7836, 765.1333, 916.6948, 1003.74, 1089.1559, 1127.8404, 1174.8028, 1218.7911, 1273.0598, 1378.9107, 1381.0889, 1479.0815, 1490.0721, 1506.3964, 3017.3928, 3059.3792, 3082.3464, 3142.8432, 3729.7599

IRC:

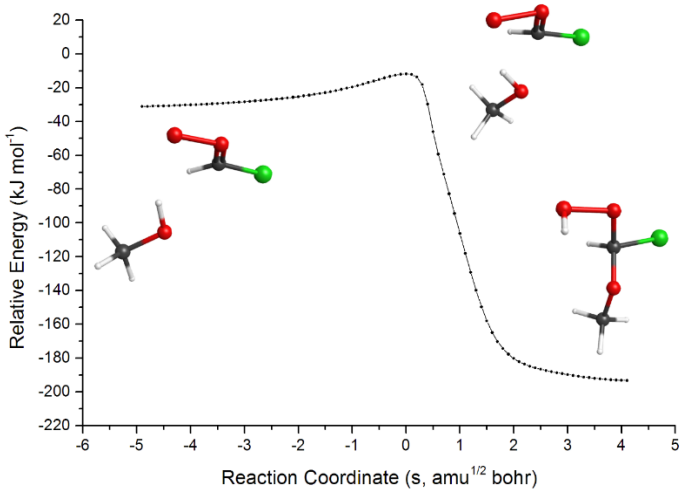


Figure S60: SCI 9 + MeOH TS-AAAH 2 IRC

8.10 sCI 10 + MeOH Reactions

CCl_2OO (sSCI 10):

```
C    0.00000000  0.00000000  0.00000000
Cl  -0.32095300 -1.65482100 -0.00000000
Cl  -1.27950500  1.12337400  0.00000000
O    1.16863500  0.46107600  0.00000000
O    2.23233700 -0.40658100  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1107.734006061150

Frequencies (cm^{-1}): 232.238, 239.6166, 290.5852, 476.344, 502.0854, 651.8358, 913.8411, 1033.6211, 1424.5393

CCl_2OO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2):

```
C    0.00000000  0.00000000  0.00000000
Cl  -0.18379500  1.48794000 -0.75521600
Cl   1.15609000 -1.10835900 -0.57190500
O   -0.67156500 -0.35235500  0.99937600
O   -1.64160100  0.51198000  1.49066500
H   -2.89756700  0.28652800  0.08600900
O   -3.20646700  0.04662900 -0.80476300
C   -4.38005900 -0.74267200 -0.69689200
H   -4.67567700 -1.02845400 -1.70559700
H   -4.21081500 -1.65491700 -0.11539600
H   -5.20612900 -0.18754900 -0.24084300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1223.353347036430

Frequencies (cm^{-1}): 24.5235, 46.6861, 53.6323, 99.3967, 120.8218, 166.1647, 241.5497, 272.6311, 294.396, 474.3288, 519.627, 655.1243, 681.5435, 892.5133, 1039.2534, 1060.0403, 1121.5912, 1173.4489, 1423.4982, 1441.2253, 1476.4621, 1496.4976, 1511.7539, 2986.1413, 3027.9077, 3090.897, 3584.8765

CCl_2OO + MeOH TS-AAAH 1:

```
C    0.00000000  0.00000000  0.00000000
Cl  -1.11256600 -0.86526500 -0.99890800
Cl  -0.22471100  1.70916100  0.05269000
O    0.49379000 -0.50123700  1.06116600
O    1.02454100 -1.82451200  0.76539900
H    1.59938300 -1.20093100 -0.52245700
O    1.59380800 -0.36774300 -1.14606300
C    2.73719100  0.43316600 -0.83969200
H    2.66838800  1.35786100 -1.40713500
H    2.79250100  0.65292800  0.22828900
H    3.63661100 -0.10911500 -1.13521000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1223.343830625610

Frequencies (cm^{-1}): -337.177, 125.2678, 129.9323, 139.9063, 223.953, 244.1493, 271.8541, 315.0992, 377.4178, 444.7636, 509.2455, 630.8715, 842.2256, 933.5874, 1024.3841, 1106.6452, 1173.4868, 1233.1287, 1396.4554, 1459.2282, 1485.2934, 1494.8383, 1509.859, 2449.149, 3024.9506, 3085.2935, 3127.063

$MeOCCl_2OOH$ (TS-AAAH 1 conformer):

```
C    0.00000000  0.00000000  0.00000000
Cl  -1.56517000  0.56909000 -0.65715300
Cl   0.94141500  1.42860900  0.63971800
O   -0.16150200 -0.74553000  1.17668800
O   -0.99058100 -1.89880400  0.88606900
H   -0.32491100 -2.59259700  0.76907600
O    0.62827500 -0.64788900 -1.00571800
C    1.95441700 -1.14440700 -0.74902900
H    2.65938900 -0.31699200 -0.69384600
H    1.99228200 -1.71770900  0.17673400
H    2.18737200 -1.78111300 -1.59640300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1223.422835294570

Frequencies (cm^{-1}): 69.2192, 113.8692, 136.7599, 174.9054, 197.8604, 253.5992, 275.6333, 369.9271, 389.1487, 426.7878, 449.7171, 731.9791, 833.6281, 912.2077, 941.5428, 1017.8806, 1129.6444, 1172.0302, 1207.0266, 1379.157, 1472.5939, 1485.4597, 1507.6967, 3045.4021, 3115.7261, 3154.0166, 3734.0656

IRC:

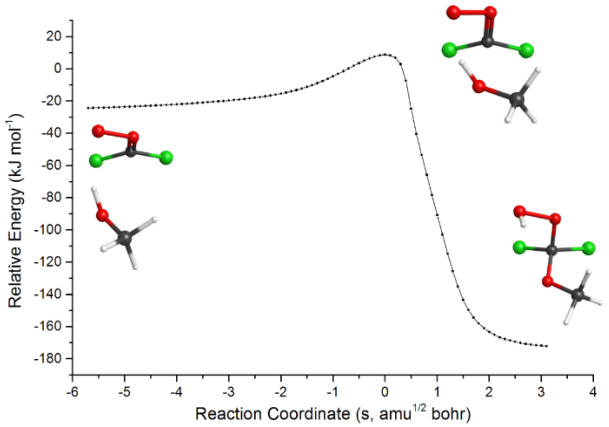


Figure S61: SCI 10 + MeOH TS-AAAH 1 IRC

CCl_2OO + MeOH TS-AAAH 2:

```
C     0.00000000  0.00000000  0.00000000
Cl    0.42869500  0.13960400  1.67781600
Cl   -1.33737800 -1.03187700 -0.32816400
O     0.14192700  0.96781700 -0.81006900
O     1.50096100  1.48953600 -0.70671800
H     1.90891700  0.01756200 -0.83239600
O     1.57382300 -0.96394600 -0.72583900
C     2.45525700 -1.73012800  0.08827400
H     1.94102200 -2.63906500  0.39437000
H     3.33059000 -1.99730800 -0.50691400
H     2.77779400 -1.17526700  0.96991900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1223.341731878740

Frequencies (cm^{-1}): -349.2092, 100.5841, 114.3361, 180.5584, 236.0631, 239.6973, 266.5437, 342.432, 392.777, 443.8602, 481.7532, 602.5251, 841.4889, 920.7466, 1031.8783, 1074.8689, 1171.209, 1214.1927, 1361.9091, 1460.1007, 1492.2681, 1498.8927, 1543.0781, 2432.4896, 3025.2043, 3087.0175, 3116.3134

$MeOCCl_2OOH$ (TS-AAAH 2- conformer):

```
C     0.00000000  0.00000000  0.00000000
Cl    0.30844000 -0.52054600  1.73221500
Cl   -1.39572000  1.16400000  0.00333200
O     1.03436100  0.78281800 -0.47859900
O     2.24306000 -0.00997000 -0.54352800
H     2.13997900 -0.44179600 -1.40587300
O    -0.19191500 -1.05247900 -0.81760300
C    -1.23040000 -1.99733600 -0.51686700
H    -2.19438500 -1.49284000 -0.47254500
H    -1.21611100 -2.70698700 -1.33759600
H    -1.02167000 -2.50093300  0.42453400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -1223.425742373930

Frequencies (cm^{-1}): 94.6569, 131.6473, 169.0406, 195.4297, 244.2999, 250.091, 276.0731, 380.3815, 397.429, 412.1632, 505.3214, 634.4813, 809.2712, 913.9577, 994.8216, 1056.7676, 1167.3307, 1174.7808, 1214.5704, 1396.1528, 1476.7505, 1488.8385, 1504.1687, 3052.3699, 3127.3747, 3156.941, 3720.2313

IRC:

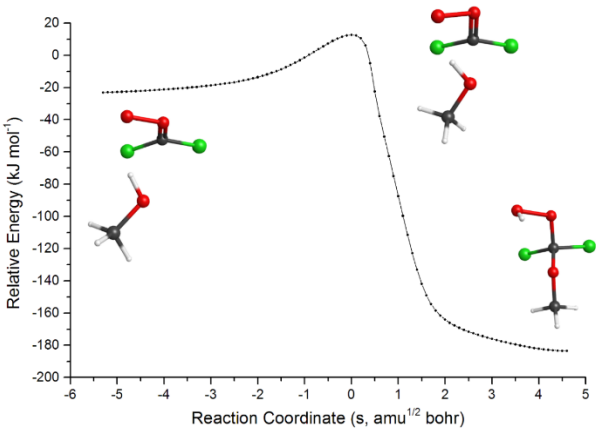


Figure S62: SCI 10 + MeOH TS-AAAH 2 IRC

7.11 sCI 11 + MeOH Reactions

7.11.1 sCI 11 + MeOH Reactions

***Syn*-PhCHOO (sCI 11):**

```
C     0.00000000   0.00000000   0.00000000
C     1.30961200   0.43716900   0.00001000
C     1.58176300   1.80492500   0.00005400
C     0.53977100   2.72562700   0.00005200
C    -0.78108600   2.30264500   0.00002100
C    -1.06752100   0.92272500   0.00004200
C    -2.38250800   0.35646800   0.00009000
O    -3.51963200   0.92494400   0.00006500
O    -3.61762400   2.28848000  -0.00000800
H    -2.49236700  -0.72226600   0.00010500
H    -1.60408400   2.99612000  -0.00008700
H     0.75691300   3.78490300   0.00019700
H     2.60722600   2.14924300   0.00008200
H     2.11969200  -0.27870700  -0.00000600
H    -0.21419100  -1.06101900   0.00000100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -420.013064508086

Frequencies (cm^{-1}): 88.3646, 162.1096, 217.5734, 318.0922, 407.3053, 414.9056, 481.5131, 560.1337, 630.7232, 701.6654, 731.5477, 779.0721, 857.2183, 868.6155, 900.0217, 917.8803, 971.6719, 1011.5287, 1015.3545, 1033.4927, 1047.1435, 1105.9386, 1186.7467, 1199.6906, 1228.3736, 1345.7797, 1354.7938, 1394.6039, 1474.7785, 1515.9827, 1549.1418, 1603.1824, 1636.3827, 3162.8589, 3168.1988, 3174.4097, 3186.9126, 3195.9999, 3249.3366

***Syn*-PhCHOO + MeOH PRC 1**

```
C     0.00000000   0.00000000   0.00000000
O    -0.15173000  -0.37165500  -1.35619500
C     0.97369400  -2.11206200  -1.88426600
C     2.34970000  -1.87687700  -1.50465600
C     3.18805800  -1.18363000  -2.38514900
C     4.52868300  -1.01158800  -2.07648100
C     5.03524700  -1.51959900  -0.88428700
C     4.20041600  -2.19665200   0.00115300
C     2.86275300  -2.36483700  -0.29841000
H     2.20808100  -2.89339600   0.38299200
H     4.59882500  -2.58529900   0.92599800
H     6.08151400  -1.38757100  -0.64384900
H     5.17821300  -0.48060400  -2.76219500
H     2.78620000  -0.79621600  -3.31485200
O     0.23681300  -2.86380800  -1.19355300
O    -1.16165100  -2.66600400  -1.50932300
H    -0.74017600  -0.82147900  -1.39268700
H     0.59993300  -1.77499900  -2.84797400
H     0.18211000  -0.86946300   0.63646600
H     0.84747000   0.67246600   0.04794000
```

```
H   -0.89440500  0.51763400  0.35454600
```
DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.745136485677

Frequencies (cm^{-1}): 5.8876, 24.8738, 34.8104, 75.9019, 100.9125, 106.1885, 157.4615, 208.4032, 221.2982, 317.8839, 408.2223, 412.464, 481.0869, 555.4728, 629.928, 697.9378, 730.0744, 734.7627, 780.4849, 847.8412, 865.6918, 903.0604, 920.7686, 975.6937, 1012.4035, 1016.3116, 1034.3012, 1047.5343, 1064.4768, 1109.2782, 1120.6582, 1172.8079, 1188.4163, 1202.0928, 1230.7581, 1348.9269, 1357.735, 1400.2307, 1432.1045, 1475.0417, 1477.5039, 1494.7545, 1511.0607, 1517.5424, 1559.9437, 1604.0327, 1637.2426, 2976.2703, 3013.9061, 3080.5212, 3158.3825, 3169.9998, 3176.787, 3190.3042, 3198.1443, 3256.8414, 3539.1295

***Syn*-PhCHOO + MeOH TS-AAAH 1:**

```
C    0.00000000  0.00000000  0.00000000
O   -1.30490700 -0.53587900 -0.20885100
C   -2.18843800 -1.10948200  1.43853400
C   -3.57108700 -1.15238700  0.95062400
C   -4.17709700 -2.30344900  0.43262100
C   -5.51950600 -2.27486500  0.08705100
C   -6.26337200 -1.10694500  0.23089500
C   -5.66536300  0.04073700  0.73973300
C   -4.32818400  0.01448200  1.10433200
H   -3.86456300  0.90383500  1.51196300
H   -6.24032800  0.94876500  0.85768800
H   -7.30733100 -1.09219400 -0.05209600
H   -5.98720500 -3.16729800 -0.30575400
H   -3.58179800 -3.19368800  0.30517700
O   -1.40712600 -2.12780500  1.64383600
O   -1.32988900 -2.89054200  0.40034400
H   -1.22327200 -1.61177500 -0.26147500
H   -1.96514000 -0.29266800  2.12228100
H   -0.08553600  1.07314700  0.16531200
H    0.48968800 -0.47004500  0.85639800
H    0.60937400 -0.17783000 -0.88801400
```
DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.731055960388

Frequencies (cm^{-1}): -499.2287, 44.3264, 85.0186, 127.4953, 134.3583, 200.007, 216.8136, 258.0833, 298.7417, 370.3842, 411.0532, 418.4874, 532.5224, 563.4654, 632.2935, 704.2092, 716.0222, 777.1402, 818.2559, 868.0949, 868.7512, 961.3269, 991.0922, 1010.8938, 1021.1587, 1030.7886, 1050.9684, 1058.5619, 1104.9857, 1111.2054, 1175.692, 1185.4334, 1196.4054, 1203.857, 1252.8085, 1316.1108, 1344.8578, 1362.6655, 1458.5698, 1472.898, 1489.5711, 1493.3431, 1511.1908, 1518.486, 1527.3364, 1619.0987, 1639.226, 1996.5675, 3013.9568, 3072.7993, 3100.4944, 3113.5266, 3163.9779, 3171.8594, 3184.5299, 3193.9882, 3221.9682

MeOCPhH(OOH) (*syn*-TS-AAAH 1 conformer)

```
C    0.00000000  0.00000000  0.00000000
O   -1.32049000  0.21349900  0.49021500
C   -2.01798900  1.23621600 -0.15876500
C   -3.50322500  1.10940500  0.10381700
C   -4.34512900  2.15853700 -0.26366100
C   -5.71676900  2.05458900 -0.08058200
C   -6.26271000  0.89937500  0.47045700
C   -5.42756200 -0.14825600  0.83568600
C   -4.05209400 -0.04610600  0.65103200
H   -3.40280700 -0.86007400  0.93560700
H   -5.84415900 -1.04895400  1.26646200
H   -7.33185100  0.81877000  0.61412800
H   -6.36003100  2.87665300 -0.36438900
H   -3.92113100  3.06283200 -0.67802600
O   -1.49015200  2.51923500  0.16858400
O   -1.77794300  2.81691000  1.55737400
H   -1.12265200  2.27142200  2.01707500
H   -1.81339900  1.21137300 -1.23851300
H   -0.02043500 -0.28687600 -1.05575600
H    0.62098900  0.89055000  0.11491100
H    0.42125700 -0.81419300  0.58423000
```
DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 25.9816, 89.249, 111.9697, 135.694, 157.5966, 202.5829, 223.8857, 268.3355, 332.5705, 352.185, 417.0797, 462.8453, 485.8864, 627.5409, 635.6631, 712.6684, 722.4365, 759.4634, 857.7645, 868.9383, 915.3165, 955.7796, 972.6866, 1003.7482, 1007.7168, 1019.8906, 1022.8488, 1053.4785, 1102.2451, 1115.1425, 1176.3196, 1181.7971, 1201.5144, 1211.2941, 1222.7559, 1326.6959, 1348.5361, 1355.0293, 1370.8745, 1385.5742, 1473.7302, 1485.9149, 1490.0183, 1511.4263, 1532.002, 1626.8686, 1646.6868,

2972.4889, 3004.4532, 3064.2424, 3125.0354, 3163.5635, 3173.3317, 3183.6664, 3192.0158, 3208.2738, 3727.7627

IRC:

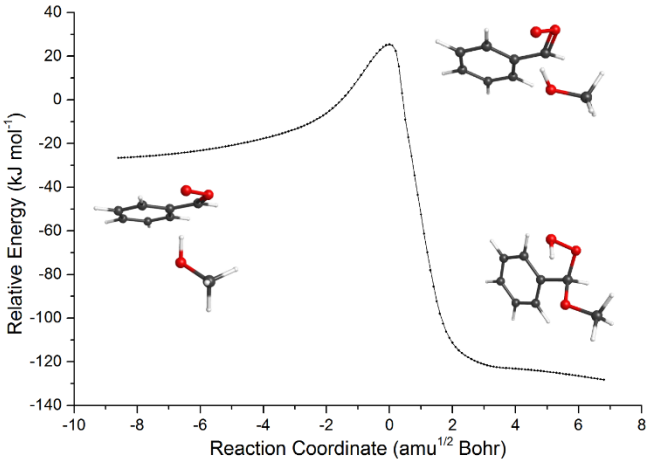


Figure S63: : SCI 10 + MeOH TS-AAAH 1 IRC

***Syn*-PhCHOO + MeOH PRC 2**

C	0.00000000	0.00000000	0.00000000
O	1.30490700	0.47087900	-0.28385100
C	2.28843800	1.19448200	1.57853400
C	3.60608700	1.17738700	0.97562400
C	4.21209700	2.32344900	0.44262100
C	5.55450600	2.28986500	0.10205100
C	6.29837200	1.12194500	0.25089500
C	5.69536300	-0.02573700	0.75973300
C	4.36318400	0.00051800	1.12933200
H	3.89956300	-0.88383500	1.54696300
H	6.27032800	-0.93376500	0.87268800
H	7.34233100	1.10219400	-0.03209600
H	6.02720500	3.18229800	-0.29075400
H	3.60679800	3.20868800	0.31017700
O	1.43212600	2.12280500	1.63883600
O	1.38988900	2.97554200	0.47034400
H	1.25327200	1.26677500	-0.44147500
H	2.05014000	0.36766800	2.24228100
H	0.08553600	-1.06814700	0.18031200
H	-0.42468800	0.49004500	0.88139800
H	-0.66937400	0.16283000	-0.85301400

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.744498988424

Frequencies (cm^{-1}): 14.2096, 19.6744, 31.8152, 79.9835, 92.7686, 104.4621, 151.2653, 163.696, 235.5262, 341.0462, 408.0337, 412.6529, 483.1751, 558.1621, 629.9173, 699.5529, 722.8306, 763.7068, 781.0625, 854.1508, 869.273, 909.0596, 917.3717, 976.4632, 1013.0243, 1015.9977, 1034.8095, 1047.4042, 1068.5917, 1108.8352, 1123.2162, 1171.9701, 1188.5031, 1202.0561, 1230.9704, 1348.5868, 1357.1142, 1400.289, 1446.554, 1474.4855, 1477.2536, 1494.7468, 1510.9691, 1517.3082, 1558.784, 1603.904, 1636.773, 2968.4286, 3002.8228, 3076.3479, 3162.3224, 3170.3288, 3176.6055, 3189.6858, 3197.922, 3253.7455, 3547.7423

***Syn*-PhCHOO + MeOH TS-AAAH 2:**

C	0.00000000	0.00000000	0.00000000
O	0.62101800	-0.85961400	0.94182600
C	-0.39484800	-2.02250500	2.13957600
C	-1.74967900	-2.01049200	1.57877600
C	-2.20696300	-2.92915100	0.62455600
C	-3.53462600	-2.90109400	0.22622700
C	-4.41212800	-1.95472600	0.74965900
C	-3.96331600	-1.03613400	1.69175600
C	-2.64079100	-1.06950000	2.10862000
H	-2.29465900	-0.36711800	2.85636600
H	-4.64254300	-0.30428000	2.10657700
H	-5.44390200	-1.93591300	0.42538100
H	-3.88703900	-3.61806100	-0.50265300

```
H   -1.50893100 -3.64255800  0.21518800
O    0.47490200 -2.98204900  2.03482000
O    0.68771500 -3.24594600  0.61187600
H    0.80816600 -1.85009400  0.51102400
H   -0.27722300 -1.48426000  3.07670900
H   -0.24044100  0.94572700  0.48475700
H    0.69651600  0.19032200 -0.82016300
H   -0.91416500 -0.43292700 -0.41361900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.730566797894

Frequencies (cm^{-1}): -586.2046, 52.0983, 77.8793, 88.2103, 159.5956, 199.5484, 211.8477, 296.2805, 310.197, 372.8817, 399.213, 413.1399, 530.1438, 542.3831, 632.1067, 703.2912, 714.4483, 780.1158, 816.5413, 861.8081, 871.0857, 950.4963, 962.8103, 1012.4804, 1020.5516, 1032.2842, 1049.6555, 1067.0181, 1086.6235, 1103.8061, 1172.1757, 1185.4289, 1196.9133, 1202.0258, 1228.2532, 1313.1798, 1339.604, 1354.0533, 1375.9332, 1464.3162, 1485.466, 1492.1693, 1499.3418, 1524.2301, 1529.895, 1618.0582, 1637.8417, 1960.4103, 3008.1558, 3062.3617, 3092.7362, 3129.2009, 3162.6398, 3172.0795, 3184.1678, 3193.8712, 3218.5359

MeOCPhH(OOH) (*syn*-TS-AAAH 2- conformer):

```
C    0.00000000  0.00000000  0.00000000
O    0.23427300  0.28882400 -1.38217500
C   -0.46216900  1.34187300 -1.98974400
C   -1.90802400  1.49944300 -1.55091300
C   -2.42640000  2.70508500 -1.08667700
C   -3.77333600  2.80631500 -0.75256900
C   -4.61617400  1.71052500 -0.88704200
C   -4.10701300  0.50677000 -1.36338700
C   -2.76265200  0.40426700 -1.69387400
H   -2.37193400 -0.53251700 -2.07086600
H   -4.75719700 -0.34962500 -1.48201400
H   -5.66332700  1.79381400 -0.62910900
H   -4.16322500  3.74797000 -0.38985000
H   -1.78117700  3.56432800 -0.98888800
O    0.28380400  2.55524000 -1.99440500
O    0.52138500  3.00273000 -0.62986500
H    1.46136600  2.79275900 -0.54530200
H   -0.43954300  1.11924000 -3.06134600
H   -0.95998400 -0.49661900  0.14689400
H    0.79877900 -0.67784700  0.29287000
H    0.03642400  0.89685700  0.61597500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.797912991077

Frequencies (cm^{-1}): 38.9272, 62.139, 117.9903, 137.3822, 171.283, 187.4489, 266.8961, 269.8304, 307.1543, 361.6836, 416.6892, 452.8227, 530.3777, 589.6905, 633.7957, 719.3825, 725.3877, 757.6922, 850.8227, 870.4348, 909.822, 927.5461, 961.8277, 992.0193, 1003.9865, 1020.0804, 1022.3112, 1055.3169, 1106.0079, 1114.9515, 1170.2386, 1182.6238, 1206.3952, 1208.5015, 1221.8909, 1321.8253, 1346.9687, 1361.2596, 1363.9753, 1379.1334, 1469.8543, 1484.2335, 1493.7506, 1512.5125, 1532.3613, 1624.5471, 1645.41, 3026.9249, 3033.0931, 3096.7044, 3122.9204, 3159.774, 3168.0868, 3178.2267, 3189.8284, 3216.5178, 3755.3171

IRC:

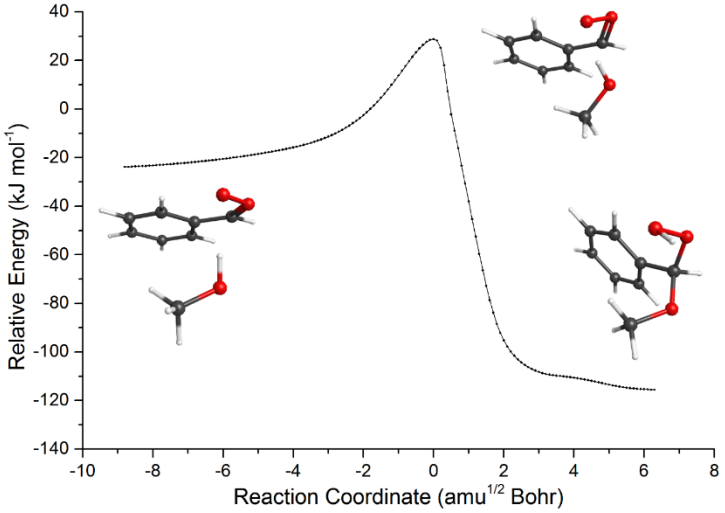


Figure S64: sCI 10 + MeOH TS-AAAH 2 IRC

7.11.2 sCI 11 + EtOH Reactions

***Syn*-PhCHOO + EtOH PRC 1.1 (For TS-AAAH 1.1 and 2.2):**

```
C     0.00000000   0.00000000   0.00000000
O    -0.79408900   0.26052400  -1.14488200
C    -5.19189400   1.68380200  -0.42558000
C    -6.33284100   0.82082600  -0.43284900
C    -6.28616800  -0.58787500  -0.45415000
C    -7.47005200  -1.30870500  -0.46317600
C    -8.69897000  -0.65731700  -0.45048200
C    -8.75701200   0.73560300  -0.42891700
C    -7.58691200   1.46813700  -0.42045300
H    -7.62728000   2.54954400  -0.40487700
H    -9.71265000   1.24060100  -0.41938500
H    -9.61475700  -1.23298900  -0.45758900
H    -7.43297300  -2.38905300  -0.48042100
H    -5.32556700  -1.07231900  -0.46409300
O    -3.95287700   1.41153100  -0.43319900
O    -3.53566300   0.09982700  -0.44696100
H    -1.73603600   0.20121100  -0.89964500
H    -5.34561100   2.75747600  -0.41302000
H    -0.21323100  -0.99972600   0.40065100
C     1.46328300   0.09601200  -0.38804900
H     2.10498300  -0.10028500   0.47287100
H     1.69925200  -0.62887400  -1.16807200
H     1.69233000   1.09144300  -0.77065400
H    -0.22112800   0.72120300   0.79796600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.005780267045

Frequencies (cm^{-1}): 10.8733, 16.8663, 25.667, 51.5719, 68.2669, 87.5008, 123.0351, 162.5405, 232.7581, 252.25, 338.042, 407.99, 412.7143, 435.5098, 483.0579, 558.069, 629.914, 699.6323, 722.3352, 762.3354, 781.0611, 815.6344, 854.1748, 869.3303, 899.7359, 908.9345, 917.237, 976.4667, 1013.0171, 1015.9642, 1034.8941, 1047.3471, 1054.7051, 1108.4887, 1120.4027, 1179.1259, 1188.4089, 1201.8297, 1230.9421, 1295.1708, 1336.6298, 1348.7015, 1356.824, 1400.6327, 1400.7137, 1473.9917, 1477.3735, 1481.8921, 1499.2657, 1517.271, 1525.5391, 1558.9306, 1603.9619, 1636.7537, 2955.8364, 2971.5934, 3026.8376, 3088.6456, 3093.385, 3162.4811, 3170.278, 3176.5233, 3189.7063, 3197.9593, 3253.5666, 3545.0272

***Syn*-PhCHOO + EtOH TS-AAAH 1.1:**

```
C     0.00000000   0.00000000   0.00000000
O    -1.39254400  -0.22068600  -0.25614300
C    -2.43714000  -0.69939100   1.32097200
C    -3.77913300  -0.40267900   0.80590600
C    -4.59797400  -1.34958100   0.17897200
C    -5.89097200  -1.00478400  -0.18453700
C    -6.37419400   0.27953500   0.04940300
C    -5.56349500   1.22576400   0.66669900
C    -4.27561000   0.88289700   1.04847100
H    -3.64807900   1.61566200   1.53965500
```

```
H   -5.93590500  2.22316300  0.85531100
H   -7.38074800  0.54151100 -0.24788400
H   -6.52372800 -1.74059200 -0.66174000
H   -4.20163000 -2.33351100 -0.01586000
O   -1.90660500 -1.87805600  1.46394700
O   -1.95154100 -2.54989700  0.16828400
H   -1.54626800 -1.28173600 -0.39002700
H   -2.06967700 -0.00553800  2.07435400
H    0.55760800 -0.38761000 -0.85701300
C    0.26892100  1.47808600  0.19378200
H    1.33458000  1.64882100  0.35298500
H   -0.04456800  2.04524900 -0.68236600
H   -0.26619800  1.86715500  1.06138600
H    0.30944400 -0.58102900  0.87443600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.993340481633

Frequencies (cm^{-1}): -498.1751, 36.0437, 63.8571, 66.9081, 105.0502, 174.6208, 209.4134, 255.3421, 259.0428, 293.4232, 350.8061, 387.6957, 413.0504, 438.201, 534.2381, 575.9907, 632.2364, 704.4611, 717.3823, 777.7924, 809.7184, 819.087, 867.3697, 868.2433, 880.0483, 960.93, 1010.6984, 1018.4652, 1025.0436, 1032.0899, 1051.1148, 1068.2236, 1093.6861, 1105.0158, 1176.265, 1182.4328, 1185.1956, 1200.6333, 1240.1988, 1304.3786, 1315.8955, 1344.2403, 1362.1539, 1376.0389, 1411.1646, 1469.3747, 1486.2221, 1496.6291, 1497.8009, 1513.0781, 1522.3832, 1527.064, 1619.211, 1638.8954, 1992.6069, 3008.1503, 3031.0684, 3036.9349, 3091.7172, 3103.9572, 3116.4506, 3163.7825, 3171.8014, 3184.2646, 3193.8281, 3221.9167

EtOCPhHOOH (*syn*-TS-AAAH 1.1):

```
C    0.00000000  0.00000000  0.00000000
O    1.38712700  0.09880400 -0.36176400
C    2.19473900  0.78006100  0.55398600
C    3.64783200  0.39900000  0.36322100
C    4.63247100  1.14922000  1.00556700
C    5.97013700  0.79921800  0.88833200
C    6.33915200 -0.30673700  0.12865100
C    5.36155600 -1.05746000 -0.51087200
C    4.01967200 -0.70830400 -0.39284900
H    3.25975400 -1.29025700 -0.89162400
H    5.64051100 -1.91734200 -1.10522100
H    7.38203500 -0.57884400  0.03603300
H    6.72578100  1.39191300  1.38618800
H    4.34854900  2.01789800  1.58344800
O    1.96578500  2.18621300  0.49692200
O    2.42944100  2.69525700 -0.77799600
H    1.74458400  2.36842500 -1.38062600
H    1.87933100  0.57518300  1.58523100
H   -0.53790500 -0.08100700 -0.94426600
C   -0.27871400 -1.21094900  0.87430600
H   -1.34588100 -1.27333900  1.09435300
H    0.02217200 -2.12797100  0.36830300
H    0.25317900 -1.15418900  1.82476700
H   -0.31997300  0.92497700  0.48535700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.064328689457

Frequencies (cm^{-1}): 22.9764, 48.7119, 73.02, 105.3045, 144.0758, 170.74, 223.5693, 234.0349, 281.3699, 307.596, 348.7012, 413.6825, 418.0568, 472.0642, 498.895, 627.1724, 635.4648, 711.7083, 721.3909, 759.1974, 811.2701, 856.3061, 869.5107, 880.3922, 924.0981, 968.281, 971.9406, 1004.4058, 1018.4217, 1022.8732, 1026.311, 1052.8713, 1079.1754, 1107.8632, 1111.5264, 1181.6971, 1199.3587, 1202.508, 1220.5294, 1313.1549, 1331.1824, 1347.372, 1355.3314, 1372.0489, 1385.964, 1403.642, 1415.2072, 1484.3295, 1488.6269, 1496.5583, 1517.1526, 1531.5116, 1626.443, 1646.4417, 2988.3544, 3031.4226, 3032.6952, 3074.4777, 3093.4545, 3106.5403, 3163.3212, 3172.8711, 3183.4212, 3191.9105, 3209.3408, 3721.6249

IRC:

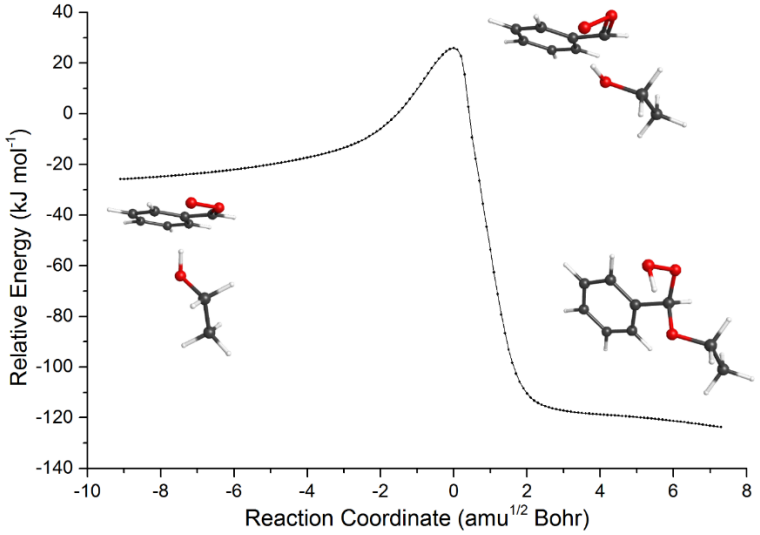


Figure S65: SCI 10 + EtOH TS-AAAH 1.1 IRC

Syn-PhCHOO + EtOH PRC 2.1 (For TS-AAAH 1.2):

C	0.00000000	0.00000000	0.00000000
O	0.83896100	0.37608100	1.07807300
C	5.31670900	1.32569200	0.10623900
C	6.38411800	0.37588300	0.17729400
C	6.22468800	-1.01386000	0.35122000
C	7.34626800	-1.82631200	0.40799000
C	8.62257700	-1.28500700	0.29448400
C	8.79201500	0.08810400	0.12153200
C	7.68508900	0.91100200	0.06363100
H	7.81204600	1.97759000	-0.06907600
H	9.78437600	0.50746200	0.03372600
H	9.48867100	-1.93143500	0.34059100
H	7.22294200	-2.89196800	0.54216100
H	5.22884300	-1.41188600	0.43726200
O	4.06089800	1.16061400	0.17589000
O	3.53980300	-0.10267900	0.34350300
H	1.76566000	0.19569100	0.83331600
H	5.55567100	2.37534200	-0.02685200
H	0.32878700	0.47755800	-0.93207300
C	-0.07993000	-1.50944200	-0.19535400
H	-0.76915300	-1.75949900	-1.00590500
H	0.90012900	-1.91965800	-0.44555900
H	-0.42896600	-1.99375700	0.71750500
H	-0.99053900	0.39764900	0.23110100

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.005883300656

Frequencies (cm^{-1}): 9.9321, 14.7492, 28.4819, 55.5768, 78.7754, 90.6251, 139.036, 162.2108, 232.4129, 266.0002, 339.6198, 407.8016, 412.3524, 423.1603, 482.6317, 557.5289, 630.2754, 698.9856, 717.4921, 752.1276, 780.3171, 805.3256, 853.6691, 867.3613, 884.0286, 908.1207, 916.1244, 975.3093, 1012.7748, 1015.9254, 1034.0445, 1047.4706, 1063.1172, 1107.7741, 1113.268, 1139.3534, 1188.2006, 1201.3673, 1230.9613, 1300.7746, 1348.2679, 1356.8968, 1390.8908, 1400.3962, 1404.5638, 1448.7324, 1477.2967, 1488.5365, 1493.7588, 1513.6539, 1517.5759, 1559.0539, 1604.081, 1636.9517, 2967.4224, 3017.1801, 3039.8098, 3077.192, 3091.7013, 3162.3343, 3169.8096, 3176.2672, 3189.2961, 3197.62, 3252.6217, 3543.6129

Syn-PhCHOO + EtOH TS-AAAH 1.2:

C	0.00000000	0.00000000	0.00000000
O	-1.31306900	0.35168700	0.45853300
C	-2.45299000	1.12877900	-0.91741400
C	-3.75704300	0.92831500	-0.27398100
C	-4.37975300	1.88822000	0.53262300
C	-5.65622600	1.65102800	1.01932600
C	-6.31426000	0.45877500	0.73016400
C	-5.69823700	-0.50048300	-0.06610200
C	-4.42924600	-0.26244100	-0.57101400
H	-3.95361200	-1.00309200	-1.20131700
H	-6.20747900	-1.42577800	-0.29762500
H	-7.30574400	0.27856100	1.12345200
H	-6.13824700	2.39733200	1.63590700

```
H   -3.84710000  2.79635000  0.76687500
O   -1.79884800  2.24881500 -1.00520200
O   -1.61611000  2.76971500  0.34751700
H   -1.30930100  1.39334100  0.72412500
H   -2.25864500  0.48696300 -1.77460900
H    0.31246500  0.69623200 -0.78359200
C    0.99030100  0.02217600  1.15121200
H    1.98127300 -0.26577400  0.79580600
H    1.06213400  1.02223000  1.57950100
H    0.68892400 -0.67206600  1.93518600
H   -0.07239300 -0.99926600 -0.43231100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.993197196119

Frequencies (cm^{-1}): -463.2392, 36.3274, 43.8928, 78.5261, 105.9804, 167.0304, 205.306, 238.2404, 262.8419, 296.4932, 339.5831, 411.0717, 415.3385, 454.2368, 531.5206, 568.9457, 632.5672, 704.0002, 716.074, 777.1425, 817.9743, 819.0298, 866.7817, 868.0899, 886.5987, 960.2947, 1009.0813, 1013.8251, 1022.1945, 1030.9465, 1050.7476, 1057.2237, 1104.164, 1114.1704, 1136.3126, 1185.0734, 1196.0791, 1201.8988, 1240.5826, 1308.5419, 1324.6003, 1344.2114, 1361.429, 1402.5604, 1418.3537, 1469.3002, 1476.881, 1496.3725, 1499.0808, 1508.3906, 1522.482, 1527.2152, 1619.2101, 1639.537, 2039.3494, 3015.6989, 3032.1768, 3059.642, 3095.176, 3108.4378, 3113.6611, 3163.2098, 3171.6911, 3184.1469, 3193.6353, 3221.2621

EtOCPhHOOH (*syn*-TS-AAAH 1.2):

```
C    0.00000000  0.00000000  0.00000000
O   -1.32072000 -0.06517100  0.55324300
C   -2.23889900  0.81518600 -0.02316300
C   -3.65630900  0.36804500  0.26700600
C   -4.70865200  1.24010200 -0.01005300
C   -6.02230600  0.84305200  0.19563600
C   -6.29936700 -0.43191200  0.67929600
C   -5.25418400 -1.30359600  0.95528800
C   -3.93645500 -0.90723300  0.74778700
H   -3.12428800 -1.58476600  0.96323400
H   -5.46125700 -2.29574800  1.33371500
H   -7.32331900 -0.74139900  0.84040200
H   -6.83036400  1.52983600 -0.01772100
H   -4.49406700  2.23635200 -0.37143100
O   -1.98110400  2.16470200  0.35879700
O   -2.26771800  2.32667700  1.77018800
H   -1.50667900  1.88741800  2.17805800
H   -2.07320300  0.88485500 -1.10746400
H    0.39937100  1.01125000  0.11246400
C    0.86957000 -1.01068200  0.71553700
H    1.88020200 -0.98813400  0.30645100
H    0.92748100 -0.78893400  1.78120300
H    0.47238000 -2.01847100  0.59628900
H   -0.05335500 -0.22118300 -1.07199300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.065496928411

Frequencies (cm^{-1}): 28.2438, 54.0097, 80.1213, 105.7036, 114.8944, 174.3511, 221.8811, 245.6859, 254.2216, 292.4857, 323.8226, 381.9474, 416.9842, 483.6083, 499.6121, 632.4632, 639.9051, 714.1252, 727.051, 763.1238, 822.8523, 855.3963, 869.934, 884.3844, 927.421, 972.4051, 974.7479, 1004.3953, 1019.1949, 1022.7967, 1042.4887, 1054.0699, 1097.6703, 1114.4713, 1145.8892, 1181.8401, 1182.409, 1201.5965, 1221.9577, 1300.5134, 1322.4273, 1343.8586, 1352.2542, 1361.9033, 1383.6114, 1408.5405, 1433.1904, 1484.6355, 1485.7053, 1500.6357, 1527.7919, 1531.7943, 1626.5624, 1646.5582, 2973.7631, 2992.3646, 3036.2617, 3037.4651, 3101.6902, 3106.203, 3163.5671, 3173.2703, 3183.8234, 3192.2102, 3208.1559, 3725.228

IRC:

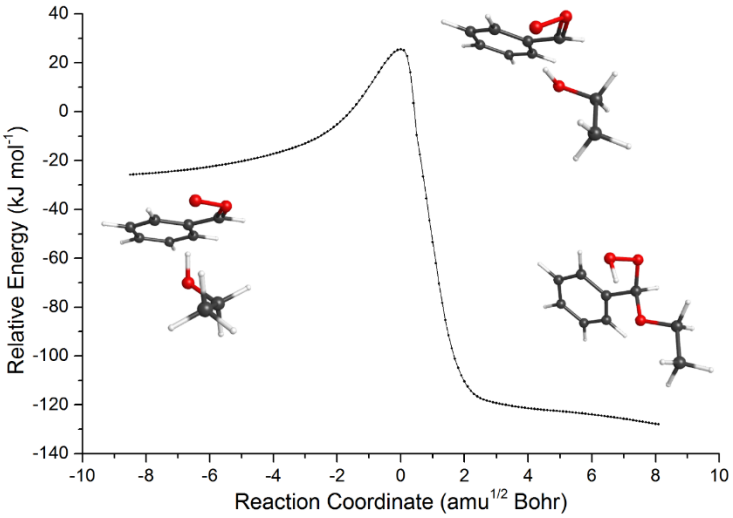


Figure S66: SCI 10 + EtOH TS-AAAH 1.2 IRC

***Syn*-PhCHOO + EtOH PRC 3 (For TS-AAAH 1.3):**

```
C     0.00000000  0.00000000  0.00000000
O    -1.40491800  0.05807400 -0.19476100
C    -4.32696800  2.78431700  0.20886900
C    -5.32156800  1.75666600  0.22977500
C    -5.21484500  0.53254200  0.92038700
C    -6.25508300 -0.38040600  0.85217900
C    -7.39893200 -0.10063000  0.11184200
C    -7.51568300  1.10697200 -0.57528700
C    -6.48784800  2.02652900 -0.51797500
H    -6.57252700  2.96424600 -1.05164400
H    -8.40449800  1.32214000 -1.15151700
H    -8.20208900 -0.82388100  0.06666800
H    -6.17033700 -1.32056900  1.37897300
H    -4.32130200  0.33248700  1.48470500
O    -3.19196800  2.85059400  0.77111700
O    -2.74991500  1.80729600  1.56159400
H    -1.78983800  0.68706300  0.44360100
H    -4.51913000  3.68383100 -0.36668700
H     0.35793800 -0.81682600 -0.62979600
C     0.70844500  1.29586700 -0.37266300
H     0.50704900  1.55646100 -1.41265300
H     0.36824500  2.11833000  0.25877400
H     1.78897100  1.19541400 -0.24483000
H     0.23398100 -0.26690900  1.03803300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.006822224458

Frequencies (cm^{-1}): 9.0638, 20.2398, 25.2503, 47.6056, 79.5987, 88.824, 155.1978, 199.9027, 220.0012, 267.0608, 317.4763, 408.5133, 412.9475, 422.9996, 481.1409, 555.3429, 630.193, 697.2542, 712.8174, 730.187, 780.3717, 807.5648, 847.6696, 865.3364, 884.2561, 903.0576, 920.1998, 975.3874, 1012.2104, 1016.352, 1034.1819, 1047.8134, 1062.3546, 1107.175, 1110.1304, 1140.1305, 1188.4057, 1201.8359, 1230.4427, 1298.9453, 1348.9136, 1357.7986, 1391.2431, 1400.1973, 1406.0245, 1438.5472, 1477.5073, 1488.157, 1494.885, 1514.3592, 1517.8233, 1559.8603, 1604.2082, 1637.3422, 2975.3363, 3018.9363, 3044.2421, 3079.4872, 3092.1126, 3158.3362, 3169.6723, 3176.5614, 3190.2791, 3197.9198, 3257.6868, 3532.8396

***Syn*-PhCHOO + EtOH TS-AAAH 1.3:**

```
C     0.00000000  0.00000000  0.00000000
O     1.28801900  0.63299000  0.01511900
C     2.16420600  1.16971000  1.66153700
C     3.55053000  1.08932900  1.18400400
C     4.23709200  2.17116400  0.62055900
C     5.57479800  2.03334000  0.28296000
C     6.23399500  0.82327900  0.48160600
C     5.55547700 -0.25575600  1.03747700
C     4.22226600 -0.11980900  1.39294200
H     3.69633900 -0.95535100  1.83733600
H     6.06523100 -1.19552800  1.19907000
```

```
H     7.27496500   0.72237400   0.20520500
H     6.10521100   2.87247500  -0.14601900
H     3.70508300   3.09434900   0.45251100
O     1.47792300   2.25945300   1.84479200
O     1.43614700   2.99086600   0.57929000
H     1.21766900   1.70757400  -0.04761700
H     1.87746100   0.39457800   2.36940200
H     0.17301800  -1.06115900   0.18750700
C    -1.01745600   0.56432800   0.97994800
H    -1.97433400   0.06255300   0.82593000
H    -0.72048300   0.40464100   2.01618400
H    -1.15970100   1.63349700   0.82939900
H    -0.37710900   0.09391100  -1.02276300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.989494064

Frequencies (cm^{-1}): -498.8902, 42.4999, 46.217, 74.0352, 118.8662, 158.6956, 209.4411, 242.6527, 276.5848, 293.3044, 358.9927, 401.9017, 413.1342, 451.8579, 531.5045, 563.0256, 632.4757, 703.27, 714.5403, 776.7378, 804.4083, 817.1448, 862.2509, 867.0207, 870.4017, 960.5873, 1001.9658, 1010.6833, 1021.5816, 1031.1448, 1051.1452, 1067.1795, 1104.1634, 1111.4841, 1142.5156, 1185.1248, 1189.8815, 1201.441, 1235.3907, 1305.4254, 1320.0823, 1343.3055, 1361.1264, 1396.8532, 1413.0701, 1420.1737, 1471.2163, 1493.1119, 1494.1715, 1508.1415, 1518.4145, 1527.2539, 1619.7989, 1639.3967, 2037.5915, 3011.4492, 3036.436, 3053.6781, 3095.2925, 3113.5683, 3116.059, 3162.5708, 3171.5047, 3183.8299, 3193.4479, 3220.4183

EtOCPhHOOH (*syn*-TS-AAAH 1.3-conformer):

```
C     0.00000000   0.00000000   0.00000000
O    -0.13082800  -0.48822900   1.34719600
C     0.26622900   0.38770500   2.36686300
C    -0.37040000  -0.03543700   3.67934000
C     0.26262100   0.25089900   4.89625500
C    -0.35756800  -0.07105700   6.10582400
C    -1.61957500  -0.67450900   6.11285700
C    -2.25614600  -0.95682500   4.90104200
C    -1.63394600  -0.64047100   3.68920500
H    -2.12685400  -0.87211000   2.74700100
H    -3.23949700  -1.42872000   4.89660700
H    -2.10277200  -0.92467700   7.05802000
H     0.14900900   0.14719500   7.04671100
H     1.24838900   0.71249400   4.89429600
O     1.68620700   0.53393500   2.43043000
O     2.28228000  -0.73003600   2.81080100
H     2.19393700  -1.24396000   1.99013200
H    -0.02024100   1.42572300   2.11283900
H    -0.13387300   1.09370000  -0.00558100
C     1.32371400  -0.38663500  -0.64957400
H     1.32398000  -0.07387000  -1.70377200
H     2.17197500   0.09717200  -0.14935700
H     1.46069500  -1.47693000  -0.62374200
H    -0.83929200  -0.44738000  -0.54954800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree):

Frequencies (cm^{-1}): 26.0766, 41.2296, 71.4569, 107.3266, 146.0047, 162.2072, 214.5502, 235.0279, 271.805, 306.6597, 343.3796, 417.3056, 441.011, 464.9306, 485.8391, 629.9851, 636.2089, 710.6321, 720.1401, 757.9295, 808.2377, 854.986, 868.8094, 874.2606, 924.8216, 966.9729, 971.274, 1003.7643, 1017.7591, 1022.8065, 1027.2599, 1053.3962, 1090.6244, 1110.7903, 1121.3324, 1181.5832, 1200.4854, 1203.0694, 1221.2933, 1315.1666, 1332.0285, 1344.9699, 1355.4841, 1371.7263, 1386.3354, 1402.0833, 1418.2078, 1484.1934, 1488.2985, 1497.3311, 1515.7714, 1531.6887, 1626.813, 1646.2686, 2974.2531, 3011.3918, 3030.4971, 3065.4712, 3089.3724, 3111.3577, 3163.3285, 3173.1513, 3183.8401, 3192.3781, 3208.2982, 3721.2965

IRC:

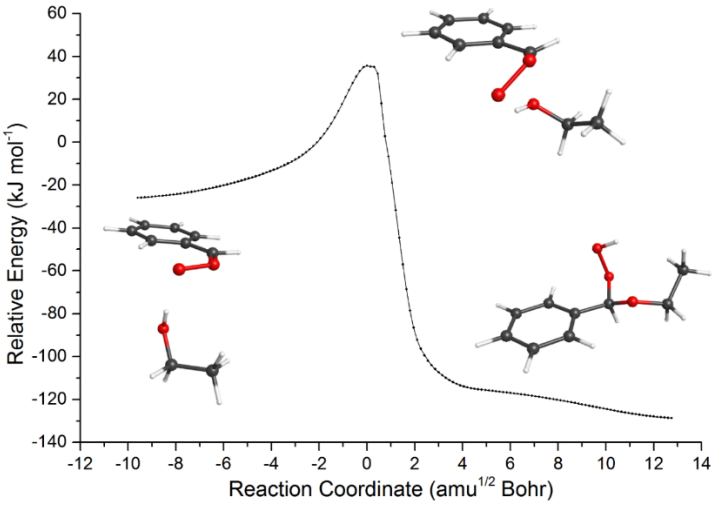


Figure S67: SCI 10 + EtOH TS-AAAH 1.3 IRC

***Syn*-PhCHOO + EtOH PRC 3.1 (For TS-AAAH 2.1):**

```
C     0.00000000  0.00000000  0.00000000
O     0.86724800 -0.27348700 -1.08653400
C     5.13993300 -1.99401000 -0.21174700
C     6.31353300 -1.18688700 -0.07897600
C     7.53793500 -1.88873200 -0.06930500
C     8.73550100 -1.21267600  0.05106600
C     8.73486800  0.17709400  0.16393100
C     7.53572100  0.88188900  0.15572700
C     6.32482800  0.21806500  0.03616100
H     5.38628500  0.74404600  0.02717600
H     7.54346300  1.95945100  0.24300500
H     9.67226300  0.70861100  0.25826100
H     9.66815300 -1.75899800  0.05736800
H     7.53357800 -2.96736500 -0.15772300
O     3.91510800 -1.66635400 -0.25349800
O     3.55260200 -0.34140900 -0.16067300
H     1.78479100 -0.31000800 -0.75793800
H     5.24922800 -3.06992600 -0.29593100
H    -0.97443800  0.22729500 -0.43751300
C    -0.12803900 -1.16777000  0.97129400
H    -0.83850000 -0.93317700  1.76801800
H    -0.47599500 -2.06048400  0.44982900
H     0.83484100 -1.39491600  1.43214700
H     0.32647000  0.89775200  0.54046400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.006304666007

Frequencies (cm^{-1}): 8.908, 18.4961, 28.1764, 49.2417, 78.3852, 91.078, 139.6751, 162.3983, 233.3261, 268.8226, 339.974, 408.0668, 412.6144, 421.7832, 483.1851, 557.4839, 629.928, 699.3454, 717.9501, 752.1557, 780.7911, 806.2782, 853.7281, 868.0194, 883.6519, 908.8557, 916.5112, 975.8322, 1013.265, 1016.0272, 1034.9444, 1047.4409, 1063.6072, 1108.9567, 1112.9182, 1139.3273, 1188.5118, 1202.3128, 1231.0644, 1300.3109, 1348.4937, 1357.6047, 1390.1777, 1400.0179, 1403.912, 1449.3833, 1477.2022, 1488.5539, 1493.7184, 1513.0958, 1517.4161, 1558.9734, 1603.8536, 1636.8615, 2968.8566, 3017.0814, 3040.224, 3077.1969, 3091.2585, 3161.2572, 3170.3741, 3176.7799, 3189.7154, 3198.0419, 3253.9452, 3544.5487

***Syn*-PhCHOO + EtOH TS-AAAH 2.1:**

```
C     0.00000000  0.00000000  0.00000000
O     0.21953300  1.31943500 -0.49702400
C    -1.23602100  2.51780000 -0.97841800
C    -2.42811200  1.88756300 -0.39839200
C    -3.15451500  1.02664400 -1.22942900
C    -4.33501100  0.44754800 -0.78717600
C    -4.80926700  0.73634800  0.48728100
C    -4.09902600  1.60233000  1.31495900
C    -2.90934600  2.17106500  0.88649300
H    -2.33643600  2.82915400  1.52097800
H    -4.47281900  1.83093900  2.30367200
H    -5.73198300  0.29101300  0.83423400
```

```
H   -4.88732300 -0.21725600 -1.43686000
H   -2.79497600  0.81783700 -2.22922400
O   -0.61550800  3.56028800 -0.51288900
O   -0.21455600  3.26924900  0.86392200
H    0.25597000  2.04365900  0.31538100
H   -1.17056000  2.47121100 -2.06260500
H   -0.29600400 -0.62288900 -0.84598300
C    1.27032600 -0.53616800  0.64087800
H    1.10545200 -1.55448100  0.99759000
H    2.08992300 -0.54804200 -0.07682300
H    1.56724400  0.07778700  1.49173700
H   -0.82180200 -0.00215800  0.72137100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.992606841398

Frequencies (cm^{-1}): -527.7177, 47.9781, 59.3307, 66.565, 127.624, 168.1251, 202.2713, 250.9578, 255.7817, 303.7309, 347.4465, 398.1398, 413.6728, 473.0111, 527.916, 545.7106, 631.8875, 703.8767, 715.064, 780.0012, 816.1715, 819.9804, 859.6323, 872.8463, 889.9874, 963.0229, 994.3944, 1013.156, 1020.6325, 1033.8082, 1050.5827, 1064.7883, 1080.1938, 1103.9251, 1133.4311, 1185.3068, 1193.92, 1199.7657, 1222.6556, 1306.4355, 1320.7459, 1341.9183, 1358.3935, 1382.2594, 1408.8959, 1425.1509, 1480.5179, 1485.8385, 1497.305, 1515.2679, 1525.7115, 1537.0255, 1618.4046, 1637.9914, 1986.1436, 3016.3761, 3031.5923, 3056.4656, 3094.3526, 3108.0439, 3127.6258, 3162.8839, 3172.0196, 3184.2556, 3193.8452, 3218.1717

EtOCPhHOOH (*syn*-TS-AAAH 2.1-conformer):

```
C    0.00000000  0.00000000  0.00000000
O   -0.37533500  1.23623900  0.60710500
C   -1.44791100  1.89836200 -0.01865300
C   -2.80507600  1.31446500  0.31860300
C   -3.83283800  1.40968300 -0.61703900
C   -5.09804900  0.91110200 -0.33152000
C   -5.34393600  0.30701800  0.89609200
C   -4.32058000  0.20427700  1.83232300
C   -3.05632600  0.70381800  1.54491100
H   -2.26097500  0.62608200  2.27164700
H   -4.50837200 -0.26402400  2.78929900
H   -6.32707300 -0.08403800  1.12122900
H   -5.88817300  0.99124700 -1.06590200
H   -3.64426700  1.88134300 -1.57367200
O   -1.33602900  3.27703000  0.27694600
O   -1.53075400  3.48084300  1.69774700
H   -0.63362600  3.32566700  2.02816600
H   -1.30771600  1.90524300 -1.10764700
H    0.24926300  0.17716900 -1.05355200
C    1.19253400 -0.55897900  0.74571900
H    1.50577600 -1.50159900  0.29555500
H    2.03136400  0.13582700  0.71024700
H    0.94255400 -0.74498800  1.79014700
H   -0.83957700 -0.70184100  0.03071100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.062153689572

Frequencies (cm^{-1}): 28.9424, 53.2702, 68.9739, 100.7676, 111.9106, 186.7496, 231.4769, 255.4566, 277.8636, 302.9254, 323.84, 370.0012, 416.8427, 469.6888, 568.9006, 579.8335, 634.7717, 704.9378, 718.8887, 776.7425, 824.6532, 860.1436, 865.7894, 901.9267, 929.5226, 952.531, 999.7314, 1014.9731, 1021.0522, 1023.0404, 1039.8012, 1051.9032, 1097.5805, 1114.8961, 1150.0633, 1181.7766, 1182.3566, 1200.0538, 1216.798, 1305.7736, 1316.2115, 1347.2193, 1350.8193, 1375.1064, 1385.7425, 1406.813, 1432.4843, 1485.0804, 1488.0821, 1500.5583, 1525.9016, 1530.4963, 1627.4898, 1644.8328, 2978.0442, 2987.4877, 3016.8695, 3037.0976, 3101.4181, 3106.2181, 3156.8847, 3166.4409, 3177.265, 3188.8856, 3200.0542, 3731.7128

IRC:

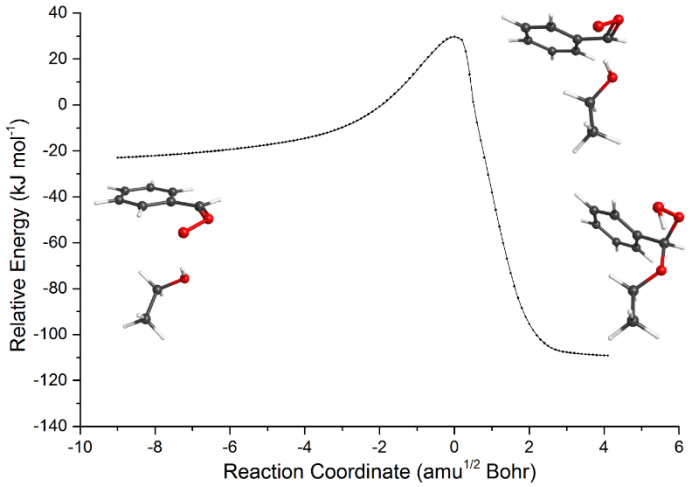


Figure S68: SCI 10 + EtOH TS-AAAH 2.1 IRC

***Syn*-PhCHOO + EtOH TS-AAAH 2.2:**

C	0.00000000	0.00000000	0.00000000
O	0.28261100	-1.10414200	0.85484100
C	-1.06429200	-2.04127500	1.90667600
C	-2.33923600	-1.59188000	1.33726800
C	-2.96371200	-0.51091900	1.97091500
C	-4.84794800	-0.70840100	0.49484600
C	-4.23838600	-1.79140000	-0.13372000
C	-4.20814900	-0.06625800	1.54871100
C	-2.98743800	-2.23058000	0.27147600
H	-2.49350000	-3.05621000	-0.21648100
H	-4.73987100	-2.29316400	-0.94997400
H	-5.82048800	-0.36849300	0.16515000
H	-4.68024900	0.77016800	2.04526800
H	-2.47336200	-0.02413600	2.80449000
O	-0.49605200	-3.19388600	1.70873600
O	-0.30670000	-3.36388200	0.26866200
H	0.19555200	-2.06048400	0.31962800
H	-0.84211300	-1.65946300	2.89979000
H	-1.06489100	0.02316200	-0.25250500
C	0.42254100	1.29732900	0.66092100
H	0.23592900	2.13968500	-0.00714300
H	-0.13575700	1.46687600	1.58251700
H	1.48454900	1.27736500	0.90432500
H	0.54818400	-0.15472100	-0.93470000

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.992564932903

Frequencies (cm^{-1}): -600.6421, 43.622, 52.1883, 81.5415, 119.6349, 188.6165, 204.5791, 239.9441, 293.005, 325.5727, 352.5144, 370.2475, 414.0696, 416.9222, 536.3071, 553.6013, 632.5844, 704.5449, 715.4652, 780.5281, 803.3706, 817.305, 859.385, 872.9835, 880.431, 963.9173, 1003.3406, 1013.8209, 1020.7181, 1033.8812, 1050.235, 1073.8536, 1089.4933, 1103.6678, 1134.218, 1174.3009, 1185.4312, 1197.996, 1219.067, 1309.0672, 1312.1257, 1321.7139, 1347.4892, 1361.3397, 1404.5867, 1428.6418, 1478.4736, 1485.5024, 1494.8777, 1509.845, 1522.809, 1526.2707, 1618.4552, 1638.0486, 1951.576, 3000.1904, 3025.2703, 3031.9549, 3092.4579, 3103.7979, 3131.0032, 3162.0725, 3171.9002, 3183.9162, 3193.8244, 3218.1443

EtOCPhHOOH (syn-TS-AAAH 2.2-Conformer):

C	0.00000000	0.00000000	0.00000000
O	-0.30199900	-0.44772400	1.33106800
C	-1.35353400	-1.34535000	1.53829400
C	-2.70609200	-0.87690000	1.01789300
C	-3.05212200	0.46891500	1.14454900
C	-4.31243400	0.91430700	0.76630200
C	-5.24633400	0.01688900	0.26081300
C	-4.91121100	-1.32640700	0.14228100
C	-3.65051500	-1.77309100	0.52257600
H	-3.39838900	-2.81841800	0.42960800
H	-5.63248800	-2.03231200	-0.24730800
H	-6.22804300	0.36165600	-0.03491300
H	-4.56539300	1.96106200	0.86967600
H	-2.33118000	1.16843100	1.54500400

```
O   -1.04509300 -2.69165000  1.20174700
O   -0.99582900 -2.84652700 -0.24980200
H   -0.07650800 -3.12657000 -0.35133700
H   -1.40797200 -1.44584900  2.62718300
H   -0.91700500  0.11825200 -0.57849100
C    0.75375100  1.30946900  0.10832100
H    1.05112700  1.65197500 -0.88391500
H    0.13575300  2.08107300  0.56747000
H    1.65267500  1.18716200  0.71258000
H    0.61412200 -0.75107400 -0.50167200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.060044436697

Frequencies (cm^{-1}): 32.7239, 55.8421, 104.4433, 117.0385, 155.3022, 186.4648, 224.2887, 243.2439, 262.1478, 285.1317, 339.5488, 364.4398, 420.2086, 466.7243, 547.7475, 597.4924, 634.4945, 718.9616, 737.7213, 748.9431, 816.8714, 837.6767, 866.1012, 871.504, 916.7168, 967.9056, 984.0006, 1005.7813, 1015.3686, 1020.6267, 1022.4819, 1054.6936, 1097.1636, 1114.9206, 1127.7952, 1181.6046, 1182.5682, 1205.2024, 1218.5604, 1305.7636, 1318.8562, 1335.2662, 1357.4486, 1358.9044, 1386.2566, 1401.8892, 1420.4347, 1483.2032, 1484.5319, 1498.2793, 1519.9616, 1530.6358, 1624.4829, 1644.362, 3023.5771, 3027.9581, 3034.4889, 3065.7914, 3097.8928, 3105.6675, 3163.5367, 3172.6363, 3183.0195, 3190.9737, 3210.9984, 3763.9756

IRC:

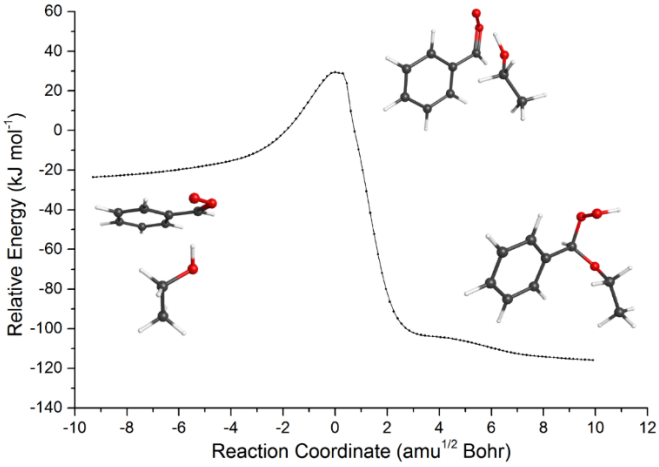


Figure S69: SCI 10 + EtOH TS-AAAH 2.2 IRC

7.11.3 sCI 11 + iPrOH Reactions

***Syn*-PhCHOO + iPrOH PRC (For TS-AAAH 1.1 and TS-AAAH 2.2):**

```
C    0.00000000  0.00000000  0.00000000
O    1.36883400 -0.37701100  0.12486300
H    1.91019900  0.19069200 -0.45413000
H   -0.11065700  1.05687600  0.28004900
C   -0.49301100 -0.17171300 -1.43475500
H   -1.53696700  0.13507100 -1.52989900
H    0.10142900  0.43412000 -2.12014400
H   -0.40939300 -1.21665600 -1.73962000
C   -0.78753800 -0.84603900  0.98809700
H   -1.84554200 -0.58030200  0.97201900
H   -0.69204800 -1.90419800  0.73738600
H   -0.40868700 -0.70123200  1.99988300
C    5.42339800 -0.41788600 -1.05331200
C    6.34547200 -1.44883000 -1.13889900
C    7.53099800 -1.40377800 -0.41271800
C    7.80958600 -0.31684300  0.41489200
C    6.90093300  0.71785700  0.51149800
C    5.69414500  0.68588900 -0.21962600
C    4.83217200  1.81218300 -0.03407300
O    3.70023600  2.08028700 -0.53964100
O    3.11858600  1.20419300 -1.43501900
H    5.14485500  2.60307500  0.63969600
H    7.11127600  1.56293000  1.15408800
H    8.73075700 -0.28419600  0.97944000
H    8.24085500 -2.21652900 -0.48847800
H    6.13549400 -2.29644900 -1.77615500
```

H 4.49993700 -0.43475900 -1.60476100

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.269634960958

Frequencies (cm^{-1}): 5.524, 20.1146, 25.9598, 48.628, 58.7809, 75.614, 148.1544, 185.855, 217.9215, 221.3416, 262.3466, 318.537, 363.873, 406.8046, 412.9557, 431.083, 480.9491, 486.4805, 555.458, 630.6434, 698.3831, 722.5291, 730.4835, 781.4284, 820.9749, 847.8809, 867.2539, 902.4496, 920.9245, 928.534, 945.0307, 967.6968, 976.5088, 1013.3447, 1016.2244, 1035.3216, 1047.7405, 1107.861, 1115.653, 1159.9456, 1185.6783, 1188.3434, 1201.1386, 1230.9062, 1317.4814, 1348.3775, 1357.2227, 1375.7653, 1392.9964, 1399.8486, 1408.2138, 1439.6593, 1477.3905, 1482.4519, 1489.6532, 1497.2377, 1508.7094, 1518.1783, 1559.4161, 1604.5122, 1637.386, 2948.2235, 3017.4725, 3027.2572, 3078.9221, 3087.5561, 3090.8726, 3096.7276, 3158.9035, 3169.574, 3176.4066, 3190.1424, 3197.8731, 3255.5717, 3541.1301

Syn-PhCHOO + iPrOH TS-AAAH 1.1

C 0.00000000 0.00000000 0.00000000
O -1.37245000 -0.25111800 -0.36975000
H -1.49440700 -1.31081900 -0.49792000
H 0.21395300 -0.56437700 0.91408900
C 0.90689300 -0.51076500 -1.11222300
H 1.95370200 -0.36681600 -0.84069600
H 0.74543000 -1.57508300 -1.28275900
H 0.71309300 0.02679500 -2.04134700
C 0.15990500 1.48774900 0.26210900
H 1.18496800 1.71317400 0.55813000
H -0.07485200 2.06009600 -0.63613800
H -0.50121900 1.82261100 1.06230900
C -4.59024300 -1.43122200 -0.20143500
C -5.84832700 -1.12209300 -0.69597700
C -6.36598800 0.16315900 -0.56220600
C -5.62661300 1.14627800 0.08623300
C -4.37549500 0.83945700 0.59879300
C -3.84366100 -0.44680700 0.45655400
C -2.55013600 -0.70514800 1.10336900
O -2.02540300 -1.87300100 1.33458600
O -1.93712400 -2.58441800 0.06149700
H -2.26708400 0.01510700 1.86813300
H -3.80483700 1.60132800 1.11447200
H -6.02653000 2.14466000 0.19781000
H -7.34400700 0.39718000 -0.96081700
H -6.42592000 -1.88678300 -1.19716800
H -4.16562800 -2.41583600 -0.31757400

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.256861960

Frequencies (cm^{-1}): -458.2734, 31.1184, 45.099, 62.8826, 84.0188, 152.5255, 203.5986, 215.7363, 233.619, 254.4291, 288.6642, 336.0429, 356.7454, 399.0265, 411.9512, 451.2733, 478.7158, 533.8098, 585.3405, 632.488, 704.2105, 717.0262, 776.3195, 812.5419, 824.4346, 867.4511, 869.9322, 929.6388, 941.2261, 949.9186, 960.3731, 1009.4384, 1020.4845, 1030.2057, 1048.4353, 1051.2179, 1104.4198, 1121.468, 1150.0248, 1184.9414, 1187.8463, 1194.6973, 1201.2577, 1247.5349, 1314.7556, 1343.4225, 1359.2402, 1361.1158, 1382.8499, 1403.7958, 1417.6017, 1464.4631, 1476.3259, 1485.904, 1492.2591, 1505.3714, 1507.7637, 1520.485, 1526.6727, 1619.2163, 1639.3622, 2046.8144, 3000.4991, 3028.2527, 3032.757, 3092.42, 3093.1707, 3101.3294, 3103.8184, 3117.6774, 3163.096, 3171.5643, 3183.5255, 3193.3261, 3220.001

iPrOCPhH(OOH) (_syn_-TS-AAAH 1.1-conformer)

C 0.00000000 0.00000000 0.00000000
O 1.35586300 0.04736500 -0.50257400
H 1.72191900 2.21997400 -1.66512300
H -0.20243100 0.93884800 0.52289200
C -0.91416600 -0.10430500 -1.20850200
H -1.95682500 -0.15287000 -0.89341400
H -0.79567900 0.75867100 -1.86346500
H -0.68654700 -1.00371200 -1.78218600
C -0.16370500 -1.17252500 0.95883200
H -1.17647200 -1.19310200 1.36372100
H 0.02075400 -2.11470900 0.44135500
H 0.52767600 -1.10368400 1.79905200
C 4.75565900 1.00558400 0.51469200
C 6.06179900 0.59245700 0.29370600
C 6.31512000 -0.55727300 -0.44822900
C 3.94323500 -0.87504800 -0.74325900
C 5.25359800 -1.28781100 -0.96548500
C 3.68668700 0.27564300 -0.00459000

C	2.27380800	0.72925400	0.29947000
O	2.10008600	2.14145100	0.19411200
O	2.46007400	2.56851700	-1.14283400
H	2.05035000	0.58610700	1.36433300
H	3.11842400	-1.44151200	-1.14797200
H	5.44196200	-2.18145100	-1.54550200
H	7.33333300	-0.87882000	-0.62161700
H	6.88289700	1.16979900	0.69702000
H	4.56102700	1.90781300	1.07807600

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.327464331759

Frequencies (cm^{-1}): 26.6052, 46.8765, 60.2004, 103.5363, 118.7242, 164.092, 210.8024, 228.0193, 235.85, 258.6981, 276.6041, 304.8564, 378.6774, 417.5072, 429.108, 435.8999, 488.2986, 512.6449, 632.5125, 639.9232, 713.3579, 724.3771, 763.0114, 828.0283, 861.973, 870.2352, 913.5441, 934.5896, 936.4849, 951.4168, 971.5787, 981.9537, 1004.7411, 1019.7133, 1022.9685, 1052.364, 1077.6194, 1109.3127, 1145.1406, 1161.8762, 1181.7709, 1199.7102, 1203.9928, 1222.4029, 1323.0763, 1340.8875, 1350.955, 1359.5704, 1378.6087, 1385.898, 1399.3233, 1411.3391, 1422.9481, 1483.4567, 1484.7657, 1485.3981, 1496.4709, 1507.5296, 1531.6029, 1626.9518, 1646.4892, 2991.3928, 3021.1954, 3030.7293, 3035.4554, 3094.0655, 3097.3961, 3101.3868, 3103.7263, 3163.3849, 3173.0534, 3183.7352, 3192.1605, 3209.1412, 3719.7377

IRC:

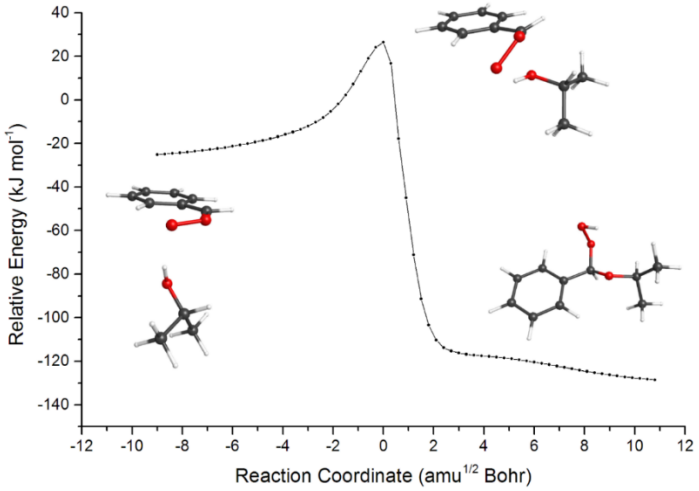


Figure S70: SCI 10 + iPrOH TS-AAAH 1.1 IRC

***Syn*-PhCHOO + iPrOH PRC (For TS-AAAH 1.2):**

C	0.00000000	0.00000000	0.00000000
O	1.39488900	-0.13097400	0.26336800
H	1.88382800	0.54085600	-0.24681200
H	-0.17762700	-0.13318200	-1.07608800
C	-0.70187400	-1.12306400	0.74717800
H	-1.77667300	-1.10234000	0.56117600
H	-0.31339900	-2.09135000	0.43162300
H	-0.53417100	-1.02296900	1.82125400
C	-0.51520200	1.37876500	0.40571600
H	-1.57911000	1.48047900	0.18067300
H	-0.37125600	1.53552700	1.47663800
H	0.02103700	2.16234900	-0.13125900
C	5.32574500	0.08057600	-0.65378500
C	6.26051700	-0.94003300	-0.72270400
C	7.39165500	-0.92331500	0.08658800
C	7.60205400	0.12446800	0.98203500
C	6.67982900	1.14844000	1.06300500
C	5.52765000	1.14482900	0.24789000
C	4.64549800	2.25671500	0.42477400
O	3.54984300	2.54374000	-0.14614800
O	3.03787700	1.70847300	-1.12007600
H	4.90429500	3.01643400	1.15491600
H	6.83706100	1.96338300	1.75762400
H	8.48107500	0.13529600	1.61096700
H	8.11195000	-1.72791000	0.02322000
H	6.10272000	-1.75788300	-1.41177800
H	4.44341500	0.08365200	-1.26901800

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.269039792

Frequencies (cm^{-1}): 11.7808, 16.0095, 20.478, 48.3763, 65.2028, 83.9372, 118.8748, 161.5982, 224.9, 232.0148, 264.4857, 335.8922, 365.8015, 407.848, 412.3528, 429.1857, 482.0736, 487.6931, 557.1539, 629.974, 698.8659, 716.4621, 748.553, 780.2831, 821.7367, 853.6205, 867.1296, 908.2439, 916.1047, 926.8809, 943.5091, 969.6169, 975.0943, 1013.0574, 1015.9675, 1034.3981, 1047.3162, 1108.2872, 1118.4867, 1160.1134, 1185.1356, 1188.2639, 1201.6852, 1230.9769, 1325.0161, 1348.466, 1356.7865, 1373.8211, 1391.2047, 1400.0497, 1406.589, 1446.7671, 1477.1894, 1482.4217, 1489.7764, 1498.996, 1508.6717, 1517.1684, 1558.8142, 1603.9035, 1636.5917, 2944.2325, 3016.455, 3026.8281, 3077.0512, 3087.4626, 3090.2414, 3097.6233, 3161.7802, 3170.1471, 3176.5581, 3189.5491, 3197.9319, 3253.2621, 3549.4271

Syn-PhCHOO + iPrOH TS-AAAH 1.2:

```
C    0.00000000  0.00000000  0.00000000
O   -1.37616400 -0.43563600 -0.04435100
H   -1.45855200 -1.49828400 -0.23822400
H    0.39096300 -0.20576800 -1.00292000
C    0.00913400  1.50142900  0.23402200
H    1.02634100  1.89034200  0.17459900
H   -0.60105500  2.01081200 -0.51071600
H   -0.38424000  1.74083900  1.22420100
C    0.84878200 -0.76401100  1.01031000
H    1.89391700 -0.47256900  0.89738000
H    0.55076900 -0.53872600  2.03558300
H    0.77140500 -1.83903000  0.85848400
C   -4.52568600 -1.59533000  0.30711400
C   -5.82096300 -1.23083800 -0.02837800
C   -6.31590500  0.02311800  0.31844800
C   -5.51478700  0.91705300  1.02048100
C   -4.22416200  0.55295000  1.37281300
C   -3.71664300 -0.70080100  1.01703300
C   -2.37090000 -1.03625000  1.50275100
O   -1.85471000 -2.23015000  1.55958300
O   -1.86423300 -2.79635300  0.21172600
H   -2.00779100 -0.40841900  2.31331900
H   -3.60394200  1.24415300  1.92931600
H   -5.89686400  1.88996000  1.29731400
H   -7.32432600  0.30201200  0.04367300
H   -6.44636200 -1.92660900 -0.57089600
H   -4.11997700 -2.55503900  0.02787300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.252983030052

Frequencies (cm^{-1}): -514.9962, 25.1887, 43.7591, 61.6484, 97.5071, 148.2604, 207.3202, 223.4838, 240.1599, 256.841, 282.3686, 339.4813, 356.7351, 373.2711, 413.4673, 440.0265, 497.4433, 544.0019, 571.2209, 632.5146, 703.4254, 714.7271, 777.108, 800.4059, 820.7787, 866.9994, 869.3418, 927.836, 934.5012, 944.631, 961.2505, 1011.3626, 1020.4881, 1031.4496, 1042.7231, 1051.6042, 1104.8034, 1131.07, 1146.7062, 1176.0334, 1184.8452, 1191.4501, 1200.5119, 1236.438, 1311.1253, 1333.5118, 1342.8914, 1359.3541, 1368.7748, 1401.2226, 1413.8314, 1428.5929, 1470.6357, 1484.5038, 1486.1323, 1497.8826, 1504.761, 1513.6262, 1527.4014, 1620.2185, 1639.3255, 2003.4603, 2990.0022, 3026.8231, 3033.4371, 3084.4635, 3092.6858, 3107.1507, 3116.9263, 3119.7959, 3162.639, 3171.1546, 3183.805, 3193.3367, 3219.8545

iPrOPhCHOOH (_syn_-TS-AAAH 1.2 & 2.2-Conformer):

```
C    0.00000000  0.00000000  0.00000000
O    1.33117000  0.44821100 -0.35657000
H    1.63890000  2.72081100 -1.28843900
H   -0.36240800 -0.39911400 -0.94829700
C    0.04954000 -1.14148200  1.01038000
H   -0.94568800 -1.57164500  1.12936100
H    0.72292400 -1.92741200  0.67032500
H    0.37751600 -0.80568600  1.99528900
C   -0.92566200  1.13283000  0.43000100
H   -1.93939800  0.74580900  0.54430700
H   -0.62341300  1.57015900  1.38107900
H   -0.94674800  1.92701200 -0.31513900
C    4.50902100  1.53264200  1.14465600
C    5.85968300  1.22838300  1.05188400
C    6.28473500  0.16982800  0.25467900
C    5.34925200 -0.57915300 -0.44655200
C    3.99421000 -0.27557300 -0.35229200
C    3.56580500  0.78363400  0.44102900
C    2.09418300  1.11507100  0.60528700
O    1.84076100  2.51937700  0.58670200
O    2.30205700  3.06716100 -0.67203200
```

```
H     1.76688100  0.86845900  1.62092300
H     3.26753400 -0.85478100 -0.90140600
H     5.67120400 -1.40178900 -1.07119200
H     7.33782300 -0.06632900  0.18075800
H     6.58204000  1.82015600  1.59800500
H     4.18244700  2.36599100  1.75137700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.323985847423

Frequencies (cm^{-1}): 30.2754, 34.3325, 69.3405, 100.9045, 130.5821, 181.3116, 210.3376, 230.7291, 242.0202, 263.0016, 288.8791, 323.0639, 369.7527, 416.7982, 418.5462, 461.0086, 479.4142, 527.3546, 632.1578, 640.2516, 702.8878, 718.9185, 760.2518, 812.9587, 863.1901, 869.6863, 903.5174, 924.9477, 940.4403, 943.4343, 973.303, 991.8132, 1004.5255, 1019.5592, 1022.8721, 1045.2079, 1056.551, 1107.1525, 1145.6568, 1161.8646, 1181.4012, 1196.4021, 1200.3832, 1217.3267, 1324.6371, 1333.9557, 1352.8462, 1370.2542, 1373.242, 1386.9301, 1397.9065, 1404.7982, 1423.1382, 1482.8902, 1484.238, 1488.8588, 1499.8081, 1506.6583, 1530.5708, 1626.5734, 1645.6333, 3014.6456, 3032.3579, 3038.417, 3047.2372, 3090.3856, 3099.5829, 3106.3879, 3111.8117, 3162.9688, 3172.4506, 3183.1471, 3191.5284, 3207.6568, 3714.5735

IRC:

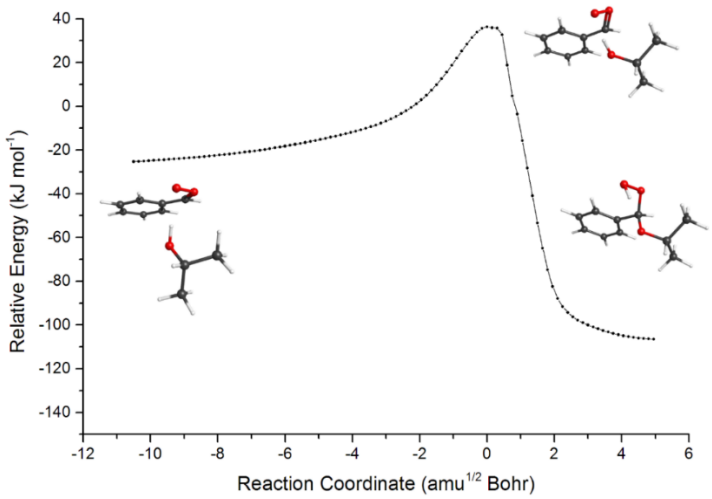


Figure S71: SCI 10 + iPrOH TS-AAAH 1.2 IRC

***Syn*-PhCHOO + iPrOH PRC (For TS-AAAH 1.3):**

```
C     0.00000000  0.00000000  0.00000000
O    -1.41928400 -0.05439800 -0.12082700
H    -1.82223900  0.42120300  0.62988500
H     0.37084800 -0.55255600 -0.86763300
C     0.50897200  1.43762200 -0.08349400
H     1.60048400  1.47054900 -0.07298600
H     0.15879400  1.90989900 -1.00159600
H     0.14346300  2.02181300  0.76388800
C     0.47417500 -0.70715300  1.26779100
H     1.56459900 -0.73973000  1.31722900
H     0.11008900 -0.18447900  2.15519800
H     0.09710200 -1.72964900  1.29411000
C    -5.23743200 -0.07388400  1.23236500
C    -6.21511900 -1.04323100  1.07473800
C    -7.41642400 -0.74451200  0.44040000
C    -7.65480400  0.53939800 -0.04816600
C    -6.69059100  1.51597500  0.10040600
C    -5.46732300  1.22766400  0.74275000
C    -4.54853900  2.32000000  0.83438700
O    -3.39124500  2.38794800  1.34903300
O    -2.83410800  1.27490100  1.94770500
H    -4.83447200  3.27831300  0.41353400
H    -6.87005400  2.51362200 -0.27884700
H    -8.58824400  0.76961800 -0.54216600
H    -8.16969900 -1.51201800  0.32328000
H    -6.03602700 -2.04206200  1.44743000
H    -4.30096900 -0.28645200  1.71690600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.269581310036

Frequencies (cm^{-1}): 4.3592, 14.3481, 25.5063, 46.5069, 57.37, 76.1091, 151.6334, 191.9359, 216.7898, 229.3837, 270.3744, 317.3272, 363.0205, 407.1623, 411.7718, 422.8567, 480.8564, 486.6515, 554.9988,

629.652, 696.4712, 703.4818, 729.9834, 781.0483, 813.6175, 847.4178, 867.5384, 902.3642, 920.4699, 921.1254, 937.4655, 966.7001, 976.6157, 1012.7824, 1016.2355, 1035.0431, 1047.2034, 1108.0012, 1125.6195, 1144.3149, 1184.4461, 1188.0666, 1201.3539, 1230.1878, 1340.6271, 1348.6143, 1357.3353, 1366.6894, 1394.5973, 1399.2847, 1410.375, 1436.3187, 1477.0742, 1482.2442, 1488.0525, 1499.9145, 1508.1824, 1517.7108, 1559.0189, 1604.041, 1636.992, 3014.8035, 3016.2361, 3022.1118, 3074.3838, 3084.1548, 3092.0595, 3094.7522, 3158.4668, 3169.6875, 3176.1611, 3190.2666, 3197.8568, 3257.3545, 3531.1779

Syn-PhCHOO + iPrOH TS-AAAH 1.3:

```
C     0.00000000  0.00000000  0.00000000
O    -1.32108200  0.49106600  0.31934900
H    -1.30406500  1.47627400  0.74943300
H    -0.16716500 -0.88105600 -0.62515500
C     0.85002300  1.00825200 -0.76464900
H     1.83556000  0.58162400 -0.95611600
H     0.40608800  1.26871600 -1.72425300
H     0.97494700  1.92720200 -0.19195100
C     0.65382500 -0.43689100  1.30602700
H     1.61960100 -0.90454400  1.10794200
H     0.81914500  0.42280700  1.95756400
H     0.02201500 -1.15217800  1.83068200
C    -4.41519900  1.84047400  0.57007300
C    -5.69046100  1.46182400  0.96123200
C    -6.29108500  0.32956000  0.41767200
C    -5.61789700 -0.42406700 -0.53755000
C    -4.34900500 -0.04171100 -0.94520300
C    -3.73476600  1.08750500 -0.39378100
C    -2.42464700  1.46533800 -0.94062500
O    -1.83869000  2.61753800 -0.79686800
O    -1.68757200  2.87727000  0.63417900
H    -2.17994800  1.01039700 -1.89862400
H    -3.82904300 -0.62089100 -1.69779300
H    -6.08280400 -1.30073500 -0.96705800
H    -7.28246300  0.03689200  0.73661900
H    -6.21695600  2.04909000  1.70116700
H    -3.92635100  2.70206900  0.99702200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.252826530138

Frequencies (cm^{-1}): -462.3727, 20.0708, 38.1303, 64.5346, 92.105, 145.1465, 205.1353, 216.8869, 228.9456, 260.3287, 283.3995, 326.0019, 377.3164, 397.7644, 412.6616, 440.3598, 506.9837, 529.6785, 567.4578, 632.556, 702.0284, 713.5167, 775.7602, 807.3183, 821.3714, 866.8259, 868.5591, 918.0507, 932.362, 945.3849, 959.7328, 1009.3448, 1020.1285, 1030.3078, 1038.7507, 1050.937, 1103.5146, 1126.7346, 1146.4847, 1176.8075, 1184.7347, 1187.537, 1199.2779, 1230.0519, 1309.4503, 1342.5893, 1356.559, 1368.7453, 1380.9744, 1403.5488, 1406.789, 1422.8211, 1471.0425, 1482.0043, 1485.5638, 1496.358, 1506.6679, 1516.2935, 1526.7217, 1619.6215, 1639.2626, 2068.9717, 3018.519, 3028.9521, 3038.0954, 3090.6793, 3100.4841, 3107.873, 3111.1703, 3114.3106, 3162.4211, 3171.238, 3183.5786, 3193.3075, 3219.5745

iPrOPhCHOOH (_syn_-TS-AAAH 1.3-Conformer):

```
C     0.00000000  0.00000000  0.00000000
O    -1.34876100  0.07286600  0.51157700
H    -1.52398500  2.23468900  1.92236600
H    -0.02778500  0.26301300 -1.06291300
C     0.91289300  0.97629000  0.73277200
H     1.93460500  0.89291600  0.35918900
H     0.58438300  2.00447400  0.58992400
H     0.92653100  0.75020600  1.80076500
C     0.45285400 -1.44346500  0.15103800
H     1.46785400 -1.56645400 -0.22830200
H     0.44280900 -1.73578600  1.20197600
H    -0.20558000 -2.11553900 -0.39812600
C    -4.70546600  1.33928400 -0.27416600
C    -6.02833800  0.98303900 -0.05309100
C    -6.33202300 -0.21498900  0.58617000
C    -5.30368800 -1.05102800  1.00075500
C    -3.97684700 -0.69559000  0.77762900
C    -3.66974500  0.50322400  0.14196000
C    -2.24011500  0.90296100 -0.16355900
O    -1.98533100  2.28772800  0.08019100
```

```
O    -2.29475500   2.59775600   1.46088800
H    -2.05557300   0.86482100  -1.24599600
H    -3.17807700  -1.34505000   1.10192000
H    -5.53098600  -1.98328300   1.50050200
H    -7.36310400  -0.49249400   0.75963100
H    -6.82289300   1.64209000  -0.37641400
H    -4.47146300   2.27794300  -0.75734000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.326832844

Frequencies (cm^{-1}): 17.4423, 29.1962, 62.2428, 105.7719, 121.3933, 169.9428, 218.1655, 234.3229, 243.9799, 269.2069, 278.1519, 312.8452, 345.8273, 411.4063, 417.0071, 453.2453, 489.8522, 518.1365, 633.2787, 642.6786, 712.7133, 723.3612, 763.2031, 825.9416, 858.8398, 867.7563, 919.3466, 932.4229, 934.7106, 943.9416, 967.8244, 979.8102, 1002.8462, 1018.3849, 1022.7916, 1052.8855, 1092.4276, 1115.128, 1144.6442, 1156.3225, 1181.5532, 1199.7601, 1206.2503, 1221.4196, 1321.6123, 1339.3815, 1349.4598, 1357.9897, 1363.4359, 1384.2559, 1401.0418, 1406.0398, 1420.1496, 1482.8174, 1485.0646, 1490.4207, 1497.9892, 1514.6741, 1531.3032, 1626.8255, 1646.3246, 2975.8694, 2997.2389, 3027.7611, 3034.7568, 3087.2846, 3099.494, 3105.6584, 3111.3651, 3163.1552, 3172.765, 3183.2158, 3191.5531, 3208.4008, 3720.8031

IRC:

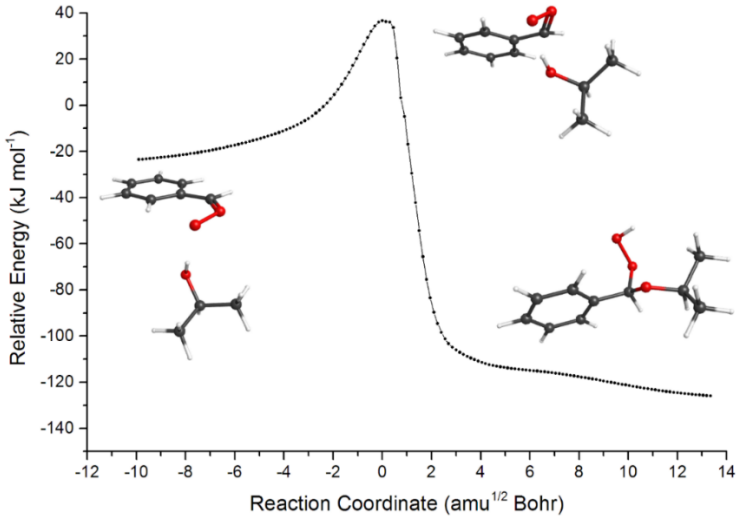


Figure S72: SCI 10 + iPrOH TS-AAAH 1.3 IRC

PRC2.1:

```
C     0.00000000   0.00000000   0.00000000
O    -0.88573400   0.31328400  -1.06873900
H    -1.80459400   0.28153300  -0.74417400
H    -0.27470200  -0.97542900   0.42582500
C     1.39579100  -0.11049200  -0.59412200
H     2.12625400  -0.38070700   0.17004200
H     1.41588500  -0.86764300  -1.37785800
H     1.69234300   0.84300000  -1.03539100
C    -0.07451300   1.04682400   1.11042100
H     0.59590300   0.79361900   1.93500300
H     0.20774400   2.02753800   0.72244000
H    -1.08895600   1.11386800   1.50565000
C    -6.32691600  -0.45127100  -0.03689000
C    -7.50699600  -1.17207800   0.05837000
C    -8.73920400  -0.53034300  -0.00899300
C    -8.80439500   0.85257700  -0.17470800
C    -7.63809400   1.58483500  -0.27198500
C    -6.38078500   0.94729900  -0.20493900
C    -5.24408400   1.80817000  -0.32086600
O    -4.00383800   1.54250800  -0.29967300
O    -3.57990500   0.24257500  -0.13875000
H    -5.40312000   2.87315400  -0.45178800
H    -7.68399300   2.65835900  -0.40140500
H    -9.76260300   1.34998700  -0.22744600
H    -9.65203200  -1.10571100   0.06718200
H    -7.46438700  -2.24476700   0.18626500
H    -5.36375800  -0.92814800   0.01255800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.269039792

Frequency (cm^{-1}): 11.7808, 16.0095, 20.478, 48.3763, 65.2028, 83.9372, 118.8748, 161.5982, 224.9, 232.0148, 264.4857, 335.8922, 365.8015, 407.848, 412.3528, 429.1857, 482.0736, 487.6931, 557.1539, 629.974, 698.8659, 716.4621, 748.553, 780.2831, 821.7367, 853.6205, 867.1296, 908.2439, 916.1047, 926.8809, 943.5091, 969.6169, 975.0943, 1013.0574, 1015.9675, 1034.3981, 1047.3162, 1108.2872, 1118.4867, 1160.1134, 1185.1356, 1188.2639, 1201.6852, 1230.9769, 1325.0161, 1348.466, 1356.7865, 1373.8211, 1391.2047, 1400.0497, 1406.589, 1446.7671, 1477.1894, 1482.4217, 1489.7764, 1498.996, 1508.6717, 1517.1684, 1558.8142, 1603.9035, 1636.5917, 2944.2325, 3016.455, 3026.8281, 3077.0512, 3087.4626, 3090.2414, 3097.6233, 3161.7802, 3170.1471, 3176.5581, 3189.5491, 3197.9319, 3253.2621, 3549.4271

Syn-PhCHOO + iPrOH TS-AAAH 2.1:

```
C    0.00000000  0.00000000  0.00000000
O   -0.00024100 -1.23263000 -0.73360400
H    0.10300100 -2.09682700 -0.07092700
H    0.99173500  0.14829300  0.44079600
C   -0.29340600  1.13343200 -0.96972100
H   -0.28604700  2.09274200 -0.45071400
H    0.45351800  1.17304600 -1.76273700
H   -1.27280100  0.99489800 -1.42937000
C   -1.02512400 -0.09782100  1.12466400
H   -1.02243900  0.81778600  1.71774700
H   -2.02653300 -0.24466000  0.71850900
H   -0.79677200 -0.93166300  1.78897800
C    3.24203600 -1.84391500  0.45141000
C    4.36483400 -1.21419200  0.96625600
C    4.95167200 -0.14683900  0.29123400
C    4.42135200  0.28591100 -0.91857000
C    3.30786900 -0.35020400 -1.44808500
C    2.70374600 -1.41527000 -0.76938100
C    1.58450800 -2.08157300 -1.44832400
O    1.13655000 -3.27607900 -1.19233700
O    0.74840400 -3.31962100  0.21747100
H    1.47773500 -1.84045000 -2.50271100
H    2.90807000 -0.02743600 -2.40109500
H    4.87839400  1.10810500 -1.45171500
H    5.82214400  0.34349700  0.70594600
H    4.78310800 -1.55420200  1.90380500
H    2.76605000 -2.66230000  0.96854300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.256158897

Frequencies (cm^{-1}): -561.8918, 41.3788, 47.1304, 62.4824, 100.623, 162.8174, 204.719, 216.4816, 237.5781, 269.056, 300.5692, 306.0923, 351.5017, 399.5065, 414.0133, 446.4492, 504.5275, 535.3404, 554.6859, 632.4426, 703.6585, 715.0361, 781.0912, 816.8334, 822.0992, 863.9261, 872.1964, 925.9512, 937.5335, 948.4317, 963.5882, 1013.1111, 1019.9471, 1034.6372, 1046.3845, 1051.6808, 1090.8309, 1103.4162, 1155.0009, 1161.4999, 1185.3764, 1193.8404, 1200.0719, 1219.6573, 1308.8992, 1323.6017, 1346.0418, 1361.7738, 1370.8157, 1397.636, 1407.1616, 1420.0979, 1476.9492, 1483.7058, 1486.9156, 1495.3571, 1508.1445, 1522.5624, 1525.4912, 1617.868, 1638.1185, 1976.4683, 2996.2601, 3028.8004, 3033.3167, 3093.5908, 3097.0013, 3099.0086, 3102.4518, 3130.516, 3162.5961, 3171.8835, 3183.7328, 3193.6355, 3218.2349

iPrOCPhHOOH (_syn_-TS-AAAH 2.1 -conformer):

```
C    0.00000000  0.00000000  0.00000000
O   -0.61507300  1.18311500  0.54708200
H   -1.15152000  3.24747700  1.85308400
H   -0.78457300 -0.62454900 -0.44056300
C    1.02506900  0.36407900 -1.06920600
H    1.46560000 -0.53968000 -1.49275900
H    0.57830400  0.92707000 -1.88877000
H    1.82331900  0.96844100 -0.63664500
C    0.62482800 -0.74334500  1.16815100
H    1.11386700 -1.65430000  0.82223000
H    1.37207800 -0.11714800  1.65771000
H   -0.13170000 -1.01523500  1.90299600
C   -3.32599900  0.45237400  1.17656300
C   -4.57979800 -0.12528400  1.33631500
C   -5.50902000 -0.07993400  0.30274000
C   -5.17919400  0.54568500 -0.89420500
```

```
C    -3.92519000   1.12285800 -1.05143700
C    -2.99116700   1.08453200 -0.01804500
C    -1.64617700   1.75393700 -0.22164200
O    -1.66512000   3.14535800  0.03929000
O    -2.01364000   3.36645200  1.42757700
H    -1.39267800   1.74975900 -1.28769500
H    -3.67219300   1.61196900 -1.98421300
H    -5.89527000   0.58153300 -1.70416800
H    -6.48390800  -0.53155000  0.42855500
H    -4.83307200  -0.60930600  2.27012700
H    -2.60359000   0.41901800  1.97863200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.323342262

Frequencies (cm^{-1}): 13.6699, 33.4494, 52.3782, 94.3565, 108.425, 182.53, 211.9723, 213.7601, 244.6322, 272.4035, 300.0948, 315.4674, 366.2189, 406.0719, 417.8971, 435.3312, 483.1573, 570.7463, 579.2747, 635.1322, 698.6366, 718.6748, 775.7987, 837.7639, 865.9103, 873.6331, 903.4085, 934.3776, 941.0036, 949.6952, 968.5901, 1000.2056, 1010.3144, 1020.0072, 1022.9598, 1049.7234, 1071.2329, 1108.4039, 1141.9236, 1162.9314, 1182.0252, 1199.4249, 1201.2318, 1217.1155, 1314.8789, 1341.9061, 1349.3715, 1369.2037, 1373.7223, 1379.9844, 1397.7079, 1408.9648, 1420.5959, 1482.7083, 1486.2816, 1488.2354, 1497.8025, 1508.4792, 1530.4187, 1627.7223, 1644.6515, 2996.6031, 3011.807, 3030.7426, 3036.2081, 3091.9811, 3097.038, 3102.553, 3108.6422, 3156.5081, 3166.0414, 3177.183, 3188.569, 3201.7289, 3727.415

IRC:

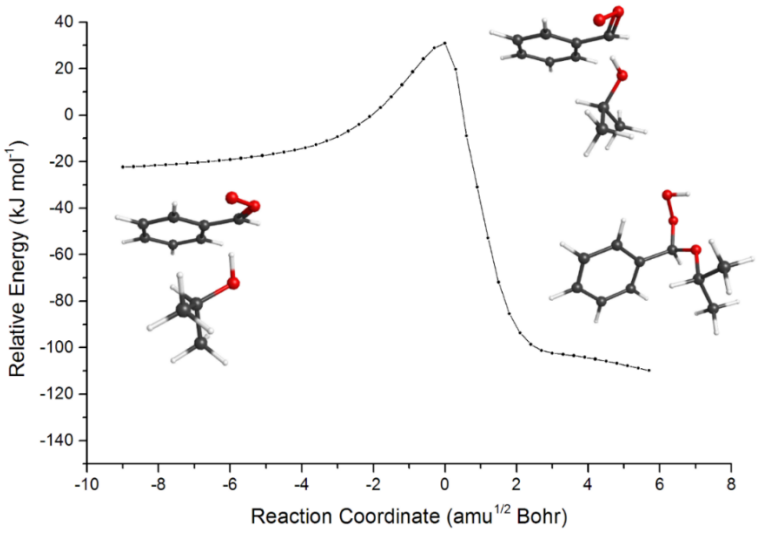


Figure S73: SCI 10 + iPrOH TS-AAAH 2.1 IRC

Syn-PhCHOO + iPrOH TS-AAAH 2.2

```
C     0.00000000   0.00000000   0.00000000
O    -0.25396000   1.24775900 -0.66910800
H    -0.42102600   2.11050100   0.00084200
H     1.02372600   0.10604200   0.37788600
C    -0.91728400  -0.26170100   1.18998100
H    -0.55621100  -1.13232300   1.73987700
H    -0.92355200   0.58748000   1.87314300
H    -1.94113400  -0.46009900   0.87766800
C    -0.01537700  -1.12311400  -1.02508100
H     0.31559500  -2.05660200  -0.56823300
H    -1.02043300  -1.28035400  -1.41817700
H     0.65218100  -0.89197500  -1.85471100
C    -3.65826300   1.93638100   0.18227000
C    -4.85530300   1.36361300   0.58283400
C    -5.38987600   0.28001100  -0.11001000
C    -4.73283300  -0.22224700  -1.22747100
C    -3.54273900   0.35705200  -1.64339500
C    -2.98695200   1.42908800  -0.93691000
C    -1.77596100   2.04334500  -1.50403000
O    -1.34901100   3.24484000  -1.23491400
O    -1.09042700   3.31080000   0.20775800
H    -1.56933400   1.77594800  -2.53688700
H    -3.04263800  -0.01896600  -2.52699000
H    -5.15104700  -1.05332700  -1.77848800
H    -6.31981300  -0.16606200   0.21611500
```

H -5.37408200 1.76117800 1.44445400
H -3.22153100 2.76510400 0.71726700

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.25068863427

Frequencies (cm^{-1}): -599.3453, 38.6752, 67.3108, 67.8589, 109.3484, 162.4867, 199.1223, 225.5842, 232.7391, 271.8878, 290.5818, 339.6278, 351.8046, 396.9057, 412.8361, 436.9443, 474.5637, 541.4957, 564.1504, 625.8242, 695.8415, 707.2387, 769.3027, 796.8716, 807.6922, 854.5216, 858.2186, 918.3605, 920.3727, 939.5057, 947.8997, 993.0733, 1008.811, 1015.7773, 1044.6064, 1052.1475, 1087.5438, 1098.0724, 1144.0798, 1155.1134, 1173.595, 1185.9193, 1192.6486, 1210.626, 1272.3494, 1299.9051, 1340.4468, 1356.2787, 1358.3761, 1363.0612, 1390.7119, 1403.5439, 1457.8046, 1462.0116, 1465.4714, 1475.6887, 1485.5312, 1502.8157, 1511.7377, 1619.0624, 1640.3139, 2013.7179, 3000.4479, 3037.3781, 3042.5467, 3107.9263, 3112.6997, 3120.0356, 3130.0119, 3140.5078, 3171.3067, 3179.0274, 3190.9888, 3201.0158, 3227.1688

IRC:

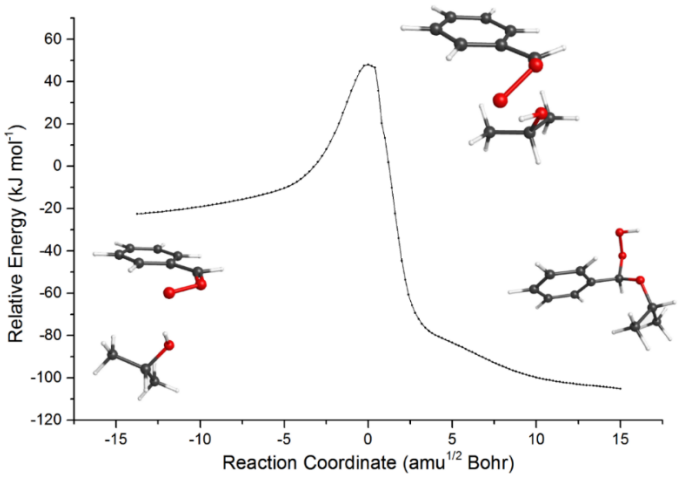


Figure S74: SCI 10 + iPrOH TS-AAAH 2.2 IRC

7.12 sCI 12 + alcohol Reactions

7.12.1 sCI 12 + MeOH Reactions

***Anti*-PhCHOO (SCI 12):**

```
C    0.00000000  0.00000000  0.00000000
C   -1.32300100 -0.41299100  0.00000000
C   -1.62553300 -1.77026900  0.00000000
C   -0.60042300 -2.71660700  0.00000000
C    0.72217400 -2.31512800  0.00000000
C    1.03722600 -0.94492600 -0.00000000
C    2.39109100 -0.46361500 -0.00000000
O    3.36717300 -1.26686700 -0.00000000
O    4.63242800 -0.74159500 -0.00000000
H    2.63324600  0.59471700 -0.00000000
H    1.51820200 -3.04521700  0.00000000
H   -0.84039600 -3.77088700  0.00000000
H   -2.65749000 -2.09363100  0.00000000
H   -2.11699700  0.32063100  0.00000000
H    0.23989100  1.05513500 -0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -420.125978241561

Frequencies (cm^{-1}): 100.215, 150.9127, 171.2266, 287.9665, 374.9567, 410.6684, 437.6771, 505.1531, 631.3959, 650.6319, 702.5733, 778.6731, 862.7444, 876.6236, 942.0391, 957.1573, 978.0935, 1004.474, 1017.6019, 1025.2752, 1047.1245, 1111.983, 1187.0727, 1200.7452, 1238.9464, 1340.8406, 1362.181, 1368.0678, 1476.9113, 1523.1209, 1541.8573, 1613.7715, 1638.8046, 3151.4785, 3170.9961, 3177.1148, 3187.0905, 3196.9555, 3205.6805

***anti*-PhCHOO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2)**

```
C    0.00000000  0.00000000  0.00000000
O   -0.15173000 -0.37165500 -1.35619500
C    0.97369400 -2.11206200 -1.88426600
C    2.34970000 -1.87687700 -1.50465600
C    3.18805800 -1.18363000 -2.38514900
C    4.52868300 -1.01158800 -2.07648100
C    5.03524700 -1.51959900 -0.88428700
C    4.20041600 -2.19665200  0.00115300
C    2.86275300 -2.36483700 -0.29841000
H    2.20808100 -2.89339600  0.38299200
H    4.59882500 -2.58529900  0.92599800
H    6.08151400 -1.38757100 -0.64384900
H    5.17821300 -0.48060400 -2.76219500
H    2.78620000 -0.79621600 -3.31485200
O    0.23681300 -2.86380800 -1.19355300
O   -1.16165100 -2.66600400 -1.50932300
H   -0.74017600 -0.82147900 -1.39268700
H    0.59993300 -1.77499900 -2.84797400
H    0.18211000 -0.86946300  0.63646600
H    0.84747000  0.67246600  0.04794000
H   -0.89440500  0.51763400  0.35454600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.747076258407

Frequencies (cm^{-1}): 15.5706, 30.842, 55.3474, 96.7646, 110.248, 120.6118, 150.5076, 178.3072, 247.1049, 289.4556, 384.6737, 411.7813, 448.2644, 503.3685, 630.717, 648.7302, 701.8937, 714.2764, 781.1642, 866.1563, 877.2138, 942.1305, 954.6093, 1007.163, 1014.7311, 1018.2635, 1028.826, 1047.6446, 1064.9563, 1112.0526, 1144.9052, 1173.0638, 1187.7698, 1202.829, 1258.9337, 1344.5382, 1365.6613, 1392.4897, 1464.675, 1478.4993, 1481.9062, 1497.0261, 1514.5204, 1528.6601, 1555.12, 1616.2755, 1639.5256, 2986.6719, 3029.0731, 3087.1758, 3133.1259, 3172.9794, 3179.7763, 3188.1803, 3197.1013, 3203.8263, 3437.7314

***Anti*-PhCHOO + MeOH TS-AAAH 1:**

```
C    0.00000000  0.00000000  0.00000000
O   -0.14173000 -0.42665400 -1.34619500
C    0.93369400 -2.01206000 -1.83926800
C    2.33470000 -1.84687600 -1.47965800
C    3.17805800 -1.16862800 -2.36515100
C    4.51868300 -0.99658600 -2.05648300
C    5.02524700 -1.50459900 -0.86428900
C    4.19041600 -2.18165300  0.02115000
C    2.84775300 -2.34983700 -0.27841300
H    2.19308100 -2.87339700  0.40298900
H    4.58882500 -2.57530100  0.94599500
```

```
H     6.07151400 -1.37257100 -0.62385100
H     5.16821300 -0.47060100 -2.74219600
H     2.77620000 -0.77621300 -3.28985300
O     0.22681300 -2.86880700 -1.17355600
O    -1.16665100 -2.59100300 -1.47932600
H    -0.88017600 -1.26147800 -1.39268800
H     0.61493300 -1.77999600 -2.84797600
H     0.16211000 -0.84446400  0.67646500
H     0.84247000  0.68746600  0.07294100
H    -0.90940500  0.51763300  0.31454700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.739981935873

Frequencies (cm^{-1}): -672.7707, 55.0472, 74.9442, 100.8268, 132.483, 173.8339, 177.3593, 272.1335, 323.5168, 371.8949, 411.1873, 417.9201, 511.0997, 612.4347, 633.9688, 647.4342, 707.6706, 787.7509, 850.6072, 867.4421, 879.452, 931.3359, 960.1905, 1007.2932, 1020.742, 1027.2917, 1043.9792, 1049.4788, 1106.9048, 1146.9291, 1177.6736, 1186.6462, 1186.7332, 1200.9303, 1234.6876, 1338.2534, 1339.8814, 1360.0379, 1451.2294, 1472.2783, 1480.9505, 1492.4773, 1503.7472, 1512.0068, 1533.3593, 1623.0042, 1642.5085, 1844.0169, 3002.3656, 3055.5157, 3089.3343, 3157.6945, 3170.9045, 3177.46, 3186.5658, 3195.9619, 3204.1984

MeOCPhH(OOH) (*anti*-TS-AAAH 1 conformer)

```
C     0.00000000  0.00000000  0.00000000
O     0.19811600  0.32961500 -1.37672900
C    -0.38167200  1.54213300 -1.81455700
C    -1.87055100  1.65303100 -1.54152700
C    -2.70036100  0.65070200 -2.04586100
C    -4.07241600  0.70362000 -1.84312800
C    -4.63157200  1.76113900 -1.13249400
C    -3.81028100  2.76262600 -0.63144900
C    -2.43448800  2.71279300 -0.83575700
H    -1.80333000  3.49998600 -0.45155300
H    -4.23837000  3.58963300 -0.08107200
H    -5.70072600  1.80422300 -0.97440400
H    -4.70518300 -0.07813900 -2.24128100
H    -2.26609700 -0.17457500 -2.59502000
O     0.25763200  2.65500700 -1.21988600
O     1.59045900  2.74477400 -1.76957700
H     2.02659500  1.97940500 -1.36372400
H    -0.18035500  1.55909100 -2.88650700
H     0.33321100  0.80625500  0.65619600
H    -1.04758200 -0.22165600  0.21011600
H     0.59986500 -0.88758500  0.18492300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.804015697086

Frequencies (cm^{-1}): 18.7928, 91.9552, 110.7903, 134.8326, 161.4189, 197.8173, 265.2678, 270.55, 337.9961, 363.9632, 413.0504, 425.3862, 503.4041, 629.1828, 640.7865, 686.3353, 719.3439, 766.4794, 871.122, 878.7808, 921.4667, 949.0772, 968.2265, 1004.1245, 1016.1008, 1020.7427, 1022.9526, 1053.582, 1090.3306, 1111.8906, 1173.2538, 1183.2111, 1204.5227, 1209.6905, 1215.8685, 1322.9936, 1349.7527, 1366.5084, 1389.78, 1398.2107, 1467.4086, 1485.4677, 1491.6195, 1513.4226, 1531.7536, 1625.1938, 1645.5923, 3022.2245, 3062.5717, 3080.0581, 3123.7714, 3164.0636, 3171.5485, 3180.6602, 3190.7915, 3206.6651, 3709.5402

IRC:

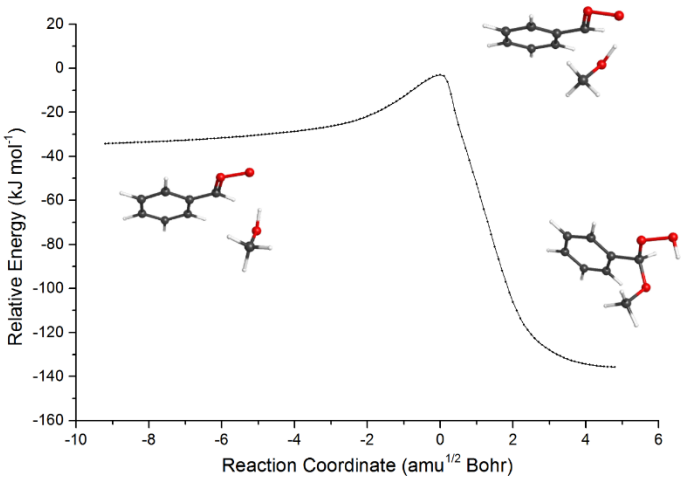


Figure S75: SCI 12 + MeOH TS-AAAH 1 IRC

***Anti*-PhCHOO + MeOH TS-AAAH 2:**

```
C     0.00000000  0.00000000  0.00000000
O    -0.44569200  1.32069100  0.23985800
C    -1.52583100  2.15251500 -1.20224900
C    -2.94322600  2.02359100 -0.89979500
C    -3.66876800  0.98090800 -1.48284200
C    -5.02306700  0.84155200 -1.21690900
C    -5.65617900  1.74206100 -0.36677100
C    -4.93623600  2.78054400  0.22006800
C    -3.58315300  2.92258900 -0.03933900
H    -3.01114200  3.71594900  0.41905400
H    -5.43291300  3.47405200  0.88437400
H    -6.71186700  1.63369000 -0.15759500
H    -5.58381800  0.03631400 -1.67069500
H    -3.17066800  0.28720100 -2.14759200
O    -0.97539500  3.31225800 -1.06076200
O     0.46382600  3.10582400 -1.07068200
H     0.24584200  2.06424700 -0.21452200
H    -1.06675800  1.46646900 -1.90674100
H     0.88632200 -0.20673200  0.60509200
H    -0.78497000 -0.70372100  0.27977000
H     0.26523300 -0.16054100 -1.05166700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.737250873

Frequencies (cm^{-1}): -655.6376, 48.5334, 73.3332, 89.9056, 127.3491, 175.1519, 203.6333, 259.3337, 331.8647, 362.6548, 401.4107, 415.2846, 511.9636, 579.3243, 633.0308, 644.6046, 706.5412, 785.498, 856.6577, 866.7714, 884.3617, 932.9324, 959.9943, 1006.9303, 1020.9872, 1027.8029, 1048.989, 1071.1774, 1106.8838, 1132.7216, 1175.9587, 1186.738, 1197.9367, 1201.4297, 1233.7963, 1332.6103, 1339.8026, 1360.8091, 1401.3347, 1455.6801, 1483.8192, 1494.6826, 1500.3366, 1511.3805, 1533.9009, 1623.503, 1642.9401, 1905.2478, 2982.4355, 3042.5745, 3077.2875, 3130.9482, 3169.0759, 3175.785, 3186.8248, 3195.6171, 3206.7993

MeOCPhH(OOH) (anti-TS-AAAH 2- conformer):

```
C     0.00000000  0.00000000  0.00000000
O     0.02383600 -1.11011200  0.88473500
C     0.69216000 -2.24594000  0.37130200
C     2.19493200 -2.18396000  0.51971600
C     3.01614900 -2.63236700 -0.51099500
C     4.39895300 -2.59672800 -0.37357000
C     4.96670400 -2.11354700  0.79949600
C     4.14926900 -1.66527200  1.83256000
C     2.76796000 -1.69892800  1.69403900
H     2.12776400 -1.34717100  2.49068400
H     4.58946700 -1.28950700  2.74640500
H     6.04252700 -2.08428700  0.90849400
H     5.03055300 -2.94426600 -1.17986500
H     2.57318300 -3.01220400 -1.42304800
```

```
O     0.27319100 -3.35238800  1.13190800
O    -1.12991100 -3.58715400  0.84665600
H    -1.54659800 -2.89315700  1.37977600
H     0.40298900 -2.39459800 -0.67616400
H    -0.59707300  0.77139800  0.48001600
H     1.00514000  0.38921700 -0.18477600
H    -0.46046400 -0.26771600 -0.95680200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -535.803878519

Frequencies (cm^{-1}): 29.927, 73.1739, 108.6865, 125.4423, 168.1175, 229.6211, 271.7461, 281.3352, 314.588, 371.7702, 416.4883, 419.542, 544.2353, 592.7976, 634.2317, 659.8782, 718.4508, 781.5515, 859.9895, 867.8298, 923.1056, 947.9059, 990.8056, 1001.7189, 1021.1035, 1022.9564, 1051.0597, 1073.0087, 1102.0963, 1110.2152, 1177.8265, 1183.0167, 1200.1052, 1212.9925, 1226.7657, 1318.5691, 1349.5126, 1359.9926, 1382.8963, 1395.364, 1477.0426, 1491.0215, 1492.9701, 1509.3572, 1530.8239, 1628.1345, 1644.8587, 2988.6033, 2995.8819, 3045.217, 3120.8952, 3161.0853, 3168.555, 3178.9955, 3189.5108, 3196.9797, 3722.9916

IRC:

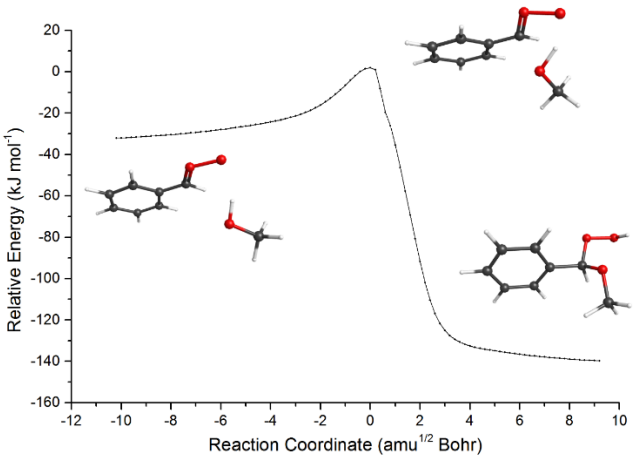


Figure S76: SCI 12 + MeOH TS-AAAH 2 IRC

7.12.2 sCI 12 + EtOH Reaction

***Anti*-PhCHOO + EtOH PRC (For TS-AAAH 1.1 and 2.2):**

```
C     0.00000000  0.00000000  0.00000000
O     1.42036400 -0.05655300 -0.03349100
H     1.73184800 -0.98602000 -0.02715800
C    -0.43538600  1.45206000 -0.01352500
H    -0.03462000  1.98079700  0.85224700
H    -0.07718000  1.95143300 -0.91462200
H    -1.52368300  1.52641000  0.01155800
H    -0.37840200 -0.49634100  0.90125800
H    -0.42093000 -0.52536200 -0.86518600
C     5.98296000  1.12029100 -0.01831400
C     7.27043100  1.63395600 -0.01654100
C     8.36027700  0.77050400 -0.01260600
C     8.16326400 -0.61103800 -0.01044400
C     6.88361200 -1.13315500 -0.01213300
C     5.77665200 -0.26729100 -0.01607400
C     4.41905700 -0.74143100 -0.01802400
O     4.18162400 -1.98305200 -0.01549700
O     2.86436700 -2.41035100 -0.01761700
H     3.57224500 -0.05985300 -0.02109600
H     6.72564200 -2.20193500 -0.01050600
H     9.01508900 -1.27684300 -0.00744800
H     9.36514800  1.17022200 -0.01124400
H     7.42444500  2.70389500 -0.01824200
H     5.12925700  1.78495100 -0.02145900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.008832394859

Frequencies (cm^{-1}): 12.1863, 25.5163, 42.3919, 61.7629, 100.2454, 107.3333, 132.6978, 177.6474, 223.0344, 274.715, 289.9043, 381.4863, 411.6668, 431.9891, 447.3013, 503.4714, 630.9827, 648.753, 701.9769, 714.9201, 781.1335, 808.996, 865.9083, 877.2325, 886.7194, 941.5006, 954.479, 1006.9897, 1014.7016, 1018.2866, 1028.7923, 1047.7195, 1063.1704, 1112.269, 1116.2056, 1151.6636, 1187.7899, 1202.8739, 1258.2801, 1305.8796, 1344.3326, 1365.6839, 1391.7122, 1395.2562, 1409.635, 1463.6697, 1479.7108,

1492.5416, 1494.7794, 1516.4763, 1528.7079, 1553.9996, 1616.1464, 1639.8462, 2983.5862, 3021.9715, 3048.2532, 3083.2197, 3095.4753, 3131.2365, 3172.8372, 3179.6508, 3188.0707, 3197.0305, 3203.8877, 3437.8625

***Anti*-PhCHOO + EtOH TS-AAAH 1.1:**

```
C     0.00000000  0.00000000  0.00000000
O     0.00477300 -0.89937800  1.10545500
H     0.63771300 -1.79460800  0.85615400
C    -0.61413600  1.32754900  0.40062500
H    -1.64957100  1.19788500  0.71585700
H    -0.05860200  1.77304100  1.22591300
H    -0.59744100  2.02225900 -0.44100400
H    -0.54697200 -0.44116600 -0.84182700
H     1.03327400  0.13511400 -0.33464700
C    -3.43692200 -1.57359200  1.80372500
C    -4.73694500 -1.15415700  1.56860200
C    -5.23414100 -1.13612900  0.26883600
C    -4.43095300 -1.53681900 -0.79550800
C    -3.12835900 -1.95226900 -0.56713100
C    -2.62461000 -1.97583700  0.73862700
C    -1.26518500 -2.41270600  1.02288300
O    -0.63283800 -3.07141400  0.10308400
O     0.76854600 -3.08093700  0.48164800
H    -0.96603500 -2.57865700  2.05034700
H    -2.49888100 -2.26628800 -1.38693200
H    -4.82234200 -1.52251700 -1.80329500
H    -6.24868600 -0.80943900  0.08470600
H    -5.36245700 -0.84303900  2.39366300
H    -3.04188300 -1.58827100  2.81088600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.00176536626

Frequencies (cm^{-1}): -728.8342, 28.9868, 52.767, 78.1697, 111.163, 158.1696, 166.9465, 228.7187, 280.9853, 325.2286, 353.2771, 394.8034, 409.9317, 417.2176, 516.0329, 622.764, 636.8714, 647.9839, 709.4911, 788.1669, 803.0847, 820.7146, 868.5454, 873.8624, 905.771, 961.4781, 975.3363, 1008.5903, 1020.794, 1028.9962, 1047.3819, 1049.9276, 1103.4668, 1107.5565, 1150.8234, 1178.4916, 1186.8962, 1200.8367, 1234.5014, 1306.568, 1334.1887, 1339.3132, 1360.2259, 1388.8647, 1408.6741, 1454.1258, 1481.5117, 1485.737, 1495.6878, 1506.6369, 1513.869, 1533.2855, 1622.4826, 1642.6837, 1835.9985, 2985.7417, 3017.8246, 3031.5663, 3093.6037, 3102.3029, 3159.1684, 3170.9653, 3177.7595, 3186.8732, 3195.8309, 3204.8664

EtOCPhHOOH (*anti*-TS-AAAH 1.1 and 1.2):

```
C     0.00000000  0.00000000  0.00000000
O    -0.05805100 -0.70699500  1.25036600
H     1.33372000 -2.73355700  0.85758800
C     1.07983600  1.05519000  0.11415100
H     0.85654400  1.75135500  0.92242100
H     2.05165100  0.60260000  0.31255000
H     1.14875800  1.61964000 -0.81658100
H    -0.96904200  0.45859800 -0.20962900
H     0.21998400 -0.70035500 -0.80959000
C    -2.98213400 -0.39662500  1.62781100
C    -4.30669100 -0.06595900  1.37740800
C    -5.04934200 -0.80620700  0.46274500
C    -4.45886300 -1.87824700 -0.19323500
C    -3.13194000 -2.21396000  0.05919400
C    -2.38322700 -1.47116500  0.96861000
C    -0.94199600 -1.80472500  1.31452800
O    -0.52010200 -2.85417200  0.46258700
O     0.67919100 -3.42855100  1.02726400
H    -0.86365200 -2.14902500  2.34691900
H    -2.68251500 -3.05481400 -0.44713400
H    -5.03074600 -2.46068400 -0.90307900
H    -6.08171900 -0.54973900  0.26682100
H    -4.75994000  0.76746500  1.89716600
H    -2.40428500  0.18225200  2.33619100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.065586589601

Frequencies (cm^{-1}):

IRC:

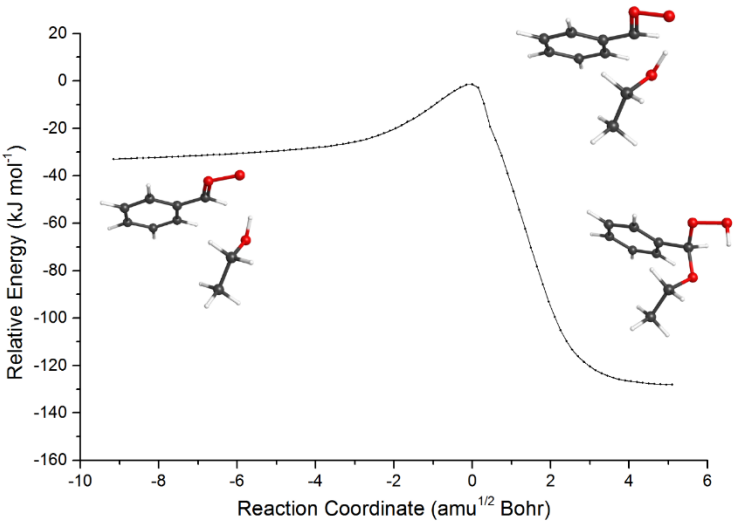


Figure S77: SCI 12 + EtOH TS-AAAH 1.1 IRC

***Anti*-PhCHOO + EtOH PRC (For TS-AAAH 1.2 and TS-AAAH 2.2):**

```
C     0.00000000  0.00000000  0.00000000
O     1.33438400  0.22453300  0.43531800
H     1.53464100  1.18446800  0.44499600
C    -1.03748000  0.52394600  0.98281300
H    -0.90523300  0.06323900  1.96232500
H    -0.95041800  1.60535900  1.10072500
H    -2.04712700  0.30278100  0.62931500
H    -0.10358500 -1.08029400 -0.11582100
H    -0.15807000  0.44849200 -0.98789000
C     6.00808900 -0.38810300  0.58223700
C     7.34780000 -0.74377000  0.58179100
C     8.32616800  0.24289100  0.53015400
C     7.96532600  1.58997400  0.47887300
C     6.63233300  1.95495800  0.47861000
C     5.63726700  0.96384300  0.53045500
C     4.23258100  1.27140900  0.53312800
O     3.84651300  2.47396700  0.48117100
O     2.48666500  2.73748400  0.48841800
H     3.47364500  0.49378500  0.57105500
H     6.34732600  2.99636200  0.43903500
H     8.73118800  2.35202900  0.43915100
H     9.37159000 -0.03402300  0.52999200
H     7.62929700 -1.78668900  0.62171800
H     5.24022300 -1.14923100  0.62195700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.008812054131

Frequencies (cm^{-1}): 13.1425, 22.3132, 38.3653, 38.8184, 98.0748, 108.5731, 128.1145, 178.1194, 217.6485, 250.4481, 288.8358, 379.3989, 410.6299, 437.0813, 462.4868, 503.3673, 630.1615, 648.1021, 701.4514, 707.5094, 780.8143, 815.7615, 866.0166, 876.8663, 898.5917, 942.6846, 953.6747, 1006.65, 1014.4996, 1018.1997, 1028.4149, 1046.5133, 1062.2851, 1111.2069, 1120.0458, 1178.7621, 1187.499, 1201.2847, 1255.2963, 1299.0544, 1342.2518, 1352.4676, 1365.0388, 1398.6846, 1404.826, 1478.0966, 1483.6406, 1490.4609, 1499.3641, 1525.7176, 1527.5327, 1553.8359, 1615.71, 1638.999, 2975.7953, 2996.7989, 3028.6683, 3092.3611, 3093.9678, 3133.6618, 3173.0595, 3179.2711, 3188.1187, 3197.6272, 3204.1933, 3442.7389

***Anti*-PhCHOO + EtOH TS-AAAH 1.2:**

```
C     0.00000000  0.00000000  0.00000000
O     0.09952900 -1.04010600 -0.97134000
H    -0.46756700 -1.93048500 -0.62019700
C    -1.37600900  0.64532700 -0.04905000
H    -1.57359400  1.05614100 -1.03895400
H    -2.15379100 -0.08197000  0.18517900
H    -1.43680800  1.45510600  0.68054900
H     0.77769900  0.73333000 -0.22156400
H     0.18913000 -0.40359300  1.00026400
```

```
C     3.59350200 -1.44523700 -1.46711200
C     4.83767300 -0.86860300 -1.26131000
C     5.28616500 -0.63400200  0.03469300
C     4.48906200 -0.97319700  1.12510000
C     3.24152700 -1.54276600  0.92518700
C     2.78845300 -1.78687200 -0.37623900
C     1.48909200 -2.39548300 -0.62898900
O     0.88327100 -2.97521000  0.35852500
O    -0.49477400 -3.17925800 -0.05668000
H     1.25272300 -2.73916400 -1.62855900
H     2.61614200 -1.80786200  1.76516400
H     4.84209700 -0.78993900  2.13050900
H     6.25731200 -0.18590600  0.19600400
H     5.45748500 -0.60432700 -2.10676900
H     3.23746400 -1.63042500 -2.47191800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.002735053783

Frequencies (cm^{-1}): -641.9891, 39.8054, 52.346, 61.6508, 119.7244, 149.305, 165.6071, 227.0856, 260.3747, 321.1441, 359.5383, 398.9513, 414.9145, 458.2878, 516.4042, 614.155, 634.1115, 646.5243, 707.7736, 787.4486, 814.1871, 835.8572, 867.2838, 873.6382, 904.5897, 959.2533, 970.8915, 1006.9521, 1021.0077, 1026.8928, 1043.7158, 1049.3076, 1105.0496, 1107.4093, 1164.3585, 1181.6317, 1186.4537, 1201.0185, 1234.029, 1313.4908, 1337.3677, 1339.063, 1360.3434, 1402.9585, 1416.675, 1455.2036, 1475.7258, 1492.0875, 1497.3358, 1507.34, 1519.7082, 1533.1446, 1623.072, 1642.4236, 1849.8384, 3001.6929, 3030.1039, 3051.0027, 3092.7119, 3105.648, 3156.618, 3170.4108, 3177.4794, 3186.4781, 3195.3385, 3204.4438

IRC:

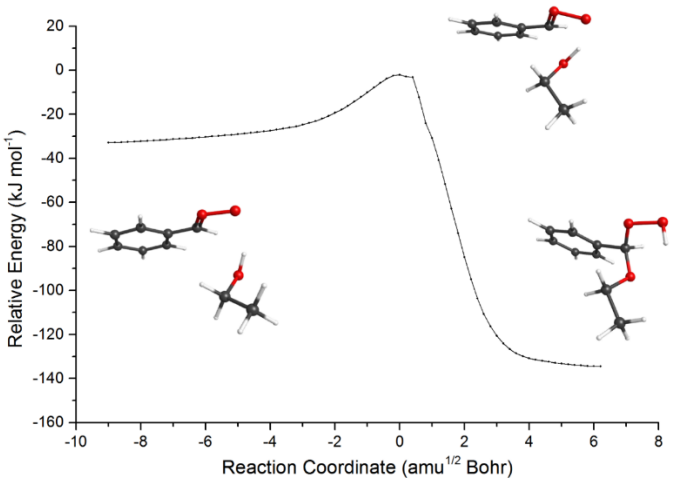


Figure S78: SCI 12 + EtOH TS-AAAH 1.2 IRC

***Anti*-PhCHOO + EtOH TS-AAAH 2.1:**

```
C     0.00000000  0.00000000  0.00000000
O     0.64421900  1.12300000  0.58665300
H     0.14376400  2.06832200  0.29455600
C    -1.27439500 -0.34662300  0.75441500
H    -1.05369800 -0.56461100  1.79894600
H    -1.98367300  0.48064000  0.71813000
H    -1.74883800 -1.22317500  0.30922400
H     0.70054500 -0.83823300  0.03093100
H    -0.23423800  0.20326900 -1.05255900
C     3.91023100  0.54884500 -0.95073600
C     5.18052300  0.08397700 -0.64302300
C     5.87243500  0.62681700  0.43448800
C     5.29422500  1.63184900  1.20690000
C     4.02449100  2.09682500  0.90662700
C     3.32767600  1.55956800 -0.18116500
C     1.99630800  2.03452200 -0.53044300
O     1.65028900  3.21745400 -0.14218500
O     0.20678500  3.30927800 -0.29463200
H     1.50679200  1.63929400 -1.41447200
H     3.56042200  2.86730400  1.50475200
H     5.83497600  2.04640700  2.04637000
H     6.86273000  0.26477300  0.67577700
H     5.63075800 -0.69651100 -1.24047800
```

```
H    3.36791400  0.13467100 -1.79077700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.999073224789

Frequencies (cm^{-1}): -620.662, 40.2806, 47.084, 77.4643, 110.8842, 155.2784, 169.6499, 219.424, 264.4289, 328.4274, 357.1942, 382.4879, 414.974, 457.5573, 513.555, 575.1512, 632.6544, 645.081, 707.3793, 785.5606, 814.8552, 858.2121, 867.2704, 878.3064, 905.6139, 959.3739, 966.586, 1006.6225, 1021.1477, 1027.4964, 1049.0347, 1059.8023, 1107.2847, 1122.8563, 1142.1866, 1186.4611, 1190.0728, 1201.5577, 1232.858, 1309.7, 1337.3814, 1339.748, 1361.3712, 1395.5444, 1410.6106, 1430.4336, 1460.4968, 1485.4288, 1496.8395, 1508.4729, 1520.8008, 1533.7634, 1623.6936, 1643.0242, 1909.5712, 2975.0725, 3031.1055, 3034.7261, 3093.8455, 3106.4746, 3133.1847, 3168.8302, 3175.5504, 3186.6452, 3195.5517, 3207.1698

EtOCPhHOOH (*anti*-TS-AAAH 2.1-conformer):

```
C    0.00000000  0.00000000  0.00000000
O    0.32817200  1.05824700  0.90013500
H   -0.74108000  3.16441200  1.40139000
C   -1.06593800 -0.86305600  0.64056600
H   -0.70620900 -1.28905600  1.57686000
H   -1.96339000 -0.28072700  0.84945000
H   -1.33576400 -1.68140700 -0.02788800
H    0.89472200 -0.59224100 -0.21882300
H   -0.35878600  0.42515000 -0.94507200
C    3.61013500  1.77015300 -0.48377600
C    4.93856700  1.38495700 -0.34462900
C    5.36510400  0.77923300  0.83135800
C    4.46062100  0.55856300  1.86564900
C    3.13313400  0.94097400  1.72504600
C    2.70189900  1.55011700  0.54786200
C    1.26374700  1.98974500  0.39640100
O    1.13652200  3.16357500  1.16378500
O   -0.16288800  3.74402100  0.88236700
H    1.02742700  2.21480800 -0.65050000
H    2.42459200  0.76726700  2.52256800
H    4.79112600  0.08810200  2.78192400
H    6.39816400  0.47796500  0.94166600
H    5.63763200  1.55657500 -1.15191500
H    3.27802700  2.24535100 -1.39823000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.065827787527

Frequencies (cm^{-1}): 27.206, 50.0811, 72.5619, 105.2008, 115.2525, 213.3984, 216.1993, 254.1711, 277.5916, 301.1416, 323.689, 377.4674, 416.3195, 462.0373, 558.6577, 592.1533, 634.936, 661.6494, 718.0493, 781.1572, 824.8609, 861.6319, 867.2556, 917.0494, 923.3011, 948.6798, 1001.1496, 1020.2935, 1022.7995, 1030.3513, 1051.4413, 1063.5231, 1096.6504, 1113.7034, 1151.9903, 1182.5892, 1183.4775, 1199.9574, 1218.0954, 1306.7241, 1317.7046, 1348.3583, 1357.0517, 1378.6951, 1388.2375, 1409.8088, 1436.7816, 1486.138, 1490.1025, 1500.1389, 1526.562, 1530.9781, 1628.1427, 1644.8801, 2980.596, 2992.855, 3014.0773, 3036.9404, 3101.0231, 3105.8954, 3161.1619, 3168.5543, 3178.7975, 3189.2364, 3196.5109, 3720.1802

IRC:

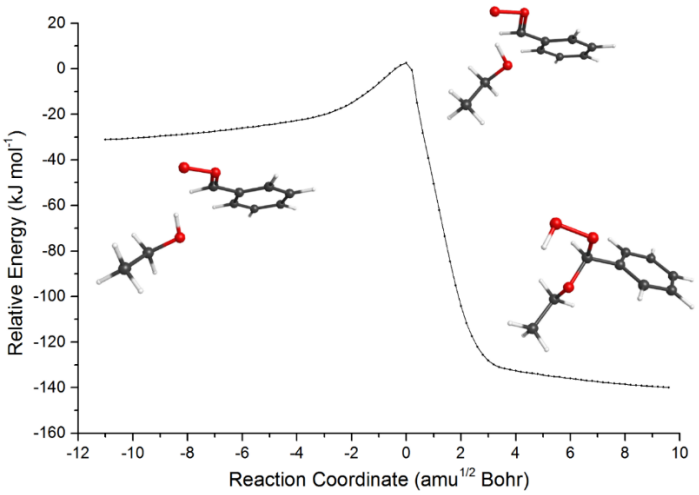


Figure S79: SCI 12 + EtOH TS-AAAH 2.1 IRC

***Anti*-PhCHOO + EtOH TS-AAAH 2.2:**

C	0.00000000	0.00000000	0.00000000
O	0.65954600	-1.12163100	-0.56965700
H	0.13412900	-2.07364200	-0.30170200
C	0.56246900	1.29179600	-0.56367000
H	1.62453800	1.38739000	-0.33664600
H	0.44318200	1.31863300	-1.64659100
H	0.04184500	2.15098400	-0.13719100
H	0.09789600	-0.01403000	1.09484000
H	-1.07030400	-0.07960900	-0.21626400
C	3.92485600	-0.70611800	1.09999900
C	5.22348900	-0.28784000	0.84985100
C	5.92385000	-0.81709800	-0.22908400
C	5.32618900	-1.76271500	-1.05943600
C	4.02870500	-2.18210600	-0.81567300
C	3.32243800	-1.65736000	0.27203500
C	1.96305700	-2.08854200	0.56470100
O	1.59535800	-3.25316700	0.14257700
O	0.14731800	-3.31035200	0.24583600
H	1.45428800	-1.68945900	1.43654400
H	3.55028900	-2.90630600	-1.45860600
H	5.87388700	-2.16693400	-1.89943200
H	6.93614200	-0.49084700	-0.42601900
H	5.68928700	0.44579100	1.49299100
H	3.37576100	-0.30252300	1.94075700

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -574.998966423

Frequencies (cm^{-1}): -704.9346, 45.7548, 51.3463, 64.9236, 114.2315, 161.7081, 177.7747, 233.6546, 282.7453, 330.2396, 336.5085, 394.6588, 400.5172, 415.2658, 517.009, 592.6445, 633.2945, 644.6808, 707.6118, 785.4254, 805.7935, 843.6328, 867.0947, 873.4482, 907.3269, 960.1015, 975.8101, 1006.5164, 1021.0864, 1027.6752, 1049.2345, 1073.7382, 1103.479, 1107.5693, 1152.334, 1176.8859, 1186.6132, 1201.4515, 1232.9025, 1309.3321, 1325.4072, 1338.9417, 1357.0253, 1361.3246, 1407.4819, 1437.9994, 1456.99, 1486.2666, 1496.2013, 1507.5394, 1517.4175, 1533.6999, 1623.5208, 1643.002, 1900.6187, 2952.3919, 3010.8677, 3032.1976, 3094.0598, 3103.6579, 3126.9774, 3168.9868, 3175.7317, 3186.7806, 3195.5656, 3207.0862

EtOCPhHOOH (anti-TS-AAAH 2.2-Conformer):

C	0.00000000	0.00000000	0.00000000
O	0.72077800	-1.02267300	-0.69260900
H	-0.50455800	-3.19847500	-0.84138400
C	0.85264600	1.20686100	0.35823500
H	1.64281600	0.94768300	1.06295000
H	1.31660500	1.62838000	-0.53325900
H	0.22885700	1.97561400	0.81822200
H	-0.46391700	-0.42752800	0.89535500
H	-0.79950800	0.29085600	-0.68136100
C	3.82436500	-1.86103700	1.07324600
C	5.19530100	-1.65772200	0.97099200
C	5.74481900	-1.22712500	-0.23130100

```
C     4.91969300 -1.00071800 -1.32817600
C     3.54896700 -1.20115200 -1.22461000
C     2.99480100 -1.63121200 -0.02133000
C     1.50785900 -1.87995700  0.10057700
O     1.32390300 -3.20548300 -0.35898000
O    -0.04757300 -3.58761500 -0.08090800
H     1.18001300 -1.81961900  1.14419200
H     2.90236600 -1.01848600 -2.07080300
H     5.34491100 -0.66672500 -2.26510300
H     6.81150100 -1.06684500 -0.31288400
H     5.83223400 -1.83419200  1.82720000
H     3.39703900 -2.20081500  2.00835400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -575.064238921656

Frequencies (cm^{-1}): 24.3769, 37.4297, 59.6508, 108.4729, 123.1154, 190.0309, 225.4854, 269.3885, 293.5402, 324.271, 336.9296, 405.1466, 416.3594, 449.6427, 533.1283, 592.2307, 634.5037, 658.8081, 717.1907, 778.545, 804.1946, 863.2313, 866.5826, 897.2175, 921.2636, 945.1278, 1000.7852, 1007.0885, 1019.0934, 1023.1505, 1050.883, 1051.5847, 1082.5702, 1106.619, 1123.6267, 1182.3417, 1198.7457, 1201.1764, 1217.2981, 1317.1555, 1330.2407, 1346.5574, 1359.7326, 1371.9005, 1397.5333, 1411.2536, 1421.9202, 1486.9473, 1488.8604, 1493.2468, 1511.3892, 1531.1341, 1627.7844, 1644.8271, 2999.1015, 3004.3378, 3032.0054, 3070.0112, 3094.4853, 3107.5698, 3160.2688, 3167.849, 3178.4728, 3189.3484, 3198.6384, 3727.8534

IRC:

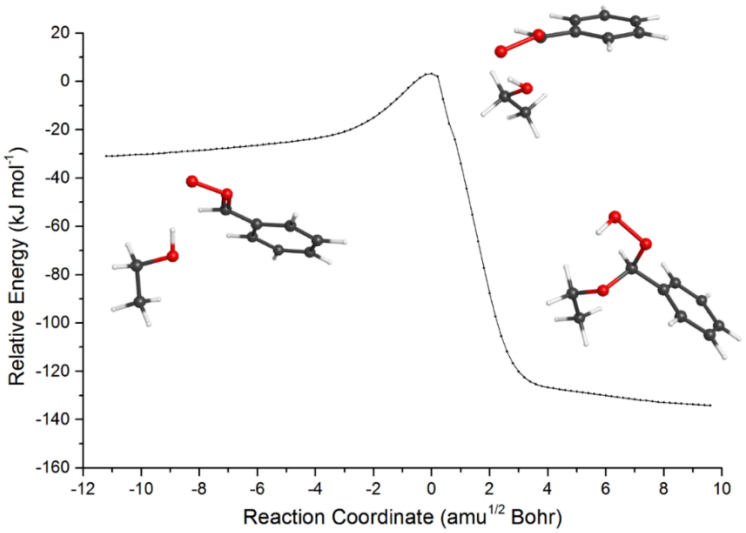


Figure S80: SCI 12 + EtOH TS-AAAH 2.2 IRC

7.12.3 sCI 12 + iPrOH Reaction

***Anti*-PhCHOO + iPrOH PRC:**

```
C     0.00000000  0.00000000  0.00000000
O     1.39736900 -0.11072600  0.27091400
H     1.68315200 -1.04761500  0.23204700
H    -0.20385400 -0.42638300 -0.99093400
C    -0.82149000 -0.76194200  1.03592900
H    -0.54312500 -1.81659400  1.05130600
H    -0.65094900 -0.34992300  2.03216700
H    -1.88805500 -0.69728000  0.81121100
C    -0.33722700  1.48192300 -0.03173300
H    -1.39074100  1.63503700 -0.26898100
H    -0.13255700  1.93662300  0.93939500
H     0.26360400  1.99480300 -0.78293700
C     5.99549000  0.92429300  0.46365000
C     7.29635300  1.40214600  0.49272800
C     8.36223400  0.51451600  0.39622900
C     8.12783400 -0.85543000  0.27027300
C     6.83457200 -1.34189400  0.24024200
C     5.75161700 -0.45143700  0.33741300
C     4.38182300 -0.88845900  0.31392000
O     4.11106500 -2.11803300  0.20063500
O     2.78273400 -2.50871500  0.18366400
H     3.55323600 -0.18843400  0.38607400
```

```
H     6.64759600 -2.40152500  0.14283600
H     8.96124300 -1.54008800  0.19564500
H     9.37751200  0.88636100  0.41865400
H     7.47943600  2.46303300  0.59014500
H     5.16019700  1.60789600  0.53808300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.271902988241

Frequencies (cm^{-1}): 11.9586, 18.9524, 33.2167, 41.5201, 96.3859, 98.8188, 114.0879, 176.7448, 211.4006, 222.1603, 264.263, 289.0363, 364.8903, 378.7402, 410.8692, 437.3942, 453.5015, 491.275, 502.9877, 630.3676, 648.08, 701.2961, 709.9108, 780.4048, 821.5039, 864.8304, 877.0633, 929.8619, 942.027, 945.7916, 953.1876, 967.8685, 1005.773, 1013.5877, 1018.2249, 1027.8469, 1046.6994, 1111.4609, 1129.5294, 1158.8103, 1186.9597, 1187.5743, 1201.954, 1255.7955, 1335.2757, 1345.0757, 1365.3199, 1375.7407, 1393.1487, 1398.4209, 1411.7782, 1460.0244, 1478.9941, 1483.6943, 1489.4453, 1503.7852, 1508.6699, 1527.6703, 1553.6179, 1615.5298, 1639.2531, 2961.7049, 3020.3327, 3027.9823, 3082.9446, 3088.6727, 3092.6343, 3097.6041, 3133.2274, 3173.1438, 3179.5829, 3188.2214, 3197.4873, 3204.0727, 3445.7599

***Anti*-PhCHOO + iPrOH TS-AAAH 1.1:**

```
C     0.00000000  0.00000000  0.00000000
O    -0.20643400  1.00027100 -1.00777600
H     0.31127500  1.95124500 -0.71163200
H    -0.52116700  0.31189000  0.91388800
C     1.48969400 -0.10404100  0.30980600
H     1.88359600  0.85509600  0.64593500
H     2.04203600 -0.41645300 -0.57770800
H     1.66200800 -0.83789700  1.09874300
C    -0.59186700 -1.31163800 -0.49307800
H    -0.47650700 -2.09193900  0.26071000
H    -0.08532400 -1.63372800 -1.40401800
H    -1.65353200 -1.20263200 -0.71209700
C    -3.74349200  1.20582000 -1.46569600
C    -4.95820500  0.59280400 -1.19987300
C    -5.36838700  0.41022700  0.11734500
C    -4.56278100  0.83917500  1.16875900
C    -3.34416600  1.44683100  0.90895200
C    -2.92911900  1.63663600 -0.41386200
C    -1.66251800  2.28562500 -0.72774400
O    -1.08078900  2.96284300  0.21357700
O     0.27862200  3.21401200 -0.23149500
H    -1.46080400  2.58065400 -1.75017700
H    -2.71371200  1.78452800  1.71851700
H    -4.88635600  0.69724300  2.19061000
H    -6.31672900 -0.06668900  0.32502400
H    -5.58537700  0.25942100 -2.01495000
H    -3.41691500  1.35036700 -2.48703600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.265301913881

Frequencies (cm^{-1}): -722.5638, 40.217, 49.1283, 55.3594, 103.3, 141.2833, 159.1927, 212.9605, 221.4357, 256.1938, 319.9999, 327.4772, 373.5141, 393.7634, 414.801, 429.0506, 487.7667, 523.2203, 624.9415, 638.6281, 647.7897, 708.1455, 778.8793, 788.8262, 867.8557, 868.7145, 892.2582, 922.5784, 935.6041, 946.6836, 959.0849, 994.2057, 1007.1213, 1021.1521, 1027.2894, 1049.1591, 1106.6929, 1108.5037, 1143.7774, 1180.9381, 1186.4633, 1195.3115, 1200.8782, 1234.743, 1332.0729, 1338.4123, 1355.8149, 1359.5981, 1384.6881, 1399.0573, 1414.6643, 1451.9141, 1458.3978, 1485.7179, 1490.7352, 1499.0846, 1506.59, 1510.3379, 1533.265, 1622.9182, 1642.7316, 1844.7842, 2974.4582, 3026.865, 3032.231, 3089.0641, 3096.5241, 3101.4724, 3103.5348, 3156.3241, 3170.7266, 3177.6424, 3186.747, 3195.5808, 3204.4913

iPrOCPhH(OOH) (*anti*-TS-AAAH 1.1-conformer):

```
C     0.00000000  0.00000000  0.00000000
O     0.18730500 -0.77340500 -1.21049500
H    -1.19501600 -2.85450500 -0.83819300
H     0.87567100 -0.13301600  0.63879300
C    -1.24279400 -0.47672500  0.74378600
H    -1.13212300 -1.50766800  1.07782200
H    -2.12195600 -0.39995400  0.10084300
H    -1.41777800  0.14134500  1.62583900
C    -0.10406500  1.45832800 -0.41764500
H    -0.27048400  2.09381700  0.45304600
H    -0.93798000  1.59617800 -1.10757200
H     0.80850000  1.78572200 -0.91358500
C     3.13687200 -0.43798300 -1.40055700
C     4.43513400 -0.07873900 -1.06571200
C     5.11155800 -0.76372200 -0.06117300
C     4.48199800 -1.81112800  0.59822500
C     3.18220500 -2.17623700  0.26039400
C     2.49711600 -1.48631800 -0.73734300
C     1.08901600 -1.85434100 -1.17797500
O     0.63570500 -2.90100100 -0.33558200
O    -0.50317000 -3.52140300 -0.97022300
H     1.09456100 -2.22393900 -2.20464500
H     2.70444900 -2.99959800  0.76952400
H     5.00234100 -2.35189100  1.37735500
H     6.12322400 -0.48473000  0.20084100
H     4.92006500  0.73340700 -1.59059000
H     2.61278900  0.09663100 -2.18151300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.326968105829

Frequencies (cm^{-1}): 25.8667, 30.4444, 69.6225, 102.7033, 142.1601, 169.5999, 207.9617, 226.0264, 238.7104, 272.9803, 304.7595, 342.0053, 369.373, 391.9314, 410.205, 414.5961, 489.3371, 510.8318, 633.3006, 647.6684, 702.1474, 721.2907, 763.7427, 792.9959, 872.8956, 891.2627, 912.6228, 932.2306, 942.6296, 946.7432, 971.8384, 1005.7792, 1009.1672, 1021.6224, 1022.5113, 1052.4783, 1075.2953, 1109.2424, 1134.857, 1151.1931, 1182.9073, 1203.3733, 1204.2875, 1214.8077, 1321.1963, 1347.9536, 1361.4571, 1364.985, 1382.004, 1390.8093, 1397.1376, 1401.1718, 1418.3918, 1483.7766, 1485.1003, 1491.4014, 1499.1015, 1516.1304, 1530.9106, 1624.6059, 1645.1572, 3025.6218, 3032.6521, 3037.3003, 3057.1515, 3085.6215, 3098.3248, 3105.112, 3107.8323, 3163.6638, 3171.7918, 3180.8225, 3190.1935, 3207.1995, 3705.0899

IRC:

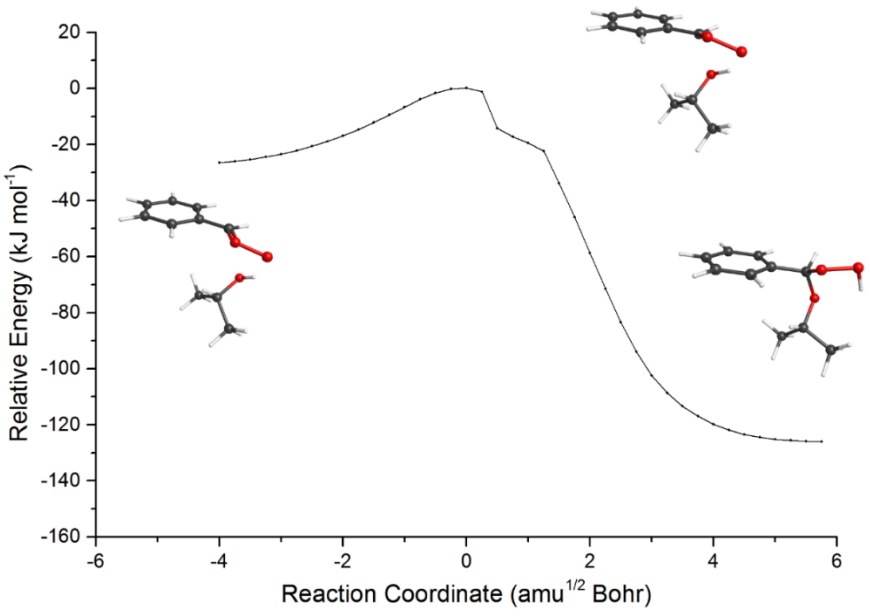


Figure S81: SCI 12 + iPrOH TS-AAAH 1.1 IRC

***Anti*-PhCHOO + iPrOH TS-AAAH 1.2:**

```
C     0.00000000  0.00000000  0.00000000
```

O	-0.36524800	1.11032700	-0.83239900
H	0.17609100	2.08993900	-0.54012300
H	1.04246800	-0.22017600	-0.26316200
C	-0.85474400	-1.20258700	-0.37341600
H	-0.78925400	-1.39886500	-1.44332600
H	-1.90099900	-1.02905700	-0.11811500
H	-0.51789200	-2.09218500	0.16126500
C	-0.04947600	0.31583500	1.49316100
H	0.37675200	-0.51459400	2.05832500
H	-1.07471400	0.45931800	1.83488000
H	0.52060200	1.21509900	1.72304000
C	-3.91141200	1.36033200	-1.23618800
C	-5.16379700	0.83944300	-0.94814100
C	-5.62225700	0.82632600	0.36515400
C	-4.82717200	1.33257700	1.39071300
C	-3.57109100	1.84540100	1.10950200
C	-3.10628300	1.86322400	-0.21009200
C	-1.80558100	2.42218400	-0.56039800
O	-1.19901400	3.15235300	0.32481100
O	0.16740200	3.32336700	-0.13481100
H	-1.59717000	2.63107800	-1.60207300
H	-2.94770900	2.23792700	1.89957400
H	-5.18903100	1.32368000	2.40955300
H	-6.59997200	0.42253600	0.59084800
H	-5.78236700	0.44751300	-1.74347700
H	-3.54690800	1.37434400	-2.25471900

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.260689493572

Frequencies (cm^{-1}): -951.3235, 31.1368, 51.0654, 67.3635, 112.9275, 139.8024, 157.4232, 214.037, 234.8559, 278.8164, 303.2765, 321.3624, 366.5955, 398.8916, 413.0956, 416.3965, 491.7897, 516.2542, 616.8907, 633.2335, 648.6774, 708.2311, 727.5656, 789.5449, 847.0038, 868.2132, 876.2698, 903.8804, 930.9437, 942.4481, 959.0645, 963.6957, 1008.4969, 1021.4777, 1027.8637, 1049.1294, 1106.7743, 1127.1741, 1143.3616, 1163.3256, 1186.5388, 1200.768, 1202.2067, 1235.8823, 1324.4974, 1337.589, 1351.0764, 1360.1117, 1370.6081, 1398.8248, 1408.3524, 1424.9896, 1452.7651, 1485.3729, 1490.2132, 1499.4925, 1506.502, 1512.2929, 1533.4292, 1623.4899, 1642.8379, 1857.6958, 2968.3109, 3029.4936, 3035.2428, 3089.463, 3095.97, 3101.7152, 3109.9383, 3157.9089, 3171.0847, 3178.1019, 3186.8232, 3195.9649, 3204.6258

iPrOPhCHOOH (*anti*-TS-AAAH 1.2-Conformer):

C	0.00000000	0.00000000	0.00000000
O	0.13601400	-1.13561900	-0.89794600
H	-1.38697900	-2.81032400	-0.31920400
H	-0.89949300	0.46862700	-0.40405000
C	1.14203800	1.00055200	-0.14763800
H	1.33554800	1.20512000	-1.20002700
H	2.06285100	0.65088100	0.31413500
H	0.85889200	1.93869400	0.33334700
C	-0.28075100	-0.36249200	1.45463500
H	-0.55577700	0.54640900	1.99271100
H	0.58888600	-0.79088900	1.94825300
H	-1.10608000	-1.06766500	1.54217100
C	3.27144900	-1.55696300	-1.21011800
C	4.60255400	-1.31369600	-0.90088500
C	5.06806500	-1.53399300	0.39139900
C	4.19638300	-2.00634200	1.36475600
C	2.86191200	-2.24779600	1.05530800
C	2.38648400	-2.01107200	-0.23248000
C	0.94782500	-2.26509800	-0.64124200
O	0.36784100	-3.10910600	0.33733400
O	-0.86878400	-3.62341800	-0.20426700
H	0.92979800	-2.79401500	-1.59589000
H	2.19581600	-2.63326600	1.81272400
H	4.55496000	-2.19432100	2.36786500
H	6.10555300	-1.34800100	0.63423400
H	5.27725500	-0.95900600	-1.66833900
H	2.91195500	-1.38759600	-2.21701200

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.319932433268

Frequencies (cm^{-1}): 42.8225, 61.8286, 77.4694, 96.6591, 153.2011, 161.8636, 211.2469, 248.2509, 259.6112, 274.2553, 313.648, 350.1282, 362.5485, 379.2745, 410.8525, 415.6965, 507.56, 527.2756, 629.5376, 640.8055, 695.9361, 719.0811, 737.0493, 788.46, 869.9759, 876.6039, 913.5727, 928.0549, 942.0476, 950.7888, 961.4174, 1003.1619, 1004.2144, 1020.3223, 1022.9561, 1044.8492, 1057.7866, 1111.08, 1147.367, 1161.2225, 1183.1232, 1196.3287, 1205.8706, 1218.6159, 1322.2775, 1353.8154, 1372.4141, 1376.0707, 1396.5002,

1400.8314, 1405.3013, 1410.3496, 1425.2147, 1481.8982, 1486.4578, 1490.8391, 1498.6904, 1509.1186, 1532.5588, 1625.212, 1645.3646, 3031.4889, 3035.7244, 3042.2747, 3050.0888, 3094.939, 3098.3768, 3121.7082, 3126.449, 3162.7053, 3169.9505, 3179.6489, 3190.1724, 3202.9866, 3688.9465

IRC:

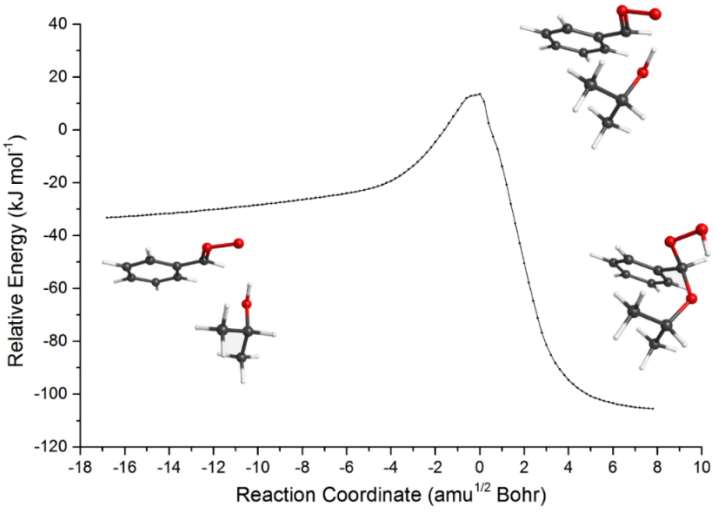


Figure S82: SCI 12 + iPrOH TS-AAAH 1.2 IRC

***Anti*-PhCHOO + iPrOH TS-AAAH 2.1:**

```
C     0.00000000  0.00000000  0.00000000
O     0.75906800  1.05904600 -0.58716900
H     0.32806000  2.05498500 -0.32294600
H     0.09526700  0.05919100  1.09440800
C    -1.47271500  0.17184400 -0.35824100
H    -1.85069800  1.13147600 -0.00484100
H    -1.60684900  0.12539000 -1.43970100
H    -2.07054600 -0.61807200  0.09903800
C     0.56879900 -1.32888500 -0.47540300
H     0.03433700 -2.16240700 -0.01728500
H     0.47474200 -1.41118300 -1.55905000
H     1.62449500 -1.41584900 -0.21959000
C     4.00806500  0.35559400  1.01910300
C     5.25467700 -0.18811700  0.74617500
C     5.96853300  0.24483700 -0.36624300
C     5.43609200  1.22013700 -1.20648100
C     4.19081000  1.76534200 -0.93921100
C     3.47155000  1.33702100  0.18143800
C     2.16601800  1.90106800  0.49944700
O     1.90762400  3.09470300  0.07407100
O     0.47485500  3.29688000  0.21348300
H     1.64870400  1.56828400  1.39391300
H     3.76284800  2.51439600 -1.58924400
H     5.99321700  1.54968500 -2.07252800
H     6.93991200 -0.17949700 -0.58148400
H     5.66942900 -0.94492000  1.39739500
H     3.44949600  0.02595400  1.88549100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.263355755823

Frequencies (cm^{-1}): -684.109, 34.0921, 45.9267, 54.8378, 105.2469, 156.3725, 158.4541, 212.5911, 222.947, 262.3847, 303.3676, 334.1804, 374.0124, 386.5773, 415.0742, 435.473, 492.4905, 520.0556, 586.6284, 633.4257, 645.7992, 707.7088, 784.1697, 818.2668, 863.0422, 866.8633, 890.7932, 927.7695, 937.0226, 948.3817, 959.6444, 1006.2299, 1013.4012, 1021.5259, 1027.2461, 1048.9202, 1106.7702, 1118.0191, 1147.9024, 1172.4779, 1186.5213, 1194.9442, 1200.6157, 1233.1169, 1323.0239, 1338.5319, 1349.4484, 1359.644, 1373.7287, 1401.1472, 1413.774, 1423.9745, 1456.2533, 1483.7912, 1488.9574, 1496.7345, 1507.0225, 1510.5772, 1533.3618, 1623.863, 1643.1158, 1909.4827, 2937.283, 3027.8575, 3032.6113, 3091.2676, 3097.5348, 3100.1216, 3101.812, 3125.6123, 3168.6984, 3175.3983, 3186.1454, 3195.1277, 3206.351

iPrOCPhHOOH (*anti*-TS-AAAH 2.1 -conformer):

```
C     0.00000000  0.00000000  0.00000000
O     0.90906800  0.76873900 -0.81013600
H     0.05484500  3.14150300 -1.11312800
H    -0.33348500  0.63796600  0.82673900
C    -1.18907900 -0.33444700 -0.88432600
H    -1.66156200  0.57271600 -1.26003800
H    -0.87199900 -0.93528200 -1.73753000
H    -1.93175400 -0.90115900 -0.32221900
C     0.67268700 -1.24654200  0.56387400
H    -0.03431000 -1.81425700  1.17079000
H     1.02547900 -1.88670700 -0.24576800
H     1.52609000 -0.99328600  1.19269400
C     4.21217300  1.26376100  0.71549500
C     5.52525400  0.83390300  0.56832800
C     5.91683600  0.18754300 -0.59874000
C     4.99168700 -0.02664000 -1.61505300
C     3.67813100  0.40058900 -1.46607400
C     3.28179300  1.04679900 -0.29783400
C     1.86288800  1.54365000 -0.12883500
O     1.87253600  2.84805900 -0.68551200
O     0.59798100  3.47116600 -0.38212400
H     1.59351800  1.61925600  0.92982300
H     2.95359500  0.22971800 -2.24913800
H     5.29390600 -0.52806100 -2.52471400
H     6.93822100 -0.14916100 -0.71523600
H     6.24034500  1.00257100  1.36214200
H     3.90884900  1.77236200  1.62201800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.327278862786

Frequencies (cm^{-1}): 20.7858, 35.2894, 48.0363, 105.1662, 113.4768, 173.0476, 211.5229, 230.839, 257.2668, 266.2381, 301.5794, 310.3398, 344.0387, 376.222, 415.4087, 455.8024, 491.9273, 549.0667, 592.5489, 635.1277, 657.3712, 718.3542, 778.3916, 846.8141, 865.3973, 867.4616, 921.0504, 934.1972, 941.5247, 946.9155, 954.8833, 1001.7221, 1019.4427, 1023.1763, 1038.2624, 1050.3783, 1073.3329, 1109.2115, 1145.5671, 1162.8586, 1182.4872, 1199.7592, 1203.745, 1216.2973, 1318.3755, 1343.3927, 1354.5859, 1366.5691, 1372.1504, 1375.7803, 1404.5495, 1418.53, 1426.2663, 1481.6375, 1486.2795, 1489.6276, 1496.2974, 1508.4365, 1531.3612, 1627.9658, 1645.1678, 2987.061, 3007.691, 3029.9322, 3036.1152, 3093.2694, 3098.9889, 3102.9993, 3103.9065, 3160.2494, 3167.9275, 3178.4014, 3189.3623, 3199.4767, 3731.3856

IRC:

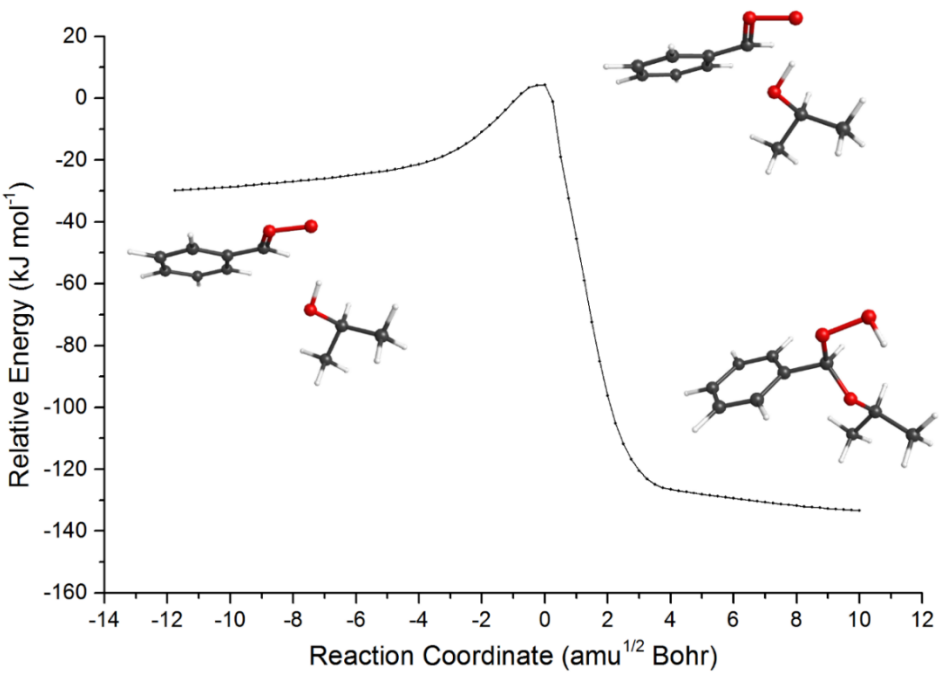


Figure S83: SCI 12 + iPrOH TS-AAAH 2.1 IRC

***Anti*-PhCHOO + iPrOH TS-AAAH 2.2:**

```
C    0.00000000  0.00000000  0.00000000
O    0.85452400  1.12701000 -0.21808000
H    0.38032500  2.11588600  0.07906700
H   -0.91672800  0.21004000 -0.56534800
C   -0.38986000 -0.19393600  1.46485000
H   -0.81170100  0.71821000  1.88701100
H    0.46777000 -0.49655000  2.06925900
H   -1.13985900 -0.98173500  1.54624700
C    0.66418000 -1.23466300 -0.59166500
H    0.00124400 -2.09878200 -0.52491200
H    1.58633400 -1.46901900 -0.05710100
H    0.91093300 -1.06742300 -1.63932800
C    3.97379300  0.36125300  1.63777100
C    5.23555600 -0.17617700  1.42966600
C    6.00440700  0.26168400  0.35637500
C    5.51211800  1.23624900 -0.50859100
C    4.25228600  1.77589000 -0.30519600
C    3.47765400  1.34202600  0.77533200
C    2.15614400  1.90355800  1.02630300
O    1.92730300  3.10748400  0.60534900
O    0.48531600  3.30601400  0.66236700
H    1.58786300  1.56472500  1.88222000
H    3.85510800  2.52410000 -0.97532000
H    6.11205700  1.56986800 -1.34396400
H    6.98740200 -0.15832400  0.19115400
H    5.61913200 -0.93236400  2.10044100
H    3.37184400  0.02615300  2.47247100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.259408548651

Frequencies (cm^{-1}): -838.8294, 32.953, 45.0048, 56.1197, 114.9307, 140.6652, 159.8283, 229.8422, 248.5201, 284.0115, 306.1636, 323.8044, 371.7821, 385.0115, 408.785, 414.9395, 471.8274, 523.156, 598.2084, 633.4297, 643.3673, 707.1798, 769.5429, 790.2226, 853.899, 866.0083, 878.2722, 903.0475, 928.1758, 943.3653, 958.225, 993.5676, 1005.7195, 1021.363, 1027.0546, 1048.7456, 1101.9144, 1107.1934, 1143.3258, 1165.693, 1186.2497, 1192.9473, 1199.3373, 1232.4318, 1293.9648, 1333.5081, 1339.8591, 1358.4358, 1367.291, 1383.1602, 1400.6526, 1419.655, 1450.9156, 1485.6904, 1489.4128, 1499.9649, 1505.5655, 1511.1343, 1533.6314, 1624.3208, 1643.2894, 1931.291, 2971.8945, 3023.7435, 3030.6487, 3082.3935, 3091.9595, 3100.0183, 3105.7971, 3166.9913, 3173.4449, 3176.6271, 3185.8432, 3194.7305, 3206.9886

iPrOCPhHOOH (*anti*-TS-AAAH 2.2-Conformer):

```
C    0.00000000  0.00000000  0.00000000
O   -0.80914600  1.10104000  0.47268000
H    0.21963800  3.41502000  0.49252000
H    0.41803000 -0.38709900  0.93032700
C    1.15434700  0.46379200 -0.88334600
H    1.73046300  1.24466900 -0.38874800
H    0.81280600  0.84964600 -1.84381500
H    1.82032500 -0.37683600 -1.08348800
C   -0.83279500 -1.10368800 -0.64452800
H   -0.20353200 -1.97334500 -0.83897800
H   -1.26150200 -0.78632700 -1.59613400
H   -1.64658700 -1.40912900  0.01151200
C   -3.84336400  1.56050100 -1.55174200
C   -5.20003000  1.26215300 -1.51547900
C   -5.78988100  0.85898900 -0.32262800
C   -5.01874800  0.75618800  0.83047900
C   -3.66170000  1.05170800  0.79244600
C   -3.06691400  1.45337800 -0.40079100
C   -1.59590600  1.81066300 -0.45278800
O   -1.55919000  3.18390600 -0.10130500
O   -0.21541100  3.67811400 -0.33187300
H   -1.20206700  1.69910300 -1.46585000
H   -3.05583000  0.96702800  1.68307200
H   -5.47544600  0.44525100  1.76057000
H   -6.84552300  0.62475200 -0.29190200
H   -5.79476500  1.34368700 -2.41527200
H   -3.38570000  1.88018200 -2.47965300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -614.324329695371

Frequencies (cm^{-1}): 28.1128, 32.1792, 63.4412, 110.9887, 115.846, 181.3467, 207.9234, 221.6357, 256.6628, 261.368, 304.2113, 329.7782, 366.1043, 371.0284, 416.3281, 446.3933, 508.0702, 536.6646, 595.6286, 634.0833, 656.6404, 718.2295, 778.2179, 821.4737, 861.0423, 867.4304, 921.2793, 924.0677, 939.2085, 943.9485, 959.0394, 1001.2831, 1018.6295, 1022.9599, 1028.6317, 1048.3876, 1052.2866, 1106.5266,

1143.493, 1165.9056, 1182.0744, 1197.9899, 1199.522, 1214.8585, 1317.109, 1342.3212, 1356.5069, 1371.2372, 1372.7923, 1396.2568, 1401.9006, 1406.4252, 1424.1898, 1482.6108, 1486.7206, 1490.851, 1499.4044, 1506.221, 1530.3838, 1627.9148, 1644.3569, 3030.5531, 3032.3777, 3040.8082, 3045.8098, 3090.4431, 3099.4589, 3108.4678, 3110.8906, 3159.4166, 3167.2716, 3177.9758, 3189.0129, 3199.0336, 3730.7798

IRC:

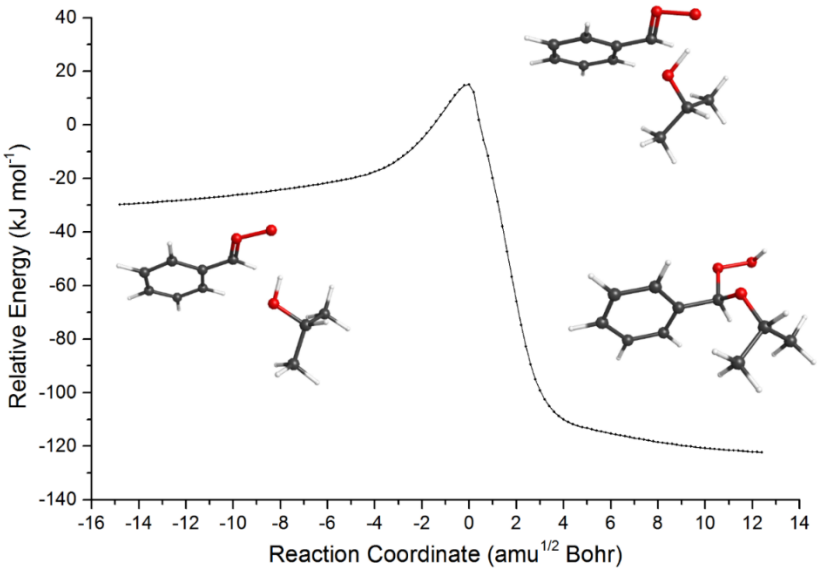


Figure S84: SCI 12 + iPrOH TS-AAAH 2.2 IRC

7.13 sCI 13 + MeOH Reaction

***Syn*-MeC(*t*-CH=CH_2)OO (sCI 13):**

```
C    0.00000000  0.00000000  0.00000000
H    0.60653400  0.89936600  0.00000000
H    0.23124700 -0.62344800  0.86706900
H    0.23124700 -0.62344800 -0.86706900
C   -1.44326700  0.29771700  0.00000000
C   -2.07091500  1.59523100  0.00000000
C   -1.42405900  2.76579200  0.00000000
H   -1.97208100  3.69670800  0.00000000
H   -0.34580200  2.83630200  0.00000000
H   -3.15384800  1.57093300  0.00000000
O   -2.27525800 -0.67626700  0.00000000
O   -1.76950900 -1.94321600  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.969910243799

Frequencies (cm^{-1}): 119.7643, 185.8068, 256.7201, 283.9639, 330.8558, 463.8314, 494.6028, 602.0009, 687.4975, 805.9873, 966.447, 968.5185, 1020.4535, 1025.849, 1041.3674, 1067.0612, 1306.36, 1334.1293, 1398.1885, 1441.7737, 1458.0968, 1487.559, 1488.7139, 1665.4753, 3033.6313, 3071.3689, 3153.2618, 3159.4576, 3169.6656, 3241.5713

SCI 13 to VHP unimolecular TS1:

```
C    0.00000000  0.00000000  0.00000000
H    0.72872500  0.69157600 -0.40019700
H   -1.19088000 -0.46583200 -0.43950400
H   -0.56371100  0.40066700  0.84135200
C    0.39500500 -1.34779200  0.10746600
C    1.70224300 -1.96464000 -0.00513100
C    2.84703000 -1.28514500  0.06894700
H    3.79862400 -1.78526700 -0.04101300
H    2.86631900 -0.21761100  0.23958200
H    1.70092900 -3.03767200 -0.15387000
O   -0.58995600 -2.21843800  0.12414000
O   -1.82160600 -1.54792500  0.00140700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.937553413712

Frequencies (cm^{-1}): -1629.7058 119.4913, 245.2927, 270.3859, 471.7263, 492.4072, 547.0806, 631.0437, 735.5808, 749.3927, 901.3281, 930.4195, 958.0064, 993.4657, 1024.401, 1033.1709, 1064.5046, 1291.0073, 1326.6722, 1345.8919, 1459.4952, 1464.4956, 1532.1167, 1679.6585, 1836.5296, 3085.2701, 3151.4623, 3167.7082, 3189.4244, 3238.6767

H_2C=C(*c*-CH=CH_2)(OOH) - VHP 1:

```
C    0.00000000  0.00000000  0.00000000
H   -0.85383100  0.63518900  0.17131800
H    2.52264900 -1.92356900  0.54860600
H    0.96842700  0.45193700 -0.12786900
C   -0.17318500 -1.31916600 -0.04089100
C   -1.44195500 -2.05030000  0.08635200
C   -2.63000600 -1.59104800 -0.29458300
H   -3.52561300 -2.17583300 -0.13952000
H   -2.74581600 -0.62688600 -0.77102700
H   -1.36093600 -3.04205800  0.51684700
O    0.83263000 -2.25585800 -0.19722300
O    2.12960500 -1.63324300 -0.28696600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.992007486332

Frequencies (cm^{-1}): 80.2441, 114.2806, 132.9152, 242.8281, 348.9691, 412.4713, 495.4987, 587.8711, 726.8709, 742.084, 854.1048, 863.8355, 920.2656, 965.1005, 977.6875, 1023.9459, 1087.7271, 1222.8676, 1330.7684, 1381.7527, 1420.9166, 1462.1516, 1686.5605, 1698.648, 3144.1138, 3152.8045, 3186.8614, 3229.5924, 3278.3523, 3744.2917

IRC:

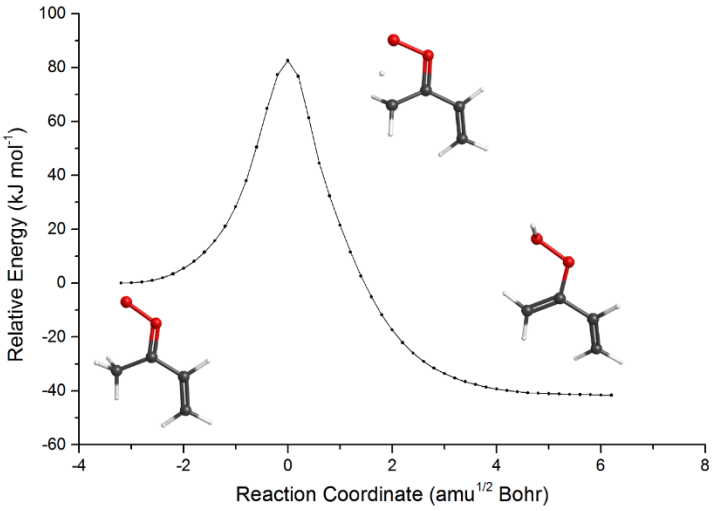


Figure S85: SCI 13 TS-Unimolcular IRC

H_2C=C(*c*-CH=CH_2)(OOH) - VHP 2:

```
C     0.00000000  0.00000000  0.00000000
H    -0.85428700  0.64062100 -0.14670400
H     2.42518000 -1.85078800  1.02794600
H     0.97542600  0.44579000  0.09154500
C    -0.17791800 -1.31894100  0.02268400
C    -1.45187600 -2.04098100 -0.10345600
C    -2.62623800 -1.59855500  0.33557200
H    -3.52859200 -2.17214600  0.17767400
H    -2.72388700 -0.65832700  0.86150500
H    -1.38506900 -3.00901400 -0.58687400
O     0.82505700 -2.26338700  0.14011800
O     2.13193600 -1.65360400  0.12708000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.992160356353

Frequencies (cm^{-1}): 86.2264, 134.3576, 163.3005, 242.8189, 346.5782, 408.4595, 499.0665, 589.1198, 726.6324, 742.5801, 852.748, 864.8869, 920.7074, 963.5385, 976.1163, 1024.0914, 1087.5473, 1223.5221, 1328.5132, 1383.4481, 1422.5958, 1461.8425, 1687.0949, 1698.0508, 3143.9638, 3154.3441, 3187.1961, 3229.045, 3278.2268, 3749.8953

***Syn*-MeC(*t*-CH=CH_2)OO + MeOH PRC (for all TS-AAAH 1, TS-AAAH 2, TS-VHP 1 and TS-VHP 2):**

```
C     0.00000000  0.00000000  0.00000000
H     0.77158500 -0.64997200  0.39846500
H    -0.24928600  0.79373200  0.70658600
H    -0.92547100 -0.56428000 -0.15274800
C     0.40346500  0.61769700 -1.27467700
C     1.56420000  0.28731500 -2.06960300
C     2.44971400 -0.66648200 -1.76787400
H     3.29164000 -0.85947500 -2.41687700
H     2.36621100 -1.28048800 -0.88289600
H     1.67844000  0.87697000 -2.97061100
O    -0.30105600  1.55396700 -1.78579100
O    -1.44208000  1.94483000 -1.11461600
C    -4.21844100 -0.33915100 -1.90259400
H    -4.94136900  0.27440200 -1.35473000
H    -4.59021700 -1.36313700 -1.92879600
H    -4.15812300  0.03104700 -2.93147100
O    -2.95147500 -0.35812800 -1.26979000
H    -2.57614700  0.54534500 -1.24744600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.588462758522

Frequencies (cm^{-1}): 24.914, 43.8241, 74.106, 103.9396, 117.0862, 123.3508, 205.2009, 230.5585, 262.2907, 306.4839, 345.2, 467.619, 491.4524, 597.919, 692.4298, 747.9653, 806.4269, 947.2099, 984.5335, 1014.9514, 1026.9293, 1046.7139, 1063.9554, 1070.3631, 1134.4684, 1173.1152, 1308.8452, 1335.4083, 1397.6581, 1434.3486, 1452.8986, 1464.1728, 1476.3412, 1495.7824, 1497.0855, 1499.7144, 1512.5521, 1670.1598,

2983.3544, 3022.3947, 3024.3394, 3075.7359, 3084.9631, 3153.5714, 3160.2551, 3173.9517, 3243.307, 3466.2752

***Syn*-MeC(*t*-CH=CH$_2$)OO + MeOH TS-AAAH 1:**

```
C     0.00000000  0.00000000  0.00000000
H     0.40087600 -0.58318700  0.82351000
H     0.70909400  0.79266800 -0.25172700
H    -0.94255400  0.44569400  0.29401500
C    -0.18553300 -0.84624400 -1.22061700
C     0.93174700 -1.59787000 -1.80032800
C     2.06576700 -1.87541500 -1.16243600
H     2.84691200 -2.44525700 -1.64575300
H     2.25243600 -1.55640400 -0.14673900
H     0.76752600 -1.94234700 -2.81349300
O    -1.06733800 -0.52496200 -2.13841100
O    -2.33507000 -0.24749600 -1.49756600
C    -1.66924800 -3.32251300 -0.97454900
H    -2.59427600 -3.76669100 -0.59843900
H    -0.84739200 -4.01520100 -0.78991500
H    -1.77807200 -3.16887400 -2.05224700
O    -1.42447600 -2.10285000 -0.29284800
H    -2.11091400 -1.30493400 -0.71335000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.570972218989

Frequencies (cm^{-1}): -838.0855, 82.3248, 119.8115, 139.1957, 160.7477, 186.2663, 233.646, 277.2996, 305.893, 325.164, 386.0633, 467.617, 504.0079, 577.9396, 693.4263, 758.2374, 877.3162, 902.8082, 974.7139, 1002.3577, 1034.994, 1045.6893, 1063.0473, 1083.9352, 1172.8255, 1179.1553, 1296.739, 1327.0241, 1381.7577, 1418.9641, 1453.2442, 1471.0311, 1482.8922, 1490.7498, 1494.7221, 1498.3756, 1513.9929, 1690.6645, 1809.1246, 3000.2796, 3040.3991, 3054.0276, 3080.1928, 3128.1695, 3153.9606, 3173.8376, 3177.8104, 3237.6581

MeOCMe(*t*-CH=CH$_2$)(OOH) (TS-AAAH 1- conformer):

```
C     0.00000000  0.00000000  0.00000000
H    -0.75448400  0.19344200  0.75944000
H    -0.23143100 -0.92995100 -0.51416700
H     0.96386400 -0.09470300  0.49092600
C     0.04527900  1.14679400 -0.99232800
C    -1.23441600  1.37108300 -1.77298600
C    -2.45297300  1.04710100 -1.36739100
H    -3.31523700  1.26136900 -1.98407700
H    -2.64428600  0.56477700 -0.41880600
H    -1.09710600  1.84833500 -2.73610500
O     0.98286800  0.90455500 -2.05914800
O     2.28460300  0.58825400 -1.51802900
C     0.38239900  3.55250100 -0.90871600
H     0.89931400  4.25790300 -0.26223900
H    -0.65317400  3.87578600 -1.03167200
H     0.87188400  3.53384600 -1.88520200
O     0.45915300  2.28789600 -0.25425800
H     2.56883400  1.44651900 -1.16851800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.633661110225

Frequencies (cm^{-1}): 56.9208, 111.9159, 139.3465, 195.2461, 210.7599, 220.4318, 259.2835, 276.3924, 329.0098, 355.6443, 407.4948, 434.0918, 526.0727, 618.3623, 688.717, 741.407, 864.5567, 908.7283, 944.5137, 980.1615, 1017.7787, 1040.1453, 1080.4826, 1125.3106, 1162.3247, 1174.4511, 1202.7467, 1295.8034, 1333.5769, 1389.5831, 1410.7389, 1455.1127, 1468.7757, 1488.3569, 1495.3127, 1496.7093, 1515.634, 1708.565, 3014.2696, 3065.4076, 3070.3183, 3117.3185, 3132.9485, 3144.1662, 3149.4392, 3158.0352, 3224.5471, 3714.8569

IRC:

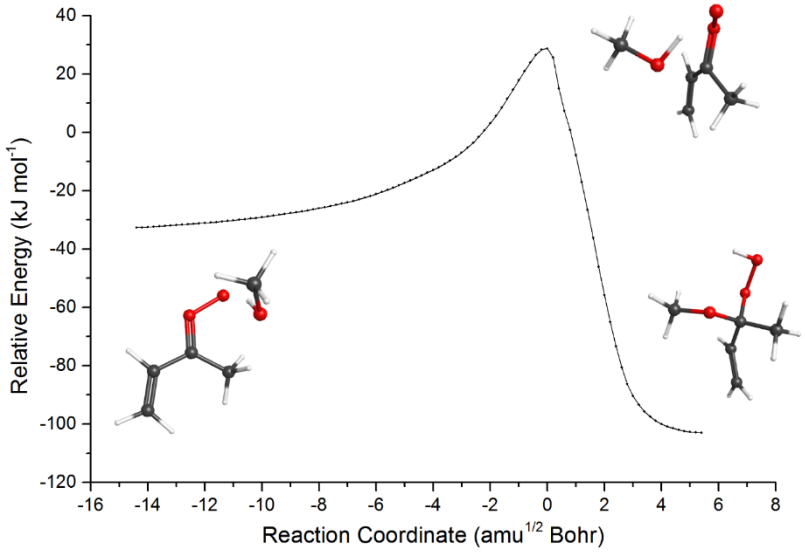


Figure S86: SCI 13 + MeOH TS-AAAH 1.1 IRC

***Syn*-MeC(*t*-CH=CH$_2$)OO + MeOH TS-AAAH 2:**

```
C     0.00000000  0.00000000  0.00000000
H    -0.16497200  1.05777400  0.18519500
H    -0.75156100 -0.56407500  0.55836800
H     0.98526700 -0.29285300  0.34291900
C    -0.16422900 -0.34601600 -1.44551000
C    -1.39580700 -0.02793800 -2.17391900
C    -2.39167400  0.70576700 -1.68513200
H    -3.27035900  0.91179300 -2.27997200
H    -2.37053700  1.12494400 -0.68875000
H    -1.43861700 -0.43082600 -3.17714200
O     0.44750000 -1.38329400 -1.95590000
O     1.85208400 -1.33305400 -1.58505700
C     1.68749600  2.02769300 -1.60345300
H     2.13132900  1.81421600 -0.62615900
H     0.86963300  2.74091000 -1.47141400
H     2.44924700  2.50213700 -2.22887900
O     1.21628900  0.86519000 -2.24936900
H     1.81202600 -0.06644300 -1.98254500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.567236975778

Frequencies (cm^{-1}): -878.1759, 86.6928, 105.3268, 133.7417, 194.7656, 209.9407, 220.5265, 248.0609, 317.923, 331.6233, 378.9442, 445.6834, 485.1212, 569.5076, 681.2661, 750.4826, 851.3126, 891.7664, 969.0745, 999.9452, 1033.2925, 1051.8877, 1067.3595, 1095.344, 1171.4937, 1178.2282, 1293.2963, 1316.317, 1352.8969, 1385.8442, 1425.438, 1453.7857, 1473.896, 1489.1535, 1490.397, 1502.3941, 1503.5969, 1691.3038, 1893.8331, 2989.0053, 3039.3539, 3042.9559, 3050.5362, 3118.3213, 3152.6411, 3174.3437, 3183.2567, 3235.2236

MeOCMe(*t*-CH=CH$_2$)(OOH) (TS-AAAH 2-conformer):

```
C     0.00000000  0.00000000  0.00000000
H    -0.80366300  0.60493300  0.41507100
H    -0.12991200 -1.02692000  0.33516900
H     0.95048400  0.36939600  0.37514100
C     0.00332100  0.03726300 -1.52080500
C    -1.25859200 -0.44957400 -2.19534100
C    -2.39316200 -0.77984200 -1.59600700
H    -3.25436800 -1.08930400 -2.17255900
H    -2.51191400 -0.76128800 -0.52124900
H    -1.17616600 -0.48246300 -3.27532900
O     0.99161900 -0.83161300 -2.06307500
O     2.30206300 -0.45337700 -1.57579800
C    -0.41990700  2.43794900 -1.59494300
H    -0.20449200  2.68786000 -0.55311000
H    -1.49311000  2.26307400 -1.70865900
H    -0.13229500  3.27789300 -2.22339000
```

O 0.34280000 1.32769600 -2.04309800
H 2.47074600 0.34122500 -2.10483600

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632524999776

Frequencies (cm^{-1}): 79.5256, 98.2195, 138.8403, 178.8241, 220.8659, 247.7769, 282.7487, 301.5822, 319.3807, 379.65, 417.6955, 465.9439, 489.4324, 596.5637, 689.2399, 730.4046, 903.5442, 906.5986, 931.9577, 980.6721, 1020.6622, 1038.7509, 1092.0426, 1136.8071, 1157.5549, 1177.4135, 1226.1477, 1274.0586, 1326.4693, 1388.4027, 1407.1824, 1454.7297, 1472.1993, 1490.5159, 1495.6356, 1503.5744, 1513.4362, 1706.3593, 3004.8058, 3056.2553, 3062.3408, 3113.2774, 3126.121, 3142.0169, 3143.2649, 3161.5094, 3222.5935, 3719.0976

IRC:

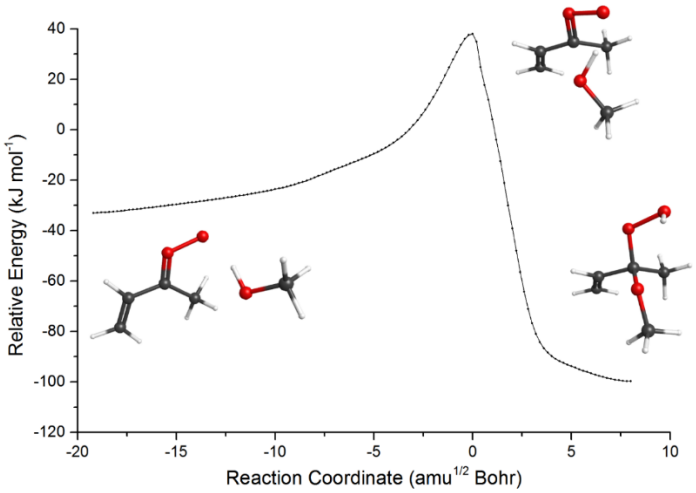


Figure S87: SCI 13 + MeOH TS-AAAH 2 IRC

***Syn*-MeC(*t*-CH=CH$_2$)OO + MeOH TS-VHP 1 (VHP1):**

C 0.00000000 0.00000000 0.00000000
H -0.54424300 -0.91083500 0.20580200
H 0.60054300 0.37334700 0.82662700
H 1.04410000 -0.11146900 -0.82411200
C -0.71582900 1.00181500 -0.67650400
C -2.04228300 0.87577600 -1.27719800
C -2.87321200 -0.14538900 -1.07763300
H -3.84145400 -0.16911200 -1.55697400
H -2.62412800 -0.98014200 -0.43769900
H -2.33170600 1.70315400 -1.91269300
O -0.20529100 2.17408900 -0.95411400
O 1.14192100 2.38884200 -0.53341700
C 3.33330900 -0.04543600 -1.04980700
H 3.40358700 -0.04063400 0.04386100
H 4.10152400 0.62088800 -1.44665100
H 3.53434200 -1.05539100 -1.40985400
O 2.05414100 0.37474900 -1.49760200
H 1.73413300 1.44006300 -1.07873300

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.549899873531

Frequencies (cm^{-1}): -1634.8686, 68.0507, 87.5771, 95.7855, 140.2903, 166.6654, 258.0168, 260.1332, 316.1095, 457.5705, 478.8841, 532.2291, 582.7649, 616.3439, 688.7195, 761.3072, 836.1762, 877.0141, 930.8757, 984.9783, 994.0627, 1028.7721, 1032.5094, 1074.48, 1088.3184, 1167.8315, 1183.5126, 1255.5664, 1306.9047, 1346.0429, 1391.34, 1441.4275, 1463.8079, 1493.9245, 1497.4344, 1501.9077, 1542.318, 1591.6989, 1686.1366, 1828.0609, 2987.7906, 3050.962, 3077.7176, 3094.6395, 3153.8027, 3173.819, 3199.2818, 3238.4141

$H_2C=C(t\text{-}CH=CH_2)(OOH)$ - VHP + MeOH complex 1 (VHP):

```
C     0.00000000  0.00000000  0.00000000
H    -0.50878300 -0.87526900  0.37037300
H     0.78956300  0.43503200  0.58944500
H     2.22467300 -0.63307200 -1.38665900
C    -0.40853000  0.55726500 -1.14433000
C    -1.52582600  0.10575000 -1.98853000
C    -2.61342800 -0.52006600 -1.54973800
H    -3.38412400 -0.83840200 -2.23745600
H    -2.77278400 -0.72787700 -0.50020100
H    -1.42511400  0.33973800 -3.04206400
O     0.17000000  1.64096500 -1.75723100
O     1.31275700  2.13798900 -1.04021100
C     4.19362100 -0.47006000 -1.46921400
H     4.36759900 -0.46697600 -0.39054300
H     4.87651200  0.23449400 -1.93766500
H     4.39285400 -1.46791700 -1.86525700
O     2.87013200 -0.04124700 -1.79239500
H     2.01430000  1.52992200 -1.36484500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.611709363723

Frequencies (cm^{-1}): 30.685, 32.1805, 70.6627, 76.0347, 88.0809, 119.7024, 144.4472, 234.335, 252.2253, 352.241, 397.8241, 425.5133, 502.4937, 588.9703, 661.8447, 741.8125, 750.0697, 842.7742, 862.0401, 927.5671, 966.8998, 988.5971, 1027.1848, 1040.7824, 1085.6352, 1090.1684, 1174.4769, 1235.8711, 1330.5595, 1369.4965, 1415.9843, 1461.1563, 1477.7971, 1499.071, 1510.3135, 1522.6267, 1671.3104, 1695.8337, 3012.6088, 3066.7565, 3121.4067, 3144.2163, 3156.9426, 3180.4491, 3228.651, 3271.4722, 3449.9287, 3755.0838

IRC:

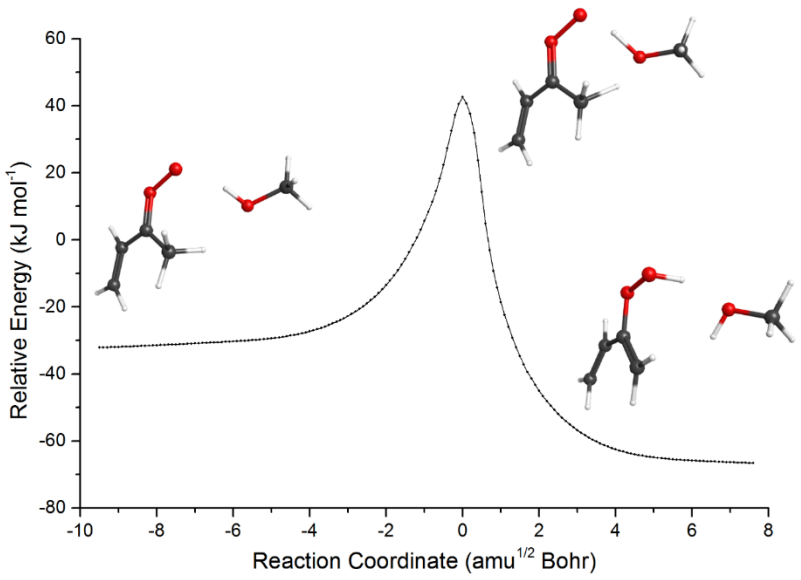


Figure S88: SCI 13 + MeOH TS-VHP 1 IRC

***Syn*-MeC(t-$CH=CH_2$)OO + MeOH TS-VHP 2:**

```
C     0.00000000  0.00000000  0.00000000
H    -0.64695100 -0.70842100  0.49743600
H     0.46698600  0.73436500  0.65259800
H     1.17844300 -0.46017800 -0.41275800
C    -0.48166700  0.53255500 -1.20706800
C    -1.67067200  0.10261100 -1.94177200
C    -2.60757900 -0.71320900 -1.46240900
H    -3.46292500 -0.98366800 -2.06499000
H    -2.55954400 -1.13134800 -0.46679200
H    -1.76158900  0.51698100 -2.93799400
O     0.17324800  1.43149200 -1.89655100
O     1.41329600  1.87369400 -1.34096000
C     2.67822900 -1.13730300 -2.02725400
H     3.26203700 -0.58818200 -2.76824500
H     1.76970400 -1.51013000 -2.51504300
H     3.26409000 -1.99176300 -1.68553000
```

```
O     2.37223600 -0.29495900 -0.92720800
H     2.03431300  0.80018800 -1.21051800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.558377802918

Frequencies (cm^{-1}): -1615.2657, 56.6032, 67.588, 91.4814, 161.698, 165.3355, 250.5688, 272.3635, 320.1989, 458.8972, 477.0006, 530.1071, 575.9207, 605.1692, 725.0645, 755.5042, 845.8735, 877.4075, 926.4459, 982.7216, 993.2076, 1026.991, 1032.0218, 1075.2299, 1093.2772, 1166.0113, 1178.9865, 1306.2134, 1343.18, 1344.6243, 1421.147, 1456.2303, 1465.604, 1490.4214, 1500.6239, 1518.2087, 1550.5315, 1562.3995, 1685.8511, 1711.0285, 2981.8636, 3048.6502, 3078.3995, 3096.1852, 3152.8376, 3172.243, 3202.5882, 3237.536

H_2C=C(*t*-CH=CH_2)(OOH) - VHP + MeOH complex 2:

```
C     0.00000000  0.00000000  0.00000000
H    -0.73838200  0.40981800  0.66994100
H     0.77962200 -0.62276600  0.40517400
H     2.51783000  1.35051400 -0.40046700
C    -0.12962100  0.20066600 -1.31390200
C    -1.17900400  0.98531300 -1.98260200
C    -1.82264300  2.02255100 -1.45575100
H    -2.60355400  2.52761600 -2.00641100
H    -1.59622200  2.39816500 -0.46669400
H    -1.40869300  0.66478400 -2.99231300
O     0.69678300 -0.31019500 -2.28651700
O     1.70728000 -1.18037100 -1.74952900
C     3.87271700  1.90658500 -1.72572700
H     4.68147900  1.39498100 -2.24139200
H     3.17129400  2.29736800 -2.46551300
H     4.29079400  2.73149400 -1.14570000
O     3.25171800  0.94036700 -0.87220600
H     2.40359700 -0.52606500 -1.51225100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.612602736691

Frequencies (cm^{-1}): 22.2291, 33.5023, 68.5741, 73.6105, 87.7532, 114.8705, 159.8132, 233.4556, 247.5103, 351.506, 418.3882, 427.0611, 506.2616, 586.6772, 712.1176, 745.0963, 754.1749, 842.9497, 864.8917, 927.5201, 962.9135, 988.1507, 1028.1188, 1034.8061, 1085.4246, 1088.7949, 1175.601, 1233.2169, 1329.2888, 1368.341, 1417.3535, 1461.6545, 1477.6041, 1499.1267, 1507.8784, 1512.1078, 1675.361, 1695.9423, 3018.0917, 3074.7407, 3124.6733, 3142.9642, 3156.1579, 3182.4234, 3226.9053, 3272.5457, 3428.8634, 3779.1881

IRC:

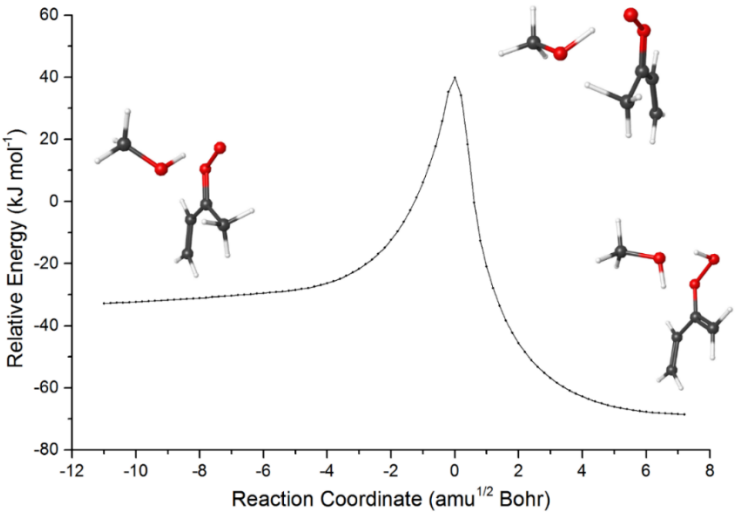


Figure S89: SCI 13 + MeOH TS-VHP 2 IRC

7.14 sCI 14 + MeOH Reaction

***Syn*-MeC(*c*-CH=CH_2)OO (SCI 14):**

```
C    0.00000000  0.00000000  0.00000000
H   -0.65656800  0.86538300  0.00000000
H    0.66703400  0.01468500  0.86609000
H    0.66703400  0.01468500 -0.86609000
C   -0.76366200 -1.26164800  0.00000000
C   -2.21238000 -1.32966300  0.00000000
C   -2.93582500 -2.45436600  0.00000000
H   -4.01533100 -2.41395600  0.00000000
H   -2.47265600 -3.43104900  0.00000000
H   -2.71126400 -0.36934400  0.00000000
O   -0.13119200 -2.36895700  0.00000000
O    1.23925400 -2.31735600  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.967057604002

Frequencies (cm^{-1}): 64.6788, 188.1578, 230.284, 267.6988, 325.5866, 449.0756, 484.1063, 612.6529, 669.4367, 808.0538, 953.3993, 990.6644, 1017.0077, 1031.8031, 1039.9662, 1107.4188, 1271.452, 1337.9377, 1397.7383, 1435.9307, 1440.1373, 1486.4882, 1494.0649, 1669.2668, 3025.8716, 3063.2155, 3140.5739, 3155.952, 3174.9356, 3245.2631

SCI 14 to VHP unimolecular TS:

```
C    0.00000000  0.00000000  0.00000000
H    0.32384300  0.97576500 -0.33793300
H   -0.82908600 -0.93314500 -0.48321100
H   -0.68534500  0.04323000  0.84572500
C    0.98859800 -1.00290000  0.05144500
C    2.42692500 -0.83424300 -0.06503200
C    3.31632600 -1.82623400  0.00292400
H    4.37572700 -1.62401400 -0.06169100
H    3.01279800 -2.85531800  0.13497100
H    2.75406500  0.19122100 -0.17567700
O    0.53774100 -2.23243500  0.02466200
O   -0.87062000 -2.21886900 -0.07753100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.935253863909

Frequencies (cm^{-1}): -1628.226, 90.2796, 231.2886, 260.4043, 477.3769, 494.1872, 538.0655, 643.1219, 724.3849, 741.5753, 902.608, 935.4915, 950.6345, 998.8477, 1021.4763, 1030.1866, 1085.3014, 1306.371, 1333.8692, 1358.0715, 1424.7791, 1476.8264, 1521.2911, 1680.4999, 1835.5185, 3082.2197, 3154.781, 3176.6498, 3182.7018, 3243.2943

H_2C=C(*c*-CH=CH_2)(OOH) - VHP

```
C    0.00000000  0.00000000  0.00000000
H   -0.53692200  0.93510400  0.01669100
H    1.50921200 -2.72552200  0.78148500
H    1.07537300  0.01882500 -0.03194600
C   -0.69671000 -1.13849300  0.00267900
C   -2.15703800 -1.19500500  0.02234100
C   -2.90335400 -2.29809000 -0.00449300
H   -3.98184300 -2.23179000  0.01197800
H   -2.46825700 -3.28596500 -0.04750300
H   -2.62995300 -0.22170700  0.06078500
O   -0.15610100 -2.40472800 -0.01856900
O    1.28290700 -2.36356300 -0.08722900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.995375835987

Frequencies (cm^{-1}): 101.764, 160.5583, 170.6639, 229.5668, 357.2057, 453.6878, 488.9104, 579.4645, 722.8322, 765.4586, 850.7152, 863.4612, 927.2554, 959.7883, 982.8157, 1017.0383, 1068.1228, 1306.7119, 1325.68, 1384.9565, 1417.6446, 1461.171, 1649.8771, 1707.8176, 3153.539, 3167.1987, 3184.3845, 3239.2849, 3279.7056, 3746.1208

IRC:

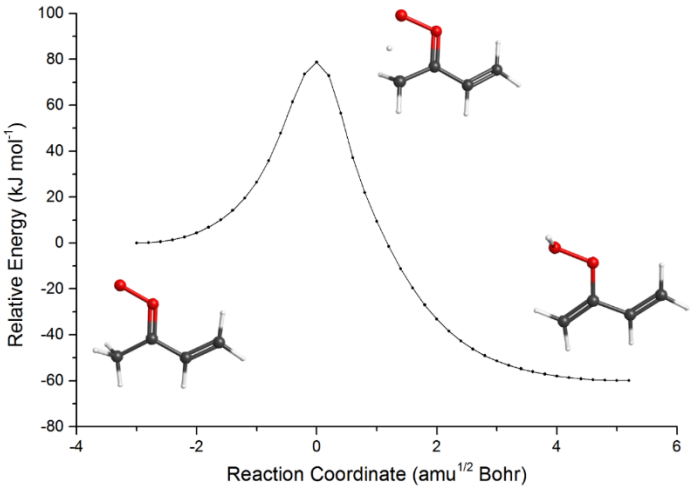


Figure S90: SCI 14 unimolecular IRC

Syn-MeC(_c_-CH=CH$_2$)OO + MeOH PRC (for all TS-AAAH 1, TS-AAAH 2, TS-VHP 1 and TS-VHP 2)

```
C     0.00000000  0.00000000  0.00000000
H    -0.63043500  0.55229300 -0.69094500
H     0.21939400  0.58258800  0.89706900
H     0.97164500 -0.20775600 -0.46116500
C    -0.63016800 -1.27217500  0.39488800
C    -1.82940500 -1.79417800 -0.23944200
C    -2.38533400 -2.97888400  0.02943500
H    -3.27907800 -3.29737800 -0.48731200
H    -1.96442600 -3.65355100  0.76164300
H    -2.26702100 -1.14628200 -0.98707400
O    -0.13532500 -1.97473800  1.33367800
O     1.02307100 -1.51479200  1.94368100
C     3.93895400 -2.44649900 -0.08323000
H     4.63934600 -2.06821200  0.66894000
H     3.70417500 -3.48937500  0.15518100
H     4.43391500 -2.42091900 -1.05375200
O     2.77378400 -1.64689800 -0.17320900
H     2.29100800 -1.66198200  0.67879000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.585780875033

Frequencies (cm^{-1}): 25.9935, 40.097, 66.6378, 82.303, 108.123, 121.3715, 189.0287, 224.8479, 240.6832, 300.4706, 335.4735, 451.686, 486.0516, 604.6741, 672.3277, 755.6733, 807.2872, 936.1391, 1005.5351, 1018.4947, 1031.7417, 1047.1829, 1065.6939, 1106.6266, 1134.9164, 1173.1949, 1270.8371, 1339.3716, 1396.222, 1433.4535, 1443.5191, 1456.209, 1476.2984, 1491.4679, 1495.8877, 1506.9566, 1512.6092, 1673.9701, 2982.2018, 3013.097, 3022.8591, 3067.9145, 3084.2128, 3141.8004, 3155.7394, 3180.3412, 3245.5066, 3448.6792

Syn-MeC(_c_-CH=CH$_2$)OO + MeOH TS-AAAH 1

```
C     0.00000000  0.00000000  0.00000000
H    -0.08567400  0.33738400  1.02937100
H    -0.61133500 -0.89980400 -0.12270900
H     1.03081500 -0.23637600 -0.23285400
C    -0.54601000  1.03108500 -0.93564100
C    -1.89858100  1.54071900 -0.68957800
C    -2.60608200  2.22540800 -1.58629200
H    -3.60591000  2.56812300 -1.35945100
H    -2.21116000  2.44676400 -2.56765200
H    -2.30638100  1.32563300  0.28939700
O    -0.16348100  1.09008600 -2.18442500
O     1.28767700  1.06615400 -2.23548900
C     0.50227700  3.75706100 -0.71320200
H     1.43708000  4.28905900 -0.91047200
H    -0.10447500  3.79777700 -1.62428700
H    -0.03213900  4.26300900  0.09110900
O     0.78413000  2.42529800 -0.32757000
H     1.29221100  1.90014400 -1.18820500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.571059388384

Frequencies (cm^{-1}): -762.6231, 94.3394, 111.4285, 135.371, 164.0864, 173.6587, 231.18, 257.1679, 297.1862, 318.2439, 371.2623, 463.5919, 525.6063, 577.2888, 687.9993, 771.1838, 883.2133, 900.9161, 992.012, 1020.8168, 1026.7641, 1045.5076, 1072.7752, 1085.578, 1169.3362, 1183.5844, 1257.2503, 1335.7798, 1398.0239, 1407.8636, 1458.0064, 1469.159, 1476.0179, 1483.1201, 1490.5975, 1498.0564, 1510.2891, 1683.2331, 1802.5348, 2991.3381, 3024.9968, 3041.235, 3082.0339, 3118.27, 3153.1689, 3176.0949, 3181.0771, 3242.733

MeOC(*c*-CH=CH_2)H(OOH) (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
H    -0.30401500 -0.97772300  0.36686200
H     0.67009900  0.44027300  0.74531500
H    -0.85973100  0.64673700 -0.12719200
C     0.78135000 -0.11532300 -1.26842800
C     1.95051200 -0.99991500 -1.29068800
C     2.74828000 -1.11888100 -2.34903900
H     3.60625600 -1.77615900 -2.32825500
H     2.55649000 -0.56920700 -3.25949900
H     2.12901600 -1.57552100 -0.39146100
O     0.85339600  0.88428300 -2.10761400
O    -0.49000500  1.36746700 -2.38462400
C    -1.71923800 -1.71085600 -1.92509700
H    -2.29591200 -1.12516500 -1.20162300
H    -1.38891700 -2.63533600 -1.44493100
H    -2.38672800 -1.97815300 -2.75012800
O    -0.60865000 -1.00586000 -2.43314500
H    -0.82141800  0.11302000 -2.56389700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.635419398320

Frequencies (cm^{-1}): 81.657, 110.3725, 125.0487, 185.985, 197.0091, 232.7882, 247.1338, 273.9468, 321.5356, 328.1503, 405.3083, 500.7246, 534.9049, 576.9805, 701.7157, 747.0446, 871.1225, 909.6908, 951.0847, 986.1873, 1039.6729, 1044.5839, 1068.9901, 1141.4393, 1170.0906, 1175.5633, 1210.3978, 1256.2557, 1327.6259, 1390.209, 1407.049, 1452.659, 1468.9253, 1484.4389, 1489.8696, 1491.8352, 1513.4507, 1705.0449, 3017.5461, 3059.4797, 3072.3645, 3118.9612, 3128.2766, 3141.2926, 3144.7314, 3153.0388, 3232.2146, 3722.603

IRC:

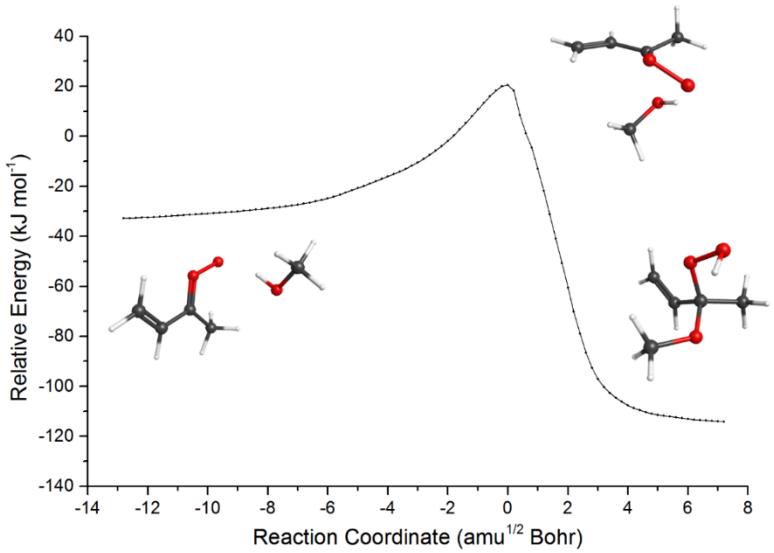


Figure S91: SCI 14 + MeOH TS-AAAH 1 IRC

***Syn*-MeC(*c*-CH=CH_2)OO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
H    -0.30401500 -0.97772300  0.36686200
H     0.67009900  0.44027300  0.74531500
H    -0.85973100  0.64673700 -0.12719200
C     0.78135000 -0.11532300 -1.26842800
C     1.95051200 -0.99991500 -1.29068800
C     2.74828000 -1.11888100 -2.34903900
```

```
H     3.60625600 -1.77615900 -2.32825500
H     2.55649000 -0.56920700 -3.25949900
H     2.12901600 -1.57552100 -0.39146100
O     0.85339600  0.88428300 -2.10761400
O    -0.49000500  1.36746700 -2.38462400
C    -1.71923800 -1.71085600 -1.92509700
H    -2.29591200 -1.12516500 -1.20162300
H    -2.38672800 -1.97815300 -2.75012800
H    -1.38891700 -2.63533600 -1.44493100
O    -0.60865000 -1.00586000 -2.43314500
H    -0.82141800  0.11302000 -2.56389700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.566246150992

Frequencies (cm^{-1}): -898.3541, 74.5053, 103.3983, 137.5303, 201.2293, 205.8703, 218.6866, 234.714, 314.8478, 323.9003, 363.7779, 445.3953, 508.1475, 571.9768, 671.6805, 743.3339, 841.2701, 898.3365, 983.7051, 1013.518, 1023.8133, 1046.5598, 1076.3158, 1097.4689, 1173.0128, 1178.6814, 1250.8728, 1332.4982, 1353.2111, 1394.8753, 1409.4878, 1458.5247, 1474.108, 1481.1093, 1489.5049, 1501.4704, 1503.2889, 1685.5511, 1890.1319, 2985.835, 3024.9454, 3035.0071, 3051.1307, 3106.1174, 3153.16, 3171.2289, 3176.524, 3244.6251

MeOC(*c*-CH=CH_2)H(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
H    -0.23878400 -0.96870700  0.43598700
H     0.86307700  0.40326000  0.52537600
H    -0.84292400  0.67407000  0.13286700
C     0.35631100 -0.13900300 -1.47966300
C     1.45511900 -1.15637500 -1.70036100
C     2.74996000 -0.89408900 -1.79755300
H     3.46443400 -1.69082100 -1.95455000
H     3.13627700  0.11329700 -1.73553100
H     1.10129700 -2.17808200 -1.77379400
O     0.86220500  1.07055800 -2.01696800
O    -0.08434500  2.13988100 -1.78842500
C    -1.67306400 -1.45451100 -1.85349500
H    -2.38173300 -1.60839700 -2.66434400
H    -2.22105700 -1.14676800 -0.95980900
H    -1.16967700 -2.40472300 -1.65092000
O    -0.77370700 -0.45461700 -2.30095400
H    -0.71864300  1.97315300 -2.50188100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.629373607742

Frequencies (cm^{-1}): 62.4547, 96.3015, 137.8425, 181.8014, 215.1059, 256.2054, 270.9022, 306.5842, 320.146, 350.1977, 394.2195, 469.6928, 554.8301, 571.5477, 680.7822, 732.8314, 895.0389, 910.8189, 945.1561, 980.9584, 1019.9358, 1051.5744, 1096.2965, 1126.5581, 1172.3789, 1175.5412, 1220.3038, 1246.8125, 1334.5329, 1389.2931, 1404.5764, 1453.9796, 1472.7258, 1489.1113, 1493.2222, 1501.0153, 1511.4571, 1702.9464, 2999.8366, 3050.7535, 3056.6972, 3111.9751, 3122.9352, 3136.4397, 3143.3837, 3157.2944, 3230.5976, 3723.1488

IRC:

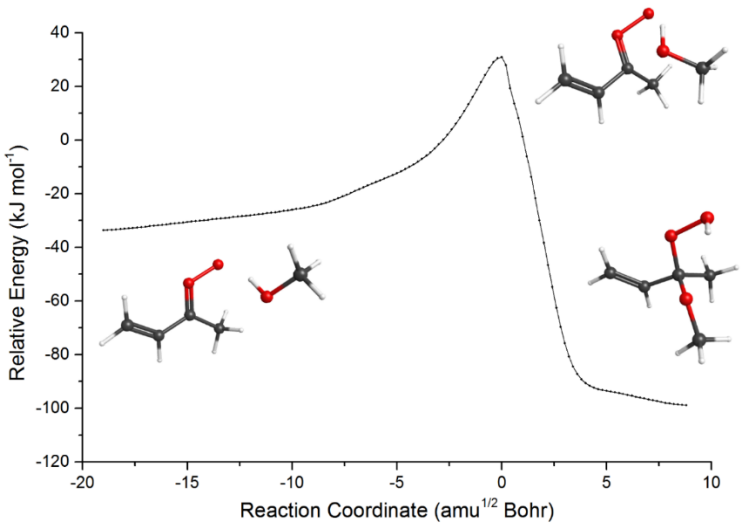


Figure S92: SCI 14 + MeOH TS-AAAH 2 IRC

***Syn*-MeC(*c*-CH=CH$_2$)OO + MeOH TS-VHP 1**

```
C     0.00000000  0.00000000  0.00000000
H     0.33715700 -1.01788200  0.14267400
H    -0.59680000  0.41023700  0.81174000
H    -0.95004100  0.18884000 -0.90284800
C     0.96990600  0.88372900 -0.50875100
C     2.26578700  0.42797900 -1.01129300
C     3.17154500  1.21030600 -1.59763100
H     4.11890100  0.80686700 -1.92575700
H     2.99315100  2.26365900 -1.76076600
H     2.46448000 -0.62453300 -0.85993300
O     0.75652700  2.15831500 -0.66996100
O    -0.55574300  2.62068900 -0.32802900
C    -3.14990500  0.79734700 -1.29274400
H    -3.32344800  0.71012500 -0.21427700
H    -3.71512700  1.65431400 -1.66400000
H    -3.52541700 -0.10173400 -1.78294500
O    -1.77272700  0.96237300 -1.59313600
H    -1.28452600  1.87425000 -1.03534600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.557300897980

Frequencies (cm^{-1}): -1602.7111, 49.5885, 83.6213, 100.5116, 141.7317, 171.9759, 237.3119, 242.6121, 320.5887, 443.7523, 488.5181, 537.7165, 587.1606, 596.6279, 698.4438, 753.1362, 848.4853, 882.8684, 926.8135, 993.9504, 1008.2994, 1020.7215, 1036.3844, 1082.7178, 1095.8461, 1167.4794, 1184.6738, 1274.2774, 1318.5833, 1348.9786, 1388.0086, 1445.2364, 1453.0724, 1494.2981, 1497.2332, 1501.3138, 1531.1002, 1584.7406, 1685.5179, 1827.8885, 2988.7661, 3051.7831, 3079.3684, 3091.0211, 3154.8757, 3179.2332, 3194.2014, 3243.9785

H$_2$C=C(*c*-CH=CH$_2$)(OOH) - VHP + MeOH complex 1

```
C     0.00000000  0.00000000  0.00000000
H     0.92119000 -0.32571100 -0.45667900
H    -0.76335000 -0.72727800  0.21430900
H    -4.78299800  1.22643800 -1.02613600
C    -0.14813000  1.29528800  0.29491100
C     0.88320100  2.29821700  0.03150100
C     0.81139600  3.59674000  0.32065000
H     1.63235300  4.25913500  0.08513300
H    -0.05553000  4.03020500  0.79781800
H     1.77031800  1.89832200 -0.44370500
O    -1.25145000  1.85880200  0.87831100
O    -2.25341800  0.86809200  1.17960800
C    -5.53262900  2.44453000  0.33911800
H    -6.30761300  1.76980100  0.70840900
H    -5.10624400  2.98531700  1.17995400
H    -5.97182300  3.16181100 -0.35669800
O    -4.45776500  1.72476400 -0.27175000
H    -2.99814500  1.19244500  0.62959600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.613684616254

Frequencies (cm^{-1}): 13.3947, 15.4245, 45.7618, 49.4964, 70.9393, 123.7863, 156.9076, 212.119, 236.085, 298.4475, 362.1725, 458.2737, 490.3456, 581.0752, 690.3511, 723.8121, 765.5693, 851.7094, 853.7473, 931.7413, 952.8346, 994.4595, 1018.6134, 1036.1868, 1071.7446, 1081.1932, 1173.8751, 1315.7346, 1325.233, 1365.8721, 1408.6303, 1457.3626, 1478.2338, 1487.2049, 1499.2871, 1509.9275, 1646.797, 1704.9043, 3017.9168, 3074.2478, 3128.9953, 3150.9467, 3165.5203, 3182.8563, 3236.811, 3279.4547, 3494.8753, 3832.5085

IRC:

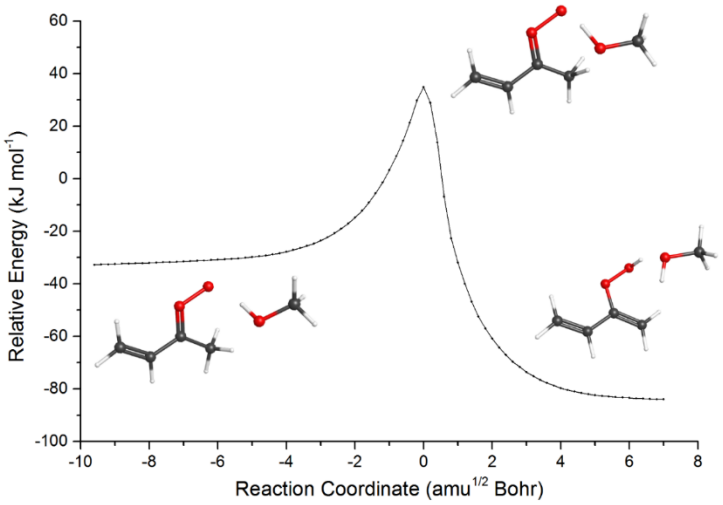


Figure S93: SCI 14 + MeOH TS-VHP 1 IRC

***Syn*-MeC(*c*-CH=CH$_2$)OO + MeOH TS-VHP 2:**

```
C     0.00000000  0.00000000  0.00000000
H     0.40223000 -0.50296400  0.86899100
H    -0.45939100  0.96689600  0.19374200
H    -1.11918500 -0.48185800 -0.50558000
C     0.81519200 -0.03905500 -1.14665700
C     2.01666000 -0.87026000 -1.23151700
C     2.80061600 -0.96872700 -2.30482000
H     3.68842300 -1.58459600 -2.28439300
H     2.58186100 -0.43740700 -3.22021700
H     2.25941900 -1.40585600 -0.32342500
O     0.51235400  0.57307500 -2.25507300
O    -0.71602800  1.31342900 -2.24803600
C    -2.34204600 -1.59622000 -2.13009100
H    -2.63589100 -1.32996000 -3.14709000
H    -1.43436600 -2.20882700 -2.18537400
H    -3.13744100 -2.19287300 -1.68168400
O    -2.13358800 -0.42233600 -1.36065700
H    -1.54977600  0.42654100 -1.90943800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.558062406780

Frequencies (cm^{-1}): -1577.1953, 47.6944, 65.8731, 92.2209, 152.1083, 177.4978, 229.039, 261.0744, 327.6184, 436.7896, 498.1808, 530.2031, 575.6606, 589.8064, 730.2677, 756.6244, 850.6865, 894.9551, 922.378, 996.4375, 1007.0399, 1021.219, 1037.7896, 1087.7138, 1097.0465, 1166.9206, 1180.0021, 1318.3827, 1339.6558, 1348.4177, 1433.8995, 1448.6514, 1464.1427, 1490.9835, 1500.9949, 1525.8548, 1539.7722, 1556.5627, 1684.9242, 1705.1507, 2982.7288, 3049.4906, 3079.929, 3093.2191, 3154.2402, 3178.0754, 3196.0141, 3243.2429

H$_2$C=C(*c*-CH=CH$_2$)(OOH) - VHP + MeOH complex 2:

```
C     0.00000000  0.00000000  0.00000000
H     0.55051700 -0.09839900 -0.92228300
H    -0.73833400 -0.74342100  0.24766400
H    -2.56335800  1.40699500 -0.09992100
C     0.30705600  1.00545900  0.82929800
C     1.34800400  1.99229500  0.53862100
C     1.71889100  2.99539300  1.33270900
H     2.50721100  3.67134500  1.03311700
H     1.25808200  3.16421900  2.29518700
H     1.83739800  1.84749200 -0.41650000
O    -0.29650500  1.25721600  2.03188700
O    -1.29746700  0.27735300  2.35829500
C    -3.74192200  2.69739600  0.82099800
H    -4.40533300  2.63629700  1.68002200
H    -2.97993700  3.45510000  1.01374800
H    -4.32669900  2.98058100 -0.05615000
O    -3.16177100  1.39956900  0.65567600
H    -2.07931600  0.65523400  1.89368000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.616065976839

Frequencies (cm^{-1}): 23.8603, 29.6498, 64.7814, 74.6211, 113.7738, 143.9865, 167.2001, 230.8387, 239.2258, 360.2382, 424.1967, 466.1218, 492.5669, 582.3303, 713.0787, 753.7369, 769.9689, 848.0198, 858.2879, 932.7486, 964.2295, 992.2776, 1021.6196, 1034.1074, 1070.4965, 1086.8463, 1175.3282, 1314.5442, 1325.5585, 1367.1996, 1411.3042, 1459.8499, 1477.9476, 1499.4089, 1508.7945, 1515.7722, 1641.6536, 1701.7583, 3018.6841, 3075.532, 3124.9865, 3151.881, 3165.8989, 3180.0372, 3238.3532, 3273.9493, 3422.8054, 3781.3958

IRC:

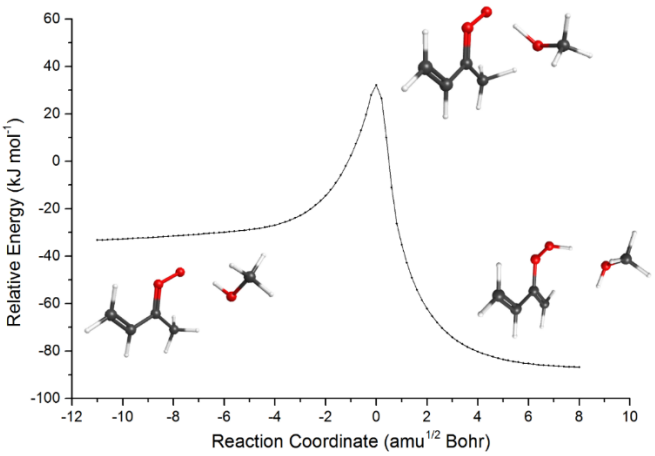


Figure S94: SCI 14 + MeOH TS-VHP 1 IRC

7.15 sCI 15 + MeOH Reaction

***Anti*-(*t*-C(CH$_3$)=CH$_2$)CHOO (SCI 15)**

```
C     0.00000000  0.00000000  0.00000000
C     0.59220500  1.38075500  0.00000000
C     1.91393300  1.62574300  0.00000000
H     2.63563500  0.82124800  0.00000000
H     2.30072000  2.63586200  0.00000000
C    -0.28985200  2.51456500  0.00000000
O    -1.54315500  2.33564300  0.00000000
O    -2.35024000  3.43693900  0.00000000
H     0.06045600  3.54171500  0.00000000
H     0.78440100 -0.75351200  0.00000000
H    -0.63248400 -0.15163100  0.87551500
H    -0.63248400 -0.15163100 -0.87551500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.958885284109

Frequencies (cm^{-1}): 155.2813, 187.2072, 188.4389, 226.6659, 367.8802, 477.4361, 509.4692, 570.4814, 695.1502, 864.4938, 948.8668, 965.3987, 969.3094, 1003.4737, 1055.2301, 1074.9328, 1303.285, 1388.4304, 1425.1941, 1441.6851, 1480.6759, 1488.9247, 1520.7186, 1655.4332, 3041.0636, 3091.9236, 3123.1928, 3147.4833, 3158.3346, 3234.4692

***Anti*-(*t*-C(CH$_3$)=CH$_2$)CHOO + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C    -1.35162900  0.49249800  0.00088700
C    -2.49079600 -0.48607800  0.00252500
H    -2.44639200 -1.13586300 -0.87228400
H    -2.44543500 -1.13400300  0.87867500
H    -3.44497100  0.03599600  0.00251000
C    -1.50691300  1.82709500  0.00021300
H    -0.65450900  2.49277500 -0.00091900
H    -2.48879600  2.27922800  0.00079700
O     0.19352100 -1.25056200  0.00062500
O     1.49007900 -1.72512500 -0.00025700
H     2.67493700 -0.34330300 -0.00172100
O     3.01541100  0.57528000 -0.00219600
C     4.43240900  0.58138800  0.00356800
H     4.84636800  0.09191200 -0.88385200
H     4.75941400  1.62061100  0.00511900
H     4.83916600  0.09150300  0.89407600
H     0.86593200  0.65668100 -0.00108400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.580667868380

Frequencies (cm^{-1}): 13.7718, 32.8242, 65.5845, 105.8112, 127.8443, 153.1073, 169.4963, 185.9234, 230.9519, 256.9799, 377.2546, 485.5563, 507.4052, 566.3871, 695.8895, 710.8898, 869.2492, 943.1853, 971.1185, 1004.1541, 1006.9222, 1057.3961, 1065.058, 1075.696, 1144.918, 1172.7052, 1337.8585, 1395.9096, 1427.3893, 1444.4607, 1461.7614, 1478.5324, 1480.5519, 1491.9574, 1496.805, 1513.7634, 1537.57, 1659.6236, 2987.0935, 3029.6623, 3041.741, 3088.1565, 3092.1515, 3124.58, 3137.2814, 3148.1036, 3235.7438, 3454.3726

***Anti*-(*t*-C(CH$_3$)=CH$_2$)CHOO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C    -1.33437000 -0.45464500  0.38772200
C    -1.75805700 -0.30822200  1.82089600
H    -1.10236300 -0.87389900  2.48379200
H    -1.70160200  0.73348900  2.13836500
H    -2.77859700 -0.66045000  1.95640600
C    -2.10329500 -0.97526300 -0.57286700
H    -1.75068900 -1.06161300 -1.59176600
H    -3.10058600 -1.33760300 -0.36364900
O     0.64246800  0.75021700  0.83802200
O     2.02074300  0.79780100  0.38655100
H     1.94032100 -0.51470600  0.11402000
O     1.33331000 -1.45395200 -0.03486400
C     1.41394900 -2.26393800  1.12778100
H     0.57995600 -2.96714700  1.13998500
H     2.34778600 -2.83107900  1.10781800
H     1.39776500 -1.66328300  2.04160400
H     0.24372400  0.09684300 -1.05044200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.569817374310

Frequencies (cm^{-1}): -782.7188, 64.6823, 107.805, 138.2962, 151.0821, 166.321, 195.8023, 233.4385, 314.512, 373.8594, 410.0961, 514.3656, 549.8572, 612.6302, 733.6879, 818.4809, 878.9537, 900.3145, 981.7368,

998.8161, 1033.2379, 1055.172, 1075.5699, 1149.5106, 1179.4536, 1180.0271, 1312.4359, 1352.7054, 1420.031, 1428.35, 1463.5662, 1476.191, 1476.7664, 1481.5667, 1494.5056, 1503.5476, 1507.8628, 1687.5762, 1831.4698, 3001.619, 3040.8477, 3056.7737, 3077.0958, 3091.5759, 3119.8549, 3144.5931, 3161.6639, 3229.6544

MeOCH(*t*-C(CH_3)=CH_2)(OOH) (TS-AAAH 1 - conformer)

```
C     0.00000000  0.00000000  0.00000000
C     1.46622600 -0.15417700  0.37776000
C     1.82638300 -0.57489400  1.77542400
H     1.42017600  0.10612700  2.52485800
H     1.41837700 -1.56103500  2.00025700
H     2.90832500 -0.61043200  1.89316200
C     2.37694700  0.08155400 -0.56126800
H     2.09696600  0.36084600 -1.56862200
H     3.43554500  0.00817800 -0.34937100
O    -0.74136900 -0.83322400  0.87410600
O    -2.07891300 -0.95835000  0.34043600
H    -2.42265900 -0.05828500  0.45414300
O    -0.50022800  1.32328800  0.02717200
C    -0.22046500  2.09862800  1.19055500
H     0.84642100  2.31627600  1.27412000
H    -0.76350200  3.03279600  1.06938000
H    -0.56360100  1.60059800  2.10019600
H    -0.17288900 -0.32408300 -1.02525900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632395945209

Frequencies (cm^{-1}): 56.8402, 103.901, 132.3332, 176.4839, 197.7068, 209.4903, 218.5771, 285.7636, 354.5077, 366.9592, 395.3467, 516.4434, 558.6762, 662.1977, 730.5469, 862.7581, 917.0333, 945.5104, 953.0185, 988.0303, 1015.3263, 1056.3884, 1075.9407, 1104.3358, 1171.8273, 1212.7271, 1300.143, 1340.7518, 1390.92, 1397.5161, 1417.544, 1452.5201, 1467.2438, 1479.5219, 1493.6394, 1500.1808, 1512.2906, 1708.0887, 3012.8558, 3034.5647, 3070.3692, 3082.6506, 3082.8536, 3109.0959, 3119.6809, 3135.158, 3214.8908, 3704.889

IRC:

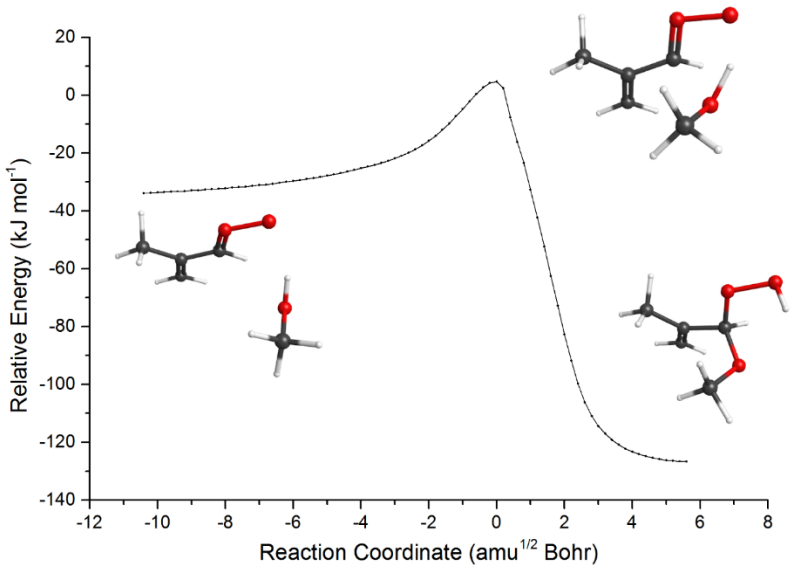


Figure S95: SCI 15 + MeOH TS-AAAH 1 IRC

***Anti*-(t-C(CH_3)=CH_2)CHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C     1.33740900  0.44912600  0.38025800
C     2.03349800 -0.27199500  1.49547100
H     1.43301000 -0.23006200  2.40513800
H     2.16750200 -1.32676000  1.25295700
H     3.00807300  0.16960300  1.69316800
C     1.84737000  1.48814200 -0.28697800
H     1.29847100  1.97385400 -1.08275000
H     2.82853700  1.88035000 -0.05677600
```

```
O   -0.33358300 -1.21400900  0.28233400
O   -1.77851800 -1.29828100  0.13998000
H   -1.83225100 -0.12774700  0.85660000
O   -1.32412800  0.78011700  1.24466100
C   -1.95823600  1.96135000  0.79311400
H   -1.28690700  2.80941300  0.93560700
H   -2.23730300  1.89932900 -0.26464600
H   -2.86710400  2.13500300  1.37419700
H   -0.51057700  0.47991000 -0.82847900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.569360591546

Frequencies (cm^{-1}): -659.489, 70.6954, 84.7336, 111.0933, 171.3362, 187.0086, 204.5444, 225.3298, 321.9371, 372.1872, 387.7743, 505.5214, 551.2006, 590.2789, 731.6951, 851.4573, 884.4112, 924.9142, 980.4668, 996.3726, 1053.2056, 1075.5023, 1077.8394, 1129.6936, 1174.696, 1198.2725, 1310.9306, 1346.462, 1406.167, 1419.9541, 1436.3955, 1467.3285, 1478.3915, 1487.0988, 1495.8697, 1500.5097, 1506.0869, 1689.9314, 1913.4559, 2987.6587, 3040.7179, 3048.4227, 3076.4978, 3092.4575, 3119.8386, 3132.4293, 3147.5363, 3226.2529

MeOCH(t-C(CH_3)=CH_2)(OOH) (TS-AAAH 2-conformer)

```
C    0.00000000  0.00000000  0.00000000
C   -1.49464400 -0.16070500 -0.16692900
C   -1.98431500 -0.61236500 -1.51200100
H   -1.61011800  0.04279100 -2.30014700
H   -1.62219400 -1.61679600 -1.73695300
H   -3.07240300 -0.61907300 -1.54749500
C   -2.29437900  0.13115700  0.85420300
H   -1.90113400  0.44736800  1.81167100
H   -3.37063400  0.05751800  0.76781000
O    0.57978200 -1.24046200 -0.31219200
O    1.98794900 -1.17301000  0.01615300
H    2.32940900 -0.66268500 -0.73411000
O    0.54415000  0.95432900 -0.89970300
C    0.48267400  2.29574500 -0.43894700
H   -0.54995200  2.63999500 -0.33426400
H    0.99366000  2.40648200  0.52320200
H    0.98726800  2.90611600 -1.18398400
H    0.25876300  0.28105100  1.02677100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.635250631972

Frequencies (cm^{-1}): 58.458, 80.1702, 133.6849, 159.3568, 168.8394, 181.0404, 255.327, 296.3797, 326.0876, 372.5139, 407.0066, 538.1223, 565.3271, 600.7901, 738.85, 849.3457, 935.129, 952.5208, 964.0001, 1008.9031, 1037.1758, 1073.9521, 1093.2642, 1102.3472, 1178.2876, 1218.7211, 1305.8119, 1340.6585, 1374.5701, 1389.0748, 1411.3601, 1456.3383, 1474.5295, 1476.3762, 1490.7585, 1499.0028, 1510.4803, 1711.3033, 2992.6173, 3006.1415, 3034.1501, 3045.0261, 3084.1391, 3110.616, 3119.5673, 3133.2807, 3212.2861, 3719.4353

IRC:

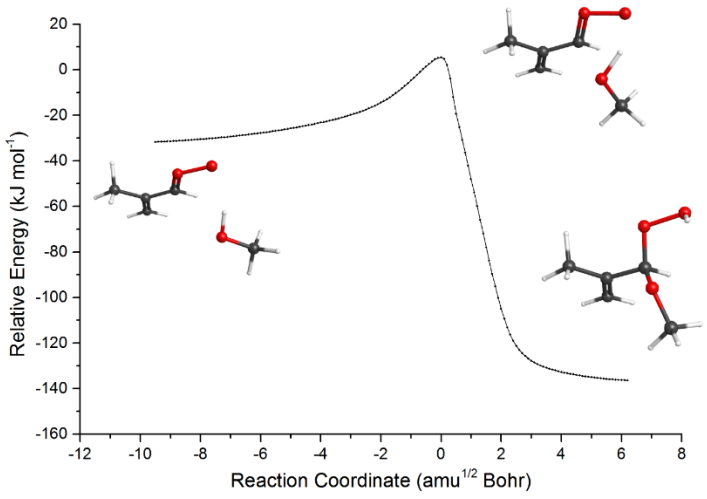


Figure S96: SCI 15 + MeOH TS-AAAH 2 IRC

7.16 sCI 16 + MeOH Reaction

***Anti*-(c-C(CH_3)=CH_2)CHOO (SCI 16):**

```
C     0.00000000  0.00000000  0.00000000
C    -1.10018900  1.02976500 -0.00098200
C    -0.86661500  2.35084600 -0.00276500
H     0.14414000  2.73314200 -0.00151000
H    -1.67268800  3.07018500 -0.00482000
C    -2.44409100  0.49223800 -0.00359500
O    -3.45597300  1.25074000  0.00266700
O    -4.69439100  0.67883200 -0.00214100
H    -2.64650700 -0.57456600 -0.01097500
H     0.97681900  0.47833900 -0.00285400
H    -0.06186600 -0.64278400  0.88050300
H    -0.06483600 -0.64720500 -0.87703600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.955058927556

Frequencies (cm^{-1}): 88.0695, 145.9678, 197.6049, 200.2049, 369.9884, 457.4961, 498.9031, 556.6127, 676.6452, 897.4329, 967.3602, 968.9331, 972.3053, 1013.4708, 1046.6039, 1076.9318, 1272.3979, 1368.1593, 1419.8447, 1446.2234, 1483.8123, 1496.3137, 1514.4736, 1663.7783, 3028.3826, 3074.6722, 3120.5265, 3149.3809, 3155.3861, 3243.6652

***Anti*-(c-C(CH_3)=CH_2)CHOO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C     0.17312000 -1.49641400 -0.00011800
C     1.55004600 -1.95252500 -0.00001900
O     1.81603500 -3.18797600 -0.00007100
O     3.13482400 -3.59122000  0.00002000
H     4.25084000 -2.14487600 -0.00031300
O     4.53408300 -1.20773400 -0.00037400
C     5.94819500 -1.11366400 -0.00007700
H     6.38825600 -1.57720000 -0.88878300
H     6.20955800 -0.05607600 -0.00049600
H     6.38784400 -1.57638800  0.88926100
H     2.38634400 -1.25766800  0.00010200
C    -0.85364400 -2.35850300 -0.00030100
H    -1.87446400 -2.00330300 -0.00037100
H    -0.69761400 -3.42765200 -0.00037800
H    -1.05422600  0.26769300 -0.00015000
H     0.46799500  0.44915000  0.87800300
H     0.46829000  0.44932000 -0.87775800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.574964983195

Frequencies (cm^{-1}): 19.4357, 31.5546, 65.5028, 92.7179, 106.2004, 127.9968, 148.0517, 173.7278, 201.321, 269.0876, 370.5015, 466.1216, 495.6894, 551.3119, 675.5708, 702.2782, 891.6975, 957.0179, 980.7744, 1010.3962, 1018.0419, 1046.5732, 1064.4058, 1079.9283, 1144.7746, 1172.8771, 1288.0747, 1393.2418, 1421.3387, 1445.8798, 1458.9555, 1478.4678, 1483.3823, 1496.1547, 1497.189, 1512.9141, 1537.5311, 1669.187, 2987.8311, 3030.6224, 3031.5657, 3079.2572, 3088.9559, 3120.7736, 3131.2995, 3153.9709, 3242.317, 3467.1509

***Anti*-(c-C(CH_3)=CH_2)CHOO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C    -0.93792100 -0.59361400  1.01290100
C    -2.25347100 -0.98322300  0.50192500
O    -3.04507700 -1.67480400  1.25303500
O    -4.36866100 -1.58266700  0.65841200
H    -4.11986400 -0.23947100  0.42207500
O    -3.42578900  0.61715200  0.36956400
C    -3.54305300  1.37286900  1.56583900
H    -4.56352000  1.75108300  1.66075700
H    -3.32132700  0.76658200  2.44956500
H    -2.85177600  2.21380900  1.52520700
H    -2.41043300 -1.04929200 -0.56806600
C    -0.63859100 -0.76816300  2.30269200
H     0.33518100 -0.50031100  2.68955900
H    -1.35127900 -1.19418500  2.99384200
H     0.93899400  0.29599900  0.46292600
H     0.22108900 -0.71375700 -0.79651500
H    -0.44705000  0.87775300 -0.47064700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.569028155585

Frequencies (cm^{-1}): -584.948, 62.6151, 99.784, 120.0388, 148.5608, 171.4914, 200.1498, 241.4905, 337.332, 363.0824, 404.922, 501.4423, 544.7969, 606.0436, 733.7, 870.6205, 895.2708, 950.6666, 989.6463, 1012.4139,

1036.4674, 1058.2634, 1076.3509, 1150.3259, 1175.9421, 1197.3096, 1274.872, 1351.3683, 1418.6756, 1445.8771, 1463.8084, 1478.5324, 1482.2457, 1490.7407, 1495.119, 1502.6708, 1507.1529, 1689.2725, 1865.4787, 3001.8542, 3028.3974, 3055.8283, 3075.9717, 3094.111, 3117.5794, 3150.4273, 3154.3081, 3239.0052

(c-C(CH_3)=CH_2)CH(OMe)(OOH) (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -1.06835600 -0.70650800  0.78703800
C    -2.47819500 -0.38945900  0.32917600
O    -3.39320700 -1.16605600  1.07411000
O    -4.66658700 -1.12253000  0.39108200
H    -4.95742300 -0.21433700  0.56707500
O    -2.80311400  0.98744200  0.40575200
C    -2.64637700  1.59239900  1.68985300
H    -3.05308900  2.59678700  1.60076400
H    -3.19291600  1.04587500  2.46049800
H    -1.59541700  1.65403800  1.98044000
H    -2.59742400 -0.62933600 -0.72943900
C    -0.80489100 -1.55506800  1.77446500
H     0.21724300 -1.76822200  2.05982000
H    -1.58745500 -2.06616100  2.31483300
H     0.99043000 -0.26692900  0.36416500
H    -0.05861900 -0.26388700 -1.05922900
H    -0.11188500  1.08433700  0.05574000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.634511077360

Frequencies (cm^{-1}): 56.2966, 110.5467, 114.677, 155.2098, 166.2685, 202.4444, 224.3661, 272.3415, 346.7086, 365.5334, 420.6209, 494.1024, 556.6518, 659.6115, 729.2715, 898.3435, 919.0368, 954.6704, 964.0329, 989.0964, 1004.1422, 1057.8923, 1077.088, 1099.3809, 1174.4066, 1210.4337, 1266.8393, 1369.1464, 1383.7783, 1397.1886, 1415.4269, 1449.2125, 1468.8691, 1476.1913, 1488.6126, 1495.5777, 1511.8166, 1714.4857, 3018.2382, 3022.2786, 3051.0122, 3067.5242, 3074.2485, 3110.3499, 3121.7738, 3142.8189, 3232.5061, 3712.0945

IRC:

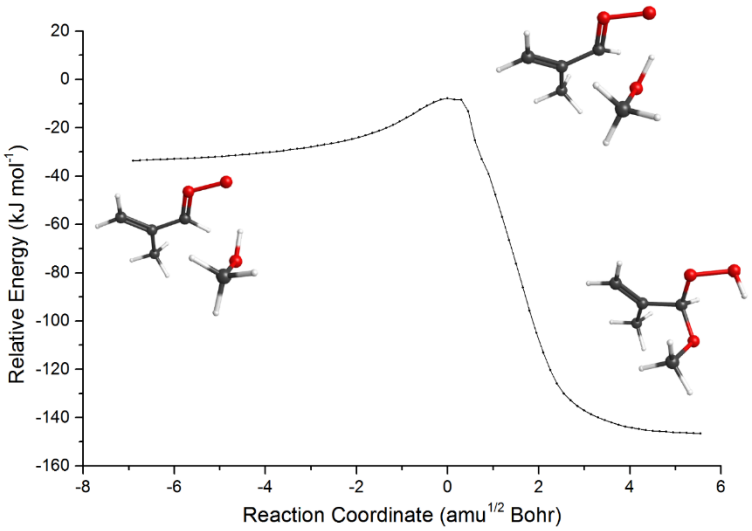


Figure S97: SCI 16 + MeOH TS-AAAH 1 IRC

***Anti*-(c-C(CH_3)=CH_2)CHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C    -0.64656600 -1.19151600  0.64952700
C    -2.00258400 -1.51265800  0.19809300
O    -2.46987100 -2.69193200  0.43242100
O    -3.90755100 -2.63032800  0.23240800
H    -3.88514000 -1.46619000  0.95071800
O    -3.33124000 -0.59608600  1.36501400
C    -3.88497200  0.61287500  0.88064100
H    -3.93457700  0.63355800 -0.21457800
H    -4.90104100  0.73642300  1.26392200
H    -3.27768300  1.45093100  1.22416600
```

```
H    -2.43029200 -0.97266900 -0.64071800
C    -0.06653600 -1.93825000  1.59144200
H     0.93987500 -1.72862400  1.92718300
H    -0.58462700 -2.76948600  2.04675600
H     0.99515700  0.17148900  0.40485700
H     0.08922900 -0.13643500 -1.07992700
H    -0.59288700  0.90273500  0.16251200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.565218768738

Frequencies (cm^{-1}): -645.4429, 43.0889, 104.9195, 111.8484, 152.0935, 179.3369, 204.9861, 213.0015, 340.4781, 350.562, 391.7097, 494.1632, 542.0624, 587.0347, 722.8776, 871.814, 889.7618, 938.8207, 994.1615, 1002.8074, 1032.8776, 1069.1575, 1073.2075, 1141.0575, 1175.9678, 1200.9799, 1270.2726, 1341.2264, 1404.6465, 1417.5088, 1444.3336, 1474.6467, 1482.396, 1491.9193, 1496.1855, 1500.1544, 1501.1615, 1690.9631, 1902.0643, 2981.3191, 3025.7378, 3041.741, 3071.0509, 3079.6458, 3116.5271, 3127.1769, 3151.813, 3241.7487

(c-C(CH_3)=CH_2)CH(OMe)(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
C     0.70192200 -1.31459200 -0.19294700
C     2.20644500 -1.24593500 -0.01387400
O     2.74021300 -2.51714200 -0.31326900
O     4.13764700 -2.50921400  0.06394100
H     4.55388900 -2.33163700 -0.79159200
O     2.75612600 -0.26431300 -0.86738600
C     3.59380100  0.70385300 -0.24520000
H     3.02407000  1.35216300  0.42715700
H     4.40555400  0.23358200  0.31406200
H     4.01095800  1.31171400 -1.04512400
H     2.45446600 -1.00056800  1.02596000
C     0.06183400 -2.44368700 -0.47508700
H    -1.01513900 -2.45148500 -0.58164900
H     0.58017800 -3.38097200 -0.60688700
H    -1.07814300 -0.12290100 -0.08505900
H     0.21570100  0.42388600  0.98499000
H     0.32722800  0.72964100 -0.74191400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.631256017719

Frequencies (cm^{-1}): 33.5536, 44.2703, 114.3224, 130.9215, 176.9173, 210.5253, 249.5735, 284.545, 359.0165, 378.4882, 380.1092, 487.6912, 552.3493, 595.3759, 716.9163, 896.7172, 952.1551, 956.8956, 966.7412, 996.7428, 1011.9531, 1069.8857, 1081.4181, 1107.1496, 1171.8705, 1209.9349, 1265.1798, 1357.4088, 1375.0891, 1391.3037, 1409.2528, 1449.2972, 1473.9212, 1477.7634, 1494.4567, 1498.8613, 1509.4174, 1714.6781, 2985.709, 3003.0549, 3018.0005, 3058.2889, 3070.9279, 3110.8303, 3116.3127, 3145.5779, 3236.4318, 3741.3122

IRC:

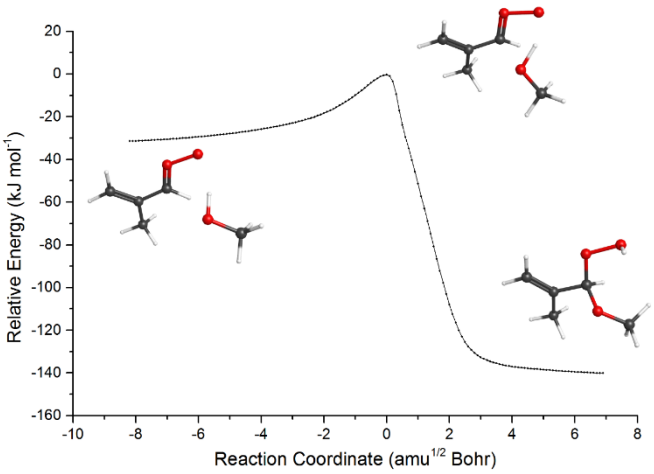


Figure S98: SCI 16 + MeOH TS-AAAH 2 IRC

7.17 sCI 17 + MeOH Reaction

***Anti*-MeC(*t*-CH=CH$_2$)OO (SCI 17):**

```
C     0.00000000  0.00000000  0.00000000
H     0.62357100  0.16058800  0.88140000
H     0.62557200  0.15998400 -0.88006800
H    -0.80398200  0.73137000 -0.00114400
C    -0.57115600 -1.37678900 -0.00010700
C     0.19904800 -2.59141900 -0.00020000
C     1.53658300 -2.61370200  0.00012000
H     2.07392500 -3.55148400  0.00010800
H     2.13525200 -1.71259100  0.00044100
H    -0.38911300 -3.49769300 -0.00046100
O    -1.85046200 -1.41251700 -0.00001300
O    -2.50898800 -2.60946400  0.00014200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.963584578150

Frequencies (cm^{-1}): 109.6602, 144.887, 246.3849, 276.8744, 328.2498, 388.5802, 479.0062, 627.327, 727.142, 789.4894, 949.9002, 991.5212, 1002.5306, 1049.1515, 1056.9369, 1067.4997, 1282.9543, 1361.8796, 1422.5154, 1431.5114, 1460.3736, 1475.1068, 1515.6467, 1661.4921, 3033.9118, 3081.2601, 3136.7787, 3147.4306, 3202.4972, 3232.7074

***Anti*-MeC(*t*-CH=CH$_2$)OO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C     0.88304700  1.08771200  0.51854500
O     1.81287900  0.65999800  1.28014700
O     2.71444000  1.54693200  1.83741100
H     4.09866100  1.62482300  0.63439200
C     0.63688000  2.45219300  0.14505200
C     1.32676300  3.54809600  0.50420700
H     1.01092200  4.51315000  0.12877800
H     2.18422800  3.48815400  1.15024200
H    -0.21705600  2.56564700 -0.51223100
O     4.73680000  1.70901200 -0.09857900
C     5.93944900  1.05354000  0.25748100
H     5.78669700 -0.01344400  0.45514900
H     6.62832200  1.14933800 -0.58178200
H     6.41002900  1.50274500  1.13918700
H     0.03460200 -0.01938600 -1.09109300
H     0.31500000 -0.96544100  0.38539200
H    -1.03613300  0.18537900  0.28947600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.584703059938

Frequencies (cm^{-1}): 25.8843, 38.2113, 45.2631, 105.7116, 107.4687, 120.5331, 133.5791, 202.5268, 253.9955, 300.5666, 333.6147, 397.9851, 477.8873, 621.0769, 726.6627, 765.58, 790.3499, 929.1159, 1001.4323, 1004.6771, 1044.0658, 1051.4322, 1064.9232, 1068.993, 1131.5076, 1172.95, 1294.6622, 1361.0548, 1420.4806, 1439.1127, 1449.3284, 1460.7951, 1474.8256, 1475.684, 1495.1431, 1512.8579, 1524.0522, 1666.2818, 2978.6508, 3017.5974, 3039.9988, 3080.7683, 3091.3675, 3141.5977, 3150.3542, 3217.6277, 3237.84, 3459.7455

***Anti*-MeC(*t*-CH=CH$_2$)OO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C     0.12532900  1.23845900 -0.82512600
O     0.89119100  2.15227400 -0.27671100
O     1.32695300  3.04712600 -1.33409800
H     1.53115900  1.95736100 -2.09847700
C    -0.96479400  1.67942600 -1.70607000
C    -1.91907700  0.88551000 -2.18187400
H    -1.93018200 -0.18367600 -2.02000400
H    -2.72570400  1.29104000 -2.77635500
H    -0.95041300  2.73808500 -1.92220500
O     1.40528400  0.85385500 -2.28967700
C     2.60192200  0.20025200 -1.89353600
H     2.44652800 -0.87909100 -1.90074400
H     3.39849700  0.44520000 -2.60059000
H     2.92503600  0.51665300 -0.89709100
H    -0.33367200 -0.83557400 -0.60979900
H     0.95051900 -0.24312100  0.46638400
H    -0.74174200  0.16708800  0.78288500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.569781495521

Frequencies (cm^{-1}): -767.1669, 65.1797, 121.6374, 129.7077, 142.6484, 171.0523, 228.1056, 288.8205, 292.5373, 322.2506, 380.9197, 465.4283, 501.8168, 601.149, 689.288, 762.959, 864.3246, 888.956, 982.5114,

996.3889, 1028.8383, 1044.6335, 1060.8987, 1074.2831, 1170.1602, 1182.8852, 1293.4997, 1322.9705, 1389.1796, 1411.7556, 1454.5335, 1466.7624, 1483.7147, 1489.2852, 1495.7958, 1497.8887, 1511.2475, 1687.459, 1824.3478, 2999.2075, 3051.9181, 3052.7933, 3081.1539, 3118.8325, 3148.3603, 3151.5214, 3197.5192, 3230.3393

MeCH(OMe)(*t*-CH=CH$_2$)(OOH) (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
C     0.37084900 -1.15706000 -0.92925600
O     0.52006300 -2.25851800 -0.03456400
O     0.88666400 -3.45452600 -0.76552600
H     0.17662600 -3.50830800 -1.42572100
C     1.61347900 -0.83765500 -1.72791800
C     2.84505500 -1.17516700 -1.38247800
H     3.69187300 -0.87796300 -1.98564200
H     3.04554100 -1.76933300 -0.50162600
H     1.42373500 -0.25809200 -2.62327400
O    -0.62895900 -1.46200600 -1.89408100
C    -1.97190900 -1.58176900 -1.42755500
H    -2.03871200 -2.22021100 -0.54447600
H    -2.53360600 -2.03511000 -2.24112900
H    -2.40572300 -0.60549400 -1.20244500
H    -0.21068000  0.88733000 -0.59537200
H    -0.86970100 -0.24074000  0.60838900
H     0.83782600  0.21343600  0.65888200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632627250236

Frequencies (cm^{-1}): 53.0269, 108.1424, 138.1621, 186.9146, 215.377, 233.95, 241.6742, 270.062, 336.4571, 360.6476, 393.1438, 435.5198, 525.5013, 616.1029, 698.731, 747.7485, 842.9752, 911.0597, 943.8465, 970.5499, 1018.5712, 1033.0092, 1068.5786, 1119.6182, 1170.0276, 1176.9824, 1201.257, 1303.2891, 1333.9515, 1383.7496, 1405.8427, 1457.6706, 1467.8675, 1485.8969, 1501.0385, 1504.3383, 1516.0817, 1713.8254, 3012.7629, 3061.4074, 3068.9798, 3114.6427, 3131.858, 3137.92, 3145.9373, 3185.2208, 3223.161, 3727.2308

IRC:

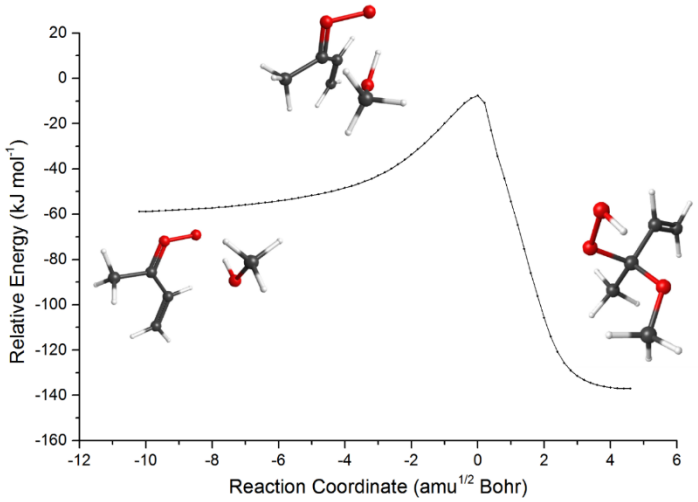


Figure S99: SCI 17 + MeOH TS-AAAH 1 IRC

***Anti*-MeC(*t*-CH=CH$_2$)OO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C    -0.70870600  0.13357800 -1.30647900
O    -1.47028100 -0.89534400 -1.58457600
O    -2.47004400 -0.46314000 -2.54653100
H    -2.66933000  0.55991200 -1.74875600
C    -0.15702400  0.91257600 -2.41528500
C     0.76536600  1.86444100 -2.28747400
H     1.14758900  2.18762100 -1.32881400
H     1.16964600  2.35917300 -3.15966600
H    -0.55020600  0.63572200 -3.38314900
O    -2.32867100  1.22451000 -0.87658400
C    -2.47501000  2.60327600 -1.13532800
```

```
H    -2.39616200   3.15518800 -0.19724400
H    -1.71034800   2.97901200 -1.82481800
H    -3.45510600   2.80196300 -1.57928900
H     0.36847500   0.96342400  0.34202200
H    -0.67814500 -0.41283500   0.74073900
H     0.85376800 -0.66967100 -0.12109000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.568643192224

Frequencies (cm^{-1}): -920.576, 76.4792, 95.9612, 121.9051, 135.8417, 199.9173, 228.0023, 273.7303, 307.3761, 331.3785, 363.2493, 453.7547, 475.2257, 590.7603, 685.9942, 745.3951, 804.7017, 886.6139, 984.9397, 999.2132, 1033.5602, 1045.4358, 1063.5703, 1092.5438, 1170.312, 1187.2818, 1291.3709, 1301.1659, 1339.9613, 1390.7399, 1413.8341, 1453.44, 1472.4898, 1485.8901, 1488.2329, 1494.7542, 1503.3946, 1680.2226, 1913.6591, 2982.2206, 3031.0433, 3049.2211, 3067.9091, 3121.3025, 3147.5985, 3155.8468, 3195.8215, 3229.6228

MeCH(OMe)(*t*-CH=CH$_2$)(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000  0.00000000  0.00000000
C     0.46269300 -0.37123700 -1.40904100
O     1.42286100 -1.38586600 -1.18205600
O     1.87080600 -1.94491600 -2.44076200
H     1.06100700 -2.38874300 -2.73794500
C     1.01246100  0.83663000 -2.13593800
C     2.28789100  1.04326200 -2.42530400
H     2.60453700  1.96349500 -2.89767100
H     3.04842600  0.30773300 -2.20784500
H     0.28460600  1.60677800 -2.36309000
O    -0.59516900 -1.02807700 -2.11887000
C    -1.55794000 -0.24119400 -2.80111700
H    -2.32769800 -0.93264700 -3.13679300
H    -2.02228300  0.50077100 -2.14466900
H    -1.13236900  0.26461000 -3.67079600
H    -0.77062700  0.76830500 -0.05382500
H    -0.40878900 -0.88268800  0.48795000
H     0.83305800  0.39000500  0.58138100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632217648743

Frequencies (cm^{-1}): 50.4929, 78.3694, 147.5809, 176.6681, 227.4822, 233.3259, 279.4559, 308.9106, 311.4334, 374.0258, 412.3931, 454.0388, 484.9057, 603.2775, 710.1398, 738.2725, 867.6822, 916.702, 948.2434, 975.0551, 1017.2446, 1045.8794, 1095.065, 1135.7773, 1162.4217, 1176.6637, 1224.9618, 1272.452, 1327.5658, 1395.2247, 1405.3098, 1455.522, 1472.0327, 1489.1136, 1491.5952, 1503.1435, 1511.9635, 1704.4032, 3008.2011, 3058.6147, 3062.7409, 3115.7617, 3129.0849, 3135.693, 3141.8604, 3177.0594, 3219.5259, 3719.2336

IRC:

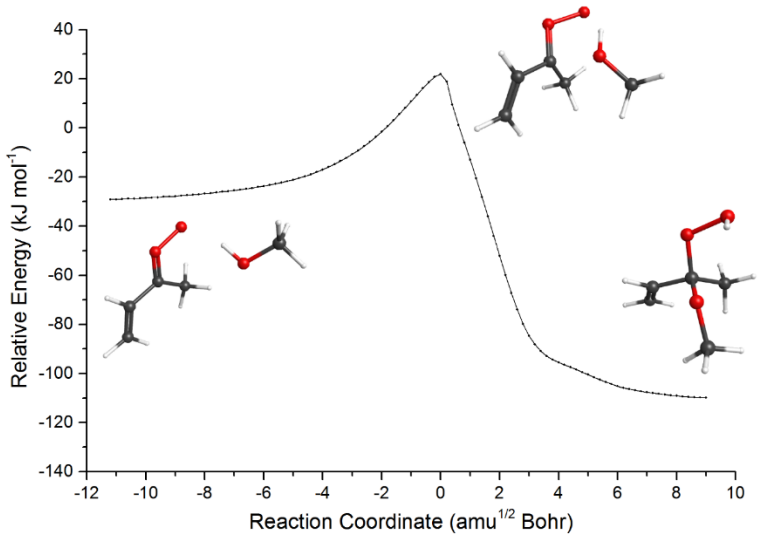


Figure S100: SCI 17 + MeOH TS-AAAH 1 IRC

7.18 sCI 18 + MeOH Reaction

***Anti*-MeC(*c*-CH=CH$_2$)OO (SCI 18):**

```
C     0.00000000  0.00000000  0.00000000
H    -0.25723500 -0.59466300 -0.87897400
H    -0.25715600 -0.59358000  0.87968800
H    -0.59237200  0.91085200 -0.00082200
C     1.45914000  0.32509500 -0.00032600
C     2.43807600 -0.72331300 -0.00021400
C     3.77777000 -0.60412800 -0.00005000
H     4.38477900 -1.50086200  0.00024200
H     4.25186800  0.36148000 -0.00020100
H     2.00244400 -1.71588000 -0.00052200
O     1.69867700  1.58159500 -0.00008900
O     2.98584400  2.04370500 -0.00013000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.964896825258

Frequencies (cm^{-1}): 109.162, 166.6448, 278.7644, 300.4088, 339.5019, 386.1221, 408.2069, 630.5678, 721.6738, 815.1076, 960.5336, 1019.4402, 1031.1058, 1034.8098, 1049.2046, 1103.5065, 1258.6473, 1337.6787, 1410.763, 1450.8149, 1455.5226, 1474.0198, 1514.0156, 1639.5914, 3030.3751, 3076.787, 3139.252, 3141.4412, 3154.6727, 3281.7687

***Anti*-MeC(*c*-CH=CH$_2$)OO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C     0.88304700  1.08771200  0.51854500
O     1.81287900  0.65999800  1.28014700
O     2.71444000  1.54693200  1.83741100
C     0.63688000  2.45219300  0.14505200
C     1.32676300  3.54809600  0.50420700
H     1.01092200  4.51315000  0.12877800
H     2.18422800  3.48815400  1.15024200
H    -0.21705600  2.56564700 -0.51223100
H     0.03460200 -0.01938600 -1.09109300
H     0.31500000 -0.96544100  0.38539200
H    -1.03613300  0.18537900  0.28947600
H     4.09866100  1.62482300  0.63439200
O     4.73680000  1.70901200 -0.09857900
C     5.93944900  1.05354000  0.25748100
H     6.62832200  1.14933800 -0.58178200
H     6.41002900  1.50274500  1.13918700
H     5.78669700 -0.01344400  0.45514900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.582447294501

Frequencies (cm^{-1}): 16.5982, 25.7365, 37.7601, 100.4047, 108.1455, 123.396, 146.4482, 185.5426, 299.9676, 303.2955, 341.0384, 390.4364, 411.7398, 627.4593, 718.8616, 744.9206, 814.5793, 946.0445, 1021.4194, 1030.8363, 1045.8771, 1049.7925, 1064.9771, 1107.0982, 1122.5881, 1172.7672, 1258.2528, 1343.3919, 1409.0598, 1433.3931, 1456.8837, 1460.3704, 1473.4692, 1475.2342, 1494.9323, 1511.3274, 1525.3197, 1646.0306, 2976.6383, 3014.309, 3034.2029, 3080.7578, 3083.0408, 3144.594, 3148.0305, 3160.6545, 3289.0268, 3526.9339

***Anti*-MeC(*c*-CH=CH$_2$)OO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C     0.12532900  1.23845900 -0.82512600
O     0.89119100  2.15227400 -0.27671100
O     1.32695300  3.04712600 -1.33409800
C    -0.96479400  1.67942600 -1.70607000
C    -1.91907700  0.88551000 -2.18187400
H    -1.93018200 -0.18367600 -2.02000400
H    -2.72570400  1.29104000 -2.77635500
H    -0.95041300  2.73808500 -1.92220500
H    -0.33367200 -0.83557400 -0.60979900
H     0.95051900 -0.24312100  0.46638400
H    -0.74174200  0.16708800  0.78288500
H     1.53115900  1.95736100 -2.09847700
O     1.40528400  0.85385500 -2.28967700
C     2.60192200  0.20025200 -1.89353600
H     2.44652800 -0.87909100 -1.90074400
H     3.39849700  0.44520000 -2.60059000
H     2.92503600  0.51665300 -0.89709100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.568328596443

Frequencies (cm^{-1}): -626.2645, 86.2011, 130.0206, 132.4837, 140.0896, 172.8764, 232.9667, 267.8174, 285.9307, 311.5298, 367.0854, 401.8609, 524.273, 614.5003, 671.7489, 784.53, 870.8943, 940.6816,

1009.6129, 1012.1592, 1019.1163, 1054.0035, 1075.1038, 1093.1554, 1171.5513, 1198.8267, 1237.4867, 1337.9658, 1400.1466, 1427.0047, 1454.7319, 1465.8815, 1478.804, 1486.372, 1495.2494, 1508.1055, 1514.9067, 1689.401, 1839.5268, 3002.1586, 3044.044, 3055.8166, 3085.0943, 3109.1649, 3146.8697, 3151.0085, 3174.4596, 3247.2472

MeCH(OMe)(*c*-CH=CH$_2$)OOH (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -0.37084900  1.15706000 -0.92925600
O    -0.52006300  2.25851800 -0.03456400
O    -0.88666400  3.45452600 -0.76552600
C    -1.61347900  0.83765500 -1.72791800
C    -2.84505500  1.17516700 -1.38247800
H    -3.69187300  0.87796300 -1.98564200
H    -3.04554100  1.76933300 -0.50162600
H    -1.42373500  0.25809200 -2.62327400
H     0.21068000 -0.88733000 -0.59537100
H     0.86970100  0.24074100  0.60838900
H    -0.83782600 -0.21343500  0.65888200
H    -0.17662600  3.50830800 -1.42572100
O     0.62895900  1.46200600 -1.89408100
C     1.97190900  1.58176900 -1.42755500
H     2.03871200  2.22021100 -0.54447600
H     2.40572300  0.60549400 -1.20244500
H     2.53360600  2.03511000 -2.24112900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.633960117161

Frequencies (cm^{-1}): 85.0038, 114.5028, 155.2295, 187.6169, 203.905, 241.4293, 266.5619, 293.9792, 323.7507, 330.9809, 395.999, 434.8846, 565.5673, 608.0416, 688.4084, 756.0026, 848.1793, 914.2384, 948.7769, 980.2946, 1026.904, 1048.6968, 1062.054, 1136.244, 1149.5669, 1175.6538, 1202.4056, 1268.0464, 1322.1785, 1401.9477, 1406.4899, 1450.0922, 1468.4954, 1482.525, 1493.9062, 1503.7794, 1516.9179, 1712.3012, 3017.4554, 3053.5366, 3075.9014, 3116.7824, 3123.7498, 3135.5733, 3143.9725, 3162.9732, 3228.9513, 3687.9468

IRC:

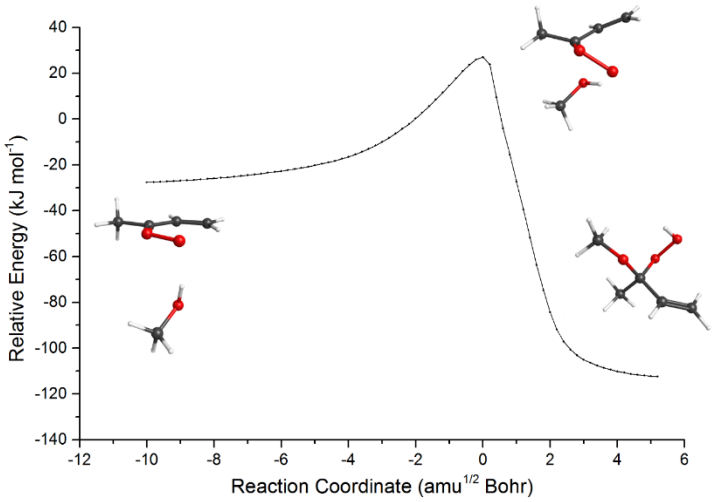


Figure S101: SCI 18 + MeOH TS-AAAH 1 IRC

***Anti*-MeC(*c*-CH=CH$_2$)OO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C    -0.70870600  0.13357900 -1.30647900
O    -1.47028200 -0.89534300 -1.58457600
O    -2.47004500 -0.46313800 -2.54653100
C    -0.15702300  0.91257600 -2.41528500
C     0.76536800  1.86444000 -2.28747400
H     1.14759200  2.18761900 -1.32881400
H     1.16964900  2.35917100 -3.15966600
H    -0.55020500  0.63572200 -3.38314900
H     0.36847600  0.96342300  0.34202200
H    -0.67814500 -0.41283400  0.74073900
H     0.85376700 -0.66967200 -0.12109000
```

```
H    -2.66932900   0.55991500 -1.74875600
O    -2.32866900   1.22451200 -0.87658400
C    -2.47500700   2.60327900 -1.13532800
H    -2.39615800   3.15519100 -0.19724400
H    -1.71034400   2.97901400 -1.82481800
H    -3.45510300   2.80196700 -1.57928900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.565930356755

Frequencies (cm^{-1}): -750.7958, 89.3021, 110.9437, 121.4114, 134.7048, 196.4151, 233.2092, 259.6859, 288.4346, 322.4595, 354.9471, 407.6249, 489.7304, 608.7449, 669.8585, 778.7637, 857.1686, 885.0278, 1016.8813, 1018.5478, 1025.5262, 1050.0386, 1082.0541, 1091.1865, 1172.5491, 1192.6724, 1228.5142, 1338.9845, 1355.843, 1403.0163, 1425.4717, 1453.6655, 1473.0618, 1479.6596, 1493.8195, 1499.7911, 1509.9584, 1683.6375, 1895.2957, 2995.2367, 3041.1596, 3046.3558, 3068.9746, 3111.3526, 3146.8659, 3153.7265, 3163.4363, 3247.5855

MeCH(OMe)(*c*-CH=CH$_2$)(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000   0.00000000   0.00000000
C     0.31531900  -1.44413800   0.39001000
O    -0.07917300  -2.16610200  -0.78666400
O     0.30275900  -3.56069000  -0.67159000
C    -0.46685500  -1.85831700   1.61428100
C    -1.51177000  -2.67101300   1.62554900
H    -2.04517700  -2.87567000   2.54401000
H    -1.86286100  -3.15669900   0.72625100
H    -0.14099800  -1.38168400   2.53243400
H     0.17186000   0.64893000   0.85674000
H     0.65835500   0.30337700  -0.81206100
H    -1.03750600   0.09107900  -0.31371900
H     1.09758000  -3.56720400  -1.22247000
O     1.71335900  -1.51859600   0.57232500
C     2.25418900  -2.47561500   1.48370100
H     3.31504300  -2.53885600   1.24907600
H     2.14626000  -2.14512300   2.51956000
H     1.79699600  -3.45686800   1.36924600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.630054775440

Frequencies (cm^{-1}): 58.0068, 99.7326, 166.3898, 198.0721, 217.4867, 224.8704, 278.0867, 305.8637, 311.0313, 351.4082, 387.6539, 457.0347, 524.2176, 614.0809, 688.6191, 736.8542, 871.4642, 918.7578, 957.0807, 985.4808, 1032.7624, 1048.9985, 1100.8213, 1126.5326, 1151.0169, 1174.8256, 1205.6266, 1268.2242, 1339.8189, 1400.414, 1401.4788, 1454.5031, 1474.461, 1484.7894, 1490.598, 1498.3971, 1510.2848, 1708.2373, 3001.1791, 3049.3925, 3055.2924, 3112.3726, 3118.3945, 3131.8428, 3142.9752, 3156.3385, 3235.4079, 3707.7349

IRC:

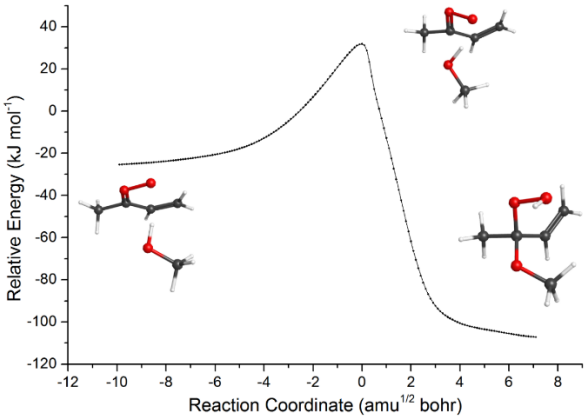


Figure S102: SCI 18 + MeOH TS-AAAH 2 IRC

7.19 sCI 19 + MeOH Reaction

***Syn*-(t-C(CH_3)=CH_2)CHOO (SCI 19):**

```
C     0.00000000  0.00000000  0.00000000
C    -1.48965400  0.20522400  0.00000000
C    -2.04373100  1.43318900  0.00000000
H    -1.43129500  2.32378000  0.00000000
H    -3.11599600  1.57604700  0.00000000
C    -2.43871800 -0.88161000  0.00000000
O    -2.24206900 -2.13492300  0.00000000
O    -0.97996900 -2.65500600  0.00000000
H    -3.49895300 -0.65506000  0.00000000
H     0.50245100  0.96683300  0.00000000
H     0.31431500 -0.57414200  0.86880400
H     0.31431500 -0.57414200 -0.86880400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.955087040803

Frequencies (cm^{-1}): 66.36, 205.1329, 253.3364, 331.8387, 350.0563, 432.3051, 556.6998, 699.1299, 723.0272, 838.6681, 895.38, 899.9555, 962.2911, 1000.2174, 1062.6115, 1076.911, 1341.447, 1384.1591, 1424.4284, 1441.7998, 1468.2878, 1484.3411, 1532.5911, 1641.4947, 3048.5667, 3120.7496, 3121.5516, 3145.4202, 3165.5799, 3231.7519

***Syn*-(t-C(CH_3)=CH_2)(OOH)CHOO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C    -0.47427500 -1.28815200  0.44552300
C    -1.55060200 -1.73028100 -0.23424600
H    -2.00941200 -2.68000600  0.00222400
H    -1.99419300 -1.15920700 -1.03869000
C     0.15560200 -2.08119700  1.55542900
H    -0.43708000 -2.97604400  1.74202700
H     1.17028300 -2.37455000  1.29018000
H     0.22499400 -1.49325400  2.46716300
O     0.95404000  0.71915300  0.41616900
O     1.75360000  0.29781700  1.46139000
H     2.86401900 -0.90854000  0.71891300
H    -0.51710000  0.48720000 -0.82005500
O     3.26380300 -1.66366900  0.24332600
C     4.64479400 -1.41781600  0.04752500
H     4.82254700 -0.50747700 -0.53510400
H     5.18590300 -1.33252500  0.99598800
H     5.05539700 -2.26264000 -0.50499900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.575828551529

Frequencies (cm^{-1}): 22.1256, 35.0219, 63.8202, 80.6349, 111.2361, 113.4253, 214.7546, 232.0569, 258.031, 331.0085, 351.2268, 436.1714, 552.8596, 700.8765, 720.5035, 758.8278, 830.1184, 880.0332, 921.5915, 978.312, 999.8135, 1063.5861, 1067.1235, 1081.8764, 1128.8439, 1172.6158, 1343.5392, 1388.1131, 1423.6297, 1438.1484, 1446.3796, 1474.846, 1476.0323, 1495.5433, 1498.0085, 1512.2441, 1546.6378, 1641.913, 2981.212, 3021.1779, 3046.9441, 3083.9456, 3113.7612, 3128.6479, 3146.1719, 3158.7785, 3233.889, 3477.295

***Syn*-(t-C(CH_3)=CH_2)(OOH)CHOO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C     1.27461200 -0.14181700 -0.71855000
C     1.90858800 -1.30327800 -0.52120500
H     2.87711800 -1.49650300 -0.96135900
H     1.48137800 -2.09319400  0.08232900
H     2.89341600  0.73787200 -1.78918000
C     1.85971100  0.97176400 -1.53653500
H     1.29494800  1.12188700 -2.45513800
H     1.82103300  1.91531900 -0.99581400
O    -0.57282000  1.11497600  0.34033900
O    -0.74632500  1.92098100 -0.85977000
H    -1.16426000  0.71295600 -1.50467300
H    -0.22285000 -0.79557700  0.70742500
O    -1.22553100 -0.36690800 -1.50257100
C    -2.53314500 -0.74616400 -1.08250700
H    -2.81096100 -0.25097100 -0.14849700
H    -3.25650900 -0.46534800 -1.85063100
H    -2.55824500 -1.82691100 -0.94829400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.561363340606

Frequencies (cm^{-1}): -497.5865, 51.8653, 115.6416, 129.5974, 166.7786, 210.1955, 223.0588, 256.7752, 314.819, 376.484, 405.0247, 490.0789, 547.304, 693.9413, 721.1861, 814.5226, 850.2223, 961.0699, 983.8656,

1003.9678, 1047.1707, 1062.4008, 1077.8109, 1116.5561, 1175.0962, 1228.626, 1316.5891, 1336.0975, 1420.4307, 1436.4182, 1459.7995, 1468.2522, 1478.7964, 1487.358, 1493.3812, 1511.0303, 1513.5155, 1673.5278, 1977.7663, 3010.8833, 3045.831, 3068.4447, 3097.6306, 3110.6648, 3119.1564, 3122.0047, 3142.2113, 3224.2608

MeOCH(t-C(CH_3)=CH_2)(OOH)(OOH) (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
C    -1.44986900  0.13508000 -0.41515100
C    -2.34422100  0.43097300  0.52313500
H    -3.39539700  0.53033200  0.28741000
H    -2.06168600  0.57175800  1.55848000
C    -1.81242800 -0.04831700 -1.86046500
H    -2.86948800  0.16190700 -2.01647000
H    -1.22565600  0.61751100 -2.49382300
H    -1.60528800 -1.06767000 -2.18615200
O     0.39742000 -1.32583900  0.36311000
O     0.13507100 -2.24037400 -0.73112900
H     0.95670600 -2.17764400 -1.23844100
H     0.16544900  0.51097400  0.95624700
O     0.82399900  0.53187800 -0.99719400
C     2.15054800  0.82466800 -0.57189500
H     2.66958100 -0.07010500 -0.22213800
H     2.67236700  1.23303100 -1.43374500
H     2.14510700  1.56840200  0.23104800
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632738441866

Frequencies (cm^{-1}): 51.5461, 101.4554, 127.9081, 167.1532, 188.3055, 205.7663, 210.0326, 242.4721, 340.6091, 356.1647, 397.9767, 535.3174, 555.5517, 686.9564, 739.8254, 849.4383, 894.3107, 944.7535, 954.2269, 986.5093, 1017.2452, 1059.5611, 1080.6286, 1116.5722, 1176.3995, 1212.7888, 1311.36, 1347.9857, 1359.6992, 1375.1092, 1411.4751, 1456.4356, 1473.6465, 1477.8778, 1490.6989, 1504.3139, 1511.1626, 1709.2968, 2999.666, 3004.6651, 3040.1325, 3060.8526, 3095.396, 3110.3154, 3123.6406, 3134.8099, 3213.2348, 3740.0786

IRC:

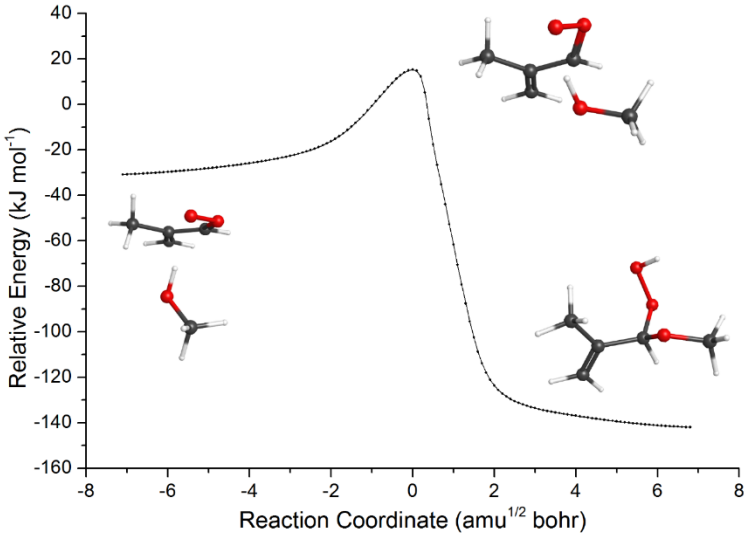


Figure S103: SCI 19 + MeOH TS-AAAH 1 IRC

***Syn*-(t-C(CH_3)=CH_2)(OOH)CHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C     1.13354900  0.41171400  0.83511700
C     1.93331900  1.34290000  0.29973400
H     2.82287200  1.68208500  0.81266800
H     1.72670800  1.78623400 -0.66562000
C     1.41916500 -0.23372100  2.16008500
H     2.42271000  0.03297800  2.49037700
H     0.69997200  0.07596900  2.91624300
H     1.33498100 -1.31663500  2.09065000
O    -0.69024500 -1.09050500  0.14017700
O    -1.20250600 -1.12479400  1.50544600
```

```
H    -1.57932400   0.18400400   1.27061600
H     0.03360300   0.32318900  -1.03639700
O    -1.48711000   1.10991400   0.67759500
C    -1.30919200   2.25535000   1.49034700
H    -1.74683500   2.09717600   2.47934000
H    -0.24889800   2.49779800   1.61661600
H    -1.80128800   3.10264300   1.01240500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.560199377383

Frequencies (cm^{-1}): -609.3191, 56.5642, 75.8973, 146.1097, 166.2448, 199.3497, 253.6514, 281.8256, 323.4909, 361.0601, 398.9398, 476.2874, 549.3093, 690.0253, 722.4279, 812.5724, 846.1588, 932.0705, 971.8623, 997.4164, 1048.7898, 1065.0395, 1081.0251, 1090.8765, 1172.7724, 1188.4097, 1305.7696, 1334.8556, 1337.6141, 1424.5885, 1439.649, 1465.7118, 1471.6956, 1482.1639, 1490.046, 1504.9929, 1520.1552, 1669.9477, 1947.4683, 2992.5158, 3045.767, 3046.3829, 3083.0201, 3110.994, 3118.368, 3137.9339, 3143.4218, 3225.1104

MeOCH(t-C(CH_3)=CH_2)(OOH)(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000   0.00000000   0.00000000
C    -1.37528400   0.36294800   0.53004000
C    -2.42315300   0.17450900  -0.26817400
H    -3.42936000   0.41031600   0.05308800
H    -2.31160700  -0.20908200  -1.27446300
C    -1.50565300   0.88513700   1.93223100
H    -2.55381000   0.94768600   2.22179500
H    -0.98449600   0.23895400   2.64009700
H    -1.05429800   1.87270200   2.02181800
O     0.83201500   1.09550700  -0.31991400
O     1.16993500   1.83344100   0.88099500
H     1.89530400   1.29445300   1.23000500
H    -0.10833700  -0.47639300  -0.98247900
O     0.72709700  -0.83969200   0.87271000
C     0.26961800  -2.18239100   0.91647500
H     0.93831100  -2.71896800   1.58495900
H    -0.75288000  -2.25194100   1.29732100
H     0.30893700  -2.64341100  -0.07630300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.630285131846

Frequencies (cm^{-1}): 45.2158, 72.201, 120.7288, 162.2713, 172.4018, 208.6577, 261.168, 294.8891, 330.6583, 352.2477, 414.5103, 505.2842, 573.9297, 674.9079, 745.633, 847.7938, 892.7613, 950.3012, 977.2349, 997.3028, 1051.2267, 1053.959, 1077.5698, 1109.1545, 1177.1445, 1220.3018, 1307.1891, 1340.6437, 1349.2769, 1386.8773, 1410.8192, 1456.3366, 1473.2274, 1478.1164, 1489.5326, 1498.6319, 1508.1524, 1702.6892, 2991.1785, 2996.5761, 3037.0007, 3044.8087, 3091.6089, 3108.818, 3120.8512, 3130.865, 3208.7612, 3729.383

IRC:

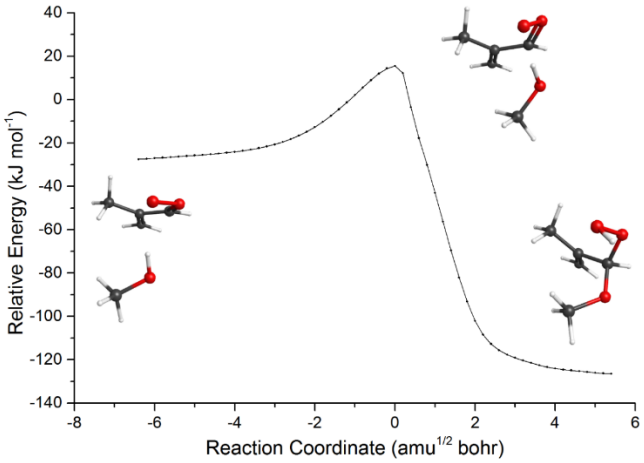


Figure S104: SCI 19 + MeOH TS-AAAH 2 IRC

7.20 sCI 20 + MeOH Reaction

***Syn*-(c-C(CH_3)=CH_2)CHOO (SCI 20):**

```
C     0.00000000  0.00000000  0.00000000
C     1.40909300  0.55003400 -0.00123100
C     1.66230500  1.87535400 -0.00174600
H     0.83456600  2.57380700 -0.00132400
H     2.67212800  2.24560500 -0.00277200
C     2.43519700 -0.44981400 -0.00193000
O     3.70446800 -0.32295600 -0.00112900
O     4.27843300  0.90894300  0.00031100
H     2.16415200 -1.49979500 -0.00318800
H    -0.72644200  0.80958000  0.00007700
H    -0.18603900 -0.61984500 -0.87916900
H    -0.18477700 -0.61895800  0.88004400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -305.958458836453

Frequencies (cm^{-1}): 107.8133, 137.0868, 282.7188, 324.3057, 341.4004, 422.381, 546.8988, 701.9436, 704.2739, 901.3552, 910.9685, 928.6035, 1006.4611, 1010.3035, 1043.7819, 1078.4389, 1276.3037, 1382.7798, 1413.606, 1430.5701, 1487.5908, 1493.3005, 1528.6233, 1629.849, 3029.4197, 3076.5837, 3118.6745, 3143.325, 3163.3386, 3281.3905

***Syn*-(c-C(CH_3)=CH_2)CHOO + MeOH PRC (for all TS-AAAH 1 and TS-AAAH 2)**

```
C     0.00000000  0.00000000  0.00000000
C    -1.27541500  0.35246000  0.73285500
C    -1.91066600  1.55060700  0.26937700
O    -2.98465700  2.11915000  0.64533800
O    -3.73449100  1.57809100  1.65988900
H    -1.45313600  2.11731800 -0.53505300
C    -1.76487600 -0.40905500  1.73261200
H    -1.23112800 -1.30342400  2.02847300
H    -2.67648300 -0.14706900  2.23871200
H     0.74172800  0.79644900  0.08419300
H     0.43584700 -0.90956400  0.40705000
H    -0.18636200 -0.16296600 -1.06309600
H    -4.97902500  0.46120400  0.83627600
O    -5.51686900 -0.19188900  0.35512500
C    -6.86128900  0.25142800  0.32085800
H    -7.29329200  0.33841400  1.32386200
H    -6.96547500  1.21761000 -0.18504400
H    -7.43669500 -0.48854400 -0.23501500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.575106574985

Frequencies (cm^{-1}): 10.1471, 27.7748, 38.0539, 87.0979, 100.836, 110.9438, 137.1059, 195.0355, 284.1901, 326.1087, 341.5296, 426.7487, 538.7278, 686.0338, 702.315, 705.8841, 887.8438, 917.8234, 936.8733, 1007.9901, 1022.9773, 1044.4295, 1062.6045, 1079.9299, 1118.4918, 1172.301, 1275.4112, 1391.0825, 1417.1748, 1426.4511, 1435.5904, 1475.2964, 1488.4734, 1495.1813, 1495.7055, 1511.0856, 1538.8979, 1634.2231, 2978.968, 3017.5212, 3030.9915, 3078.8853, 3083.6835, 3121.3402, 3151.2898, 3158.5133, 3288.8489, 3570.966

***Syn*-(c-C(CH_3)=CH_2)CHOO + MeOH TS-AAAH 1**

```
C     0.00000000  0.00000000  0.00000000
C     0.51675500  1.41126900 -0.03344500
C     1.78305400  1.62146700  0.68923000
O     2.45499800  2.72087200  0.79974100
O     2.68397700  3.26309600 -0.53703400
H     1.93775600  0.97417200  1.55289100
C    -0.14412500  2.43172700 -0.58087600
H    -1.12708800  2.28001200 -1.00703100
H     0.28420200  3.42159300 -0.61707900
H    -0.06624500 -0.37973100  1.02287000
H    -0.98962100 -0.05939100 -0.44805000
H     0.66913700 -0.66309300 -0.55048500
H     2.96867800  1.89001600 -0.92876900
O     2.95861800  0.83893600 -0.69260200
C     4.25202700  0.47871900 -0.21222100
H     4.97534200  0.56002600 -1.02578900
H     4.57026900  1.13525100  0.60125400
H     4.22056800 -0.55266500  0.13637300
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.560854529436

Frequencies (cm^{-1}): -479.8971, 62.9127, 122.8995, 129.535, 161.1575, 171.6361, 216.099, 246.5275, 330.9919, 356.8205, 386.4787, 486.2873, 533.6191, 662.8756, 696.1549, 815.9399, 904.982, 973.9241, 993.0938,

1002.3725, 1034.1714, 1048.5974, 1085.2366, 1117.4553, 1177.3882, 1240.8512, 1284.3522, 1335.0551, 1412.5971, 1445.4677, 1462.6983, 1479.9088, 1486.5, 1493.0712, 1497.4848, 1512.3141, 1527.552, 1691.1137, 2006.7518, 3014.1154, 3023.7089, 3072.3612, 3074.7243, 3093.8169, 3100.5883, 3116.4076, 3146.8317, 3247.2789

(c-C(CH_3)=CH_2)CH(OMe)(OOH) (TS-AAAH 1- conformer)

```
C     0.00000000  0.00000000  0.00000000
C     1.13993900 -0.82462500  0.53852800
C     2.29680400 -0.91676200 -0.36792600
O     3.31718100 -1.71029600 -0.27128500
O     3.92955500 -1.52185800  1.04119500
H     2.08229300 -0.69252100 -1.41127600
C     1.07724900 -1.49443300  1.69171400
H     0.16608600 -1.48642000  2.27611500
H     1.92361800 -2.05601200  2.05622900
H    -0.35665800 -0.39174300 -0.95567100
H    -0.83558800  0.00652400  0.69664300
H     0.30476800  1.03391600 -0.17405100
H     3.82780100 -0.17206700  0.73787200
O     3.37290700  0.64705500  0.14821100
C     2.92175400  1.67301100  1.01595200
H     2.20203800  1.30202400  1.75165300
H     3.77764800  2.08662600  1.55545100
H     2.46232500  2.46565100  0.42570100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.632635509339

Frequencies (cm^{-1}): 48.4904, 99.7092, 116.0528, 160.9288, 187.7106, 202.7145, 225.5375, 258.9527, 325.5542, 375.3141, 404.487, 509.23, 550.456, 696.2657, 717.0647, 865.8757, 920.47, 954.4526, 965.6292, 998.3739, 1012.5188, 1041.814, 1076.7051, 1109.0824, 1176.289, 1207.7051, 1274.6354, 1346.5272, 1366.2129, 1394.0522, 1413.2954, 1448.7571, 1473.4474, 1478.0961, 1489.9387, 1494.9926, 1511.2663, 1718.7349, 2956.6092, 3003.4331, 3018.8551, 3061.6921, 3072.8739, 3109.6769, 3123.9222, 3147.7452, 3237.6489, 3717.9736

IRC:

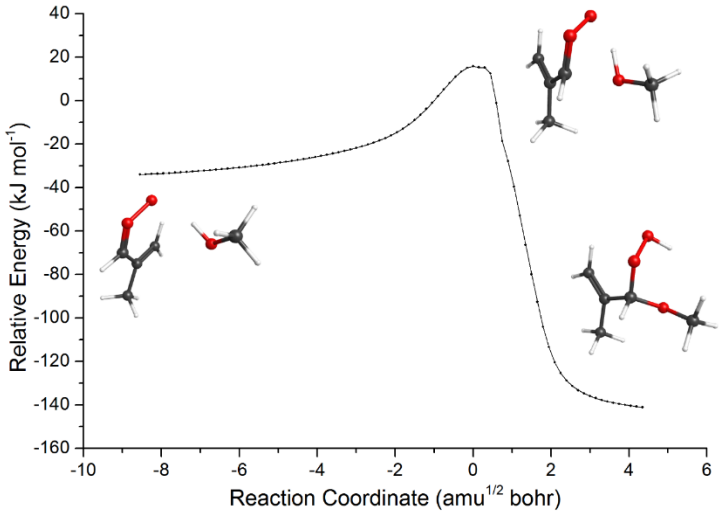


Figure S105: SCI 20 + MeOH TS-AAAH 1 IRC

***Syn*-(c-C(CH_3)=CH_2)CHOO + MeOH TS-AAAH 2**

```
C     0.00000000  0.00000000  0.00000000
C     1.13993900 -0.82462500  0.53852800
C     2.29680400 -0.91676200 -0.36792600
O     3.31718100 -1.71029600 -0.27128500
O     3.92955500 -1.52185800  1.04119500
H     2.08229300 -0.69252100 -1.41127600
C     1.07724900 -1.49443300  1.69171400
H     0.16608600 -1.48642000  2.27611500
H     1.92361800 -2.05601200  2.05622900
H    -0.35665800 -0.39174300 -0.95567100
```

```
H    -0.83558800   0.00652400   0.69664300
H     0.30476800   1.03391600  -0.17405100
H     3.82780100  -0.17206700   0.73787200
O     3.37290700   0.64705500   0.14821100
C     2.92175400   1.67301100   1.01595200
H     2.20203800   1.30202400   1.75165300
H     3.77764800   2.08662600   1.55545100
H     2.46232500   2.46565100   0.42570100
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.557801857095

Frequencies (cm^{-1}): -660.086, 80.4593, 133.5406, 142.9411, 154.8788, 166.2208, 249.7319, 275.1392, 328.6534, 361.2989, 380.2959, 469.0288, 534.7261, 668.0583, 705.926, 820.9719, 894.4838, 927.0534, 983.5234, 1011.3398, 1033.5095, 1052.4586, 1075.3072, 1094.0705, 1176.3196, 1207.2082, 1268.1618, 1330.169, 1364.2138, 1417.6595, 1441.2384, 1470.8803, 1483.5643, 1492.3808, 1494.4067, 1503.4012, 1533.0661, 1685.6296, 1929.5845, 3000.7029, 3026.0919, 3052.9511, 3071.2966, 3089.4242, 3114.4803, 3119.4497, 3143.0007, 3249.5065

(c-C(CH_3)=CH_2)CH(OMe)(OOH) (TS-AAAH 2-conformer)

```
C     0.00000000   0.00000000   0.00000000
C    -1.22157500  -0.87039500  -0.12328100
C    -2.42525200  -0.36863900   0.65690000
O    -3.54129300  -1.24819100   0.67906900
O    -4.13154600  -1.34081300  -0.65108800
H    -2.16889600  -0.37564200   1.72249000
C    -1.21711800  -2.02673300  -0.77581600
H    -0.31883400  -2.37779300  -1.26745400
H    -2.09320900  -2.65372500  -0.83729700
H    -0.16137900   0.99082900  -0.42733900
H     0.85246800  -0.45617000  -0.50020000
H     0.26246700   0.15612300   1.04994400
H    -5.00307000  -0.96595400  -0.46701800
O    -2.76733500   0.96419300   0.39013800
C    -2.92104900   1.38101500  -0.96700900
H    -2.63551700   2.43132600  -1.00529100
H    -3.95824200   1.28012000  -1.28809900
H    -2.29220200   0.80570300  -1.64634600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -421.627862112355

Frequencies (cm^{-1}): 66.8653, 114.679, 138.0062, 167.1785, 174.1108, 226.3255, 230.7328, 270.2669, 319.7034, 373.0137, 417.6876, 503.9122, 563.5972, 694.8214, 708.1143, 859.0233, 922.3731, 940.0218, 955.5642, 965.0974, 1016.6917, 1040.3734, 1079.7386, 1114.2941, 1172.8202, 1218.3001, 1267.4309, 1349.4037, 1360.2419, 1384.3626, 1417.4342, 1451.6072, 1475.375, 1479.1867, 1491.4335, 1496.7307, 1508.0246, 1716.2885, 3014.8233, 3021.7435, 3027.0625, 3068.4693, 3086.3357, 3105.9688, 3108.8032, 3144.0238, 3237.6666, 3762.024

IRC:

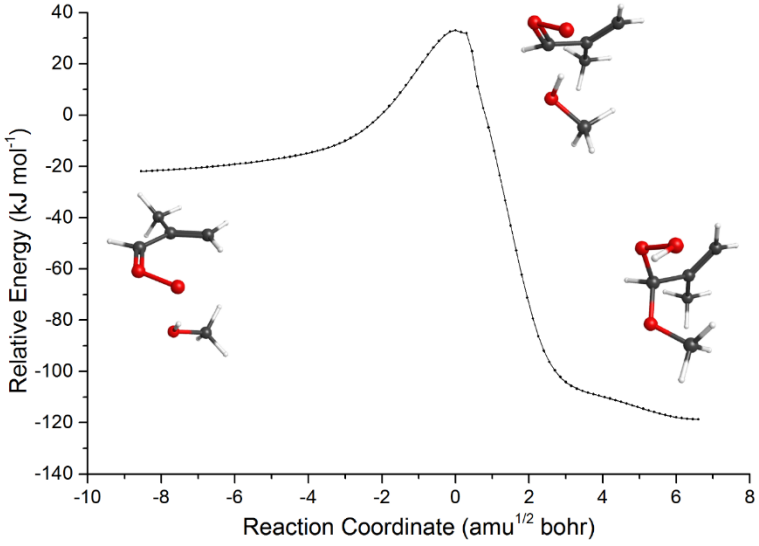


Figure S106: SCI 20 + MeOH TS-AAAH 2 IRC

7.21 sCI 21 + MeOH Reaction

Cyclopropenone oxide (SCI 21):

```
C     0.00000000  0.00000000  0.00000000
C     0.75397600  1.17398400  0.00000000
C     1.39625200 -0.00230500  0.00000000
H     2.32892700 -0.53763900  0.00000000
H     0.82441100  2.24895400  0.00000000
O    -1.08740000 -0.58862500  0.00000000
O    -0.91943800 -2.04538400  0.00000000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -265.409611101032

Frequencies (cm^{-1}): 214.4015, 222.1463, 468.1776, 548.9594, 745.3178, 770.1877, 869.2331, 959.1246, 991.219, 1045.1757, 1200.6748, 1512.5543, 1868.0469, 3242.1528, 3286.7569

Cyclopropenone oxide + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2)

```
C     0.00000000  0.00000000  0.00000000
O    -1.26649700 -0.07215400 -0.62834400
H    -1.65357800  0.84186400 -0.71448900
H    -0.05396400  0.49497900  0.97536500
H     0.72969000  0.53516900 -0.61679500
H     0.36305200 -1.01710400  0.15076100
C    -4.11076400  0.50033800 -0.23207900
C    -4.87551900 -0.63735800 -0.01118300
C    -3.92223100 -0.66904200 -0.95604200
H    -3.36827700 -1.20532200 -1.70422900
H    -5.63788100 -1.16613500  0.53531400
O    -3.81019700  1.67608700  0.04416500
O    -2.69691500  2.16909300 -0.78215200
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -381.041056144537

Frequencies (cm^{-1}): 44.3167, 77.8384, 102.9195, 105.9903, 157.702, 207.0088, 238.375, 312.1732, 483.6495, 556.8688, 773.8948, 790.4758, 876.6819, 943.5287, 946.6752, 1010.8583, 1050.0199, 1068.1426, 1156.2587, 1173.7362, 1236.0249, 1472.0976, 1488.918, 1493.3004, 1495.8014, 1523.0658, 1858.2756, 2980.8509, 3024.1495, 3073.7501, 3140.2132, 3251.2983, 3302.8284

Cyclopropenone oxide + MeOH TS-AAAH 1

```
C     0.00000000  0.00000000  0.00000000
O     0.96142400  0.53419600  0.89602500
H     0.89210900  1.65130100  0.90604000
H    -0.08716500  0.60762700 -0.90525000
H    -0.97882500 -0.03889100  0.48479900
H     0.28607800 -1.01677700 -0.27847600
C     2.67219100  1.14449300  0.05417700
C     3.62927600  0.15161800 -0.22590900
C     3.61805100  0.68273200  0.98974700
H     4.02519200  0.71865700  1.98424600
H     4.06772100 -0.54860400 -0.91513000
O     2.15092700  2.18173900 -0.50239400
O     1.34669800  2.85791000  0.53003600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -381.028117045846

Frequencies (cm^{-1}): -644.2091, 110.4283, 130.014, 142.6107, 211.0331, 278.1369, 293.7581, 397.1501, 512.8567, 557.5529, 740.7099, 804.3892, 872.8344, 936.196, 945.9391, 1000.6174, 1062.7642, 1072.948, 1173.6882, 1185.0732, 1199.7395, 1473.4815, 1478.8441, 1494.62, 1502.0628, 1509.133, 1721.0789, 1823.8712, 2997.1701, 3053.9177, 3060.9889, 3250.2623, 3288.9621

1-Methyoxycyclopropene 1-hydroperoxide (TS-AAAH 1 conformer)

```
C     0.00000000  0.00000000  0.00000000
O    -1.11281400  0.33917300  0.82513500
H    -2.87234000 -1.38679100  0.62877100
H    -0.29624700 -0.65788800 -0.81993600
H     0.71743000 -0.51241100  0.63633900
H     0.46586000  0.90019700 -0.41205400
C    -2.15887100  0.96600400  0.13998500
C    -2.09142500  2.34768900 -0.36633900
C    -2.78787200  2.15662100  0.71397200
H    -3.39561700  2.55208900  1.50735100
H    -1.71781500  3.01590500 -1.12126900
O    -2.88941900  0.04516700 -0.62770300
O    -3.59885700 -0.84470500  0.28518700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -381.096784151500

Frequencies (cm^{-1}): 82.4144, 108.9546, 172.9877, 222.0824, 255.9041, 303.7746, 409.8895, 425.1572, 541.6014, 599.6041, 682.4044, 769.3497, 884.9707, 900.2029, 949.9072, 978.6792, 1023.4284, 1073.5159, 1090.478, 1173.8794, 1217.8071, 1260.2434, 1375.6449, 1470.7521, 1491.6957, 1507.5412, 1689.4085, 3002.6378, 3060.0028, 3121.3004, 3244.6825, 3287.3025, 3718.1433

IRC:

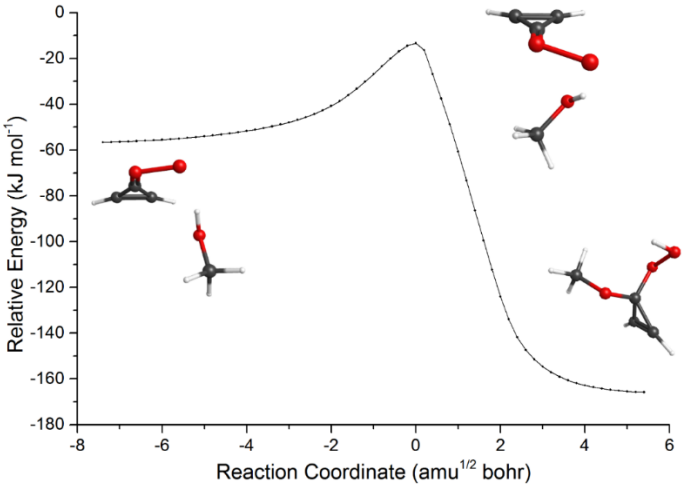


Figure S107: SCI 21 + MeOH TS-AAAH 1 IRC

Cyclopropenone oxide + MeOH TS-AAAH 2

```
C     0.00000000  0.00000000  0.00000000
O     0.85203600  0.84231700 -0.73728900
H     1.00518800  1.80984200 -0.21135700
H    -0.57097300  0.55685600  0.74849300
H     0.56380600 -0.78345800  0.52966500
H    -0.69409700 -0.50063400 -0.67747300
C     2.81526700  0.83950400 -0.21048700
C     3.53071900 -0.33186100 -0.50367400
C     2.98021900 -0.22532900  0.70086600
H     2.82176200 -0.65463900  1.67405300
H     4.13193800 -0.90604800 -1.18682500
O     2.90404900  2.10707200 -0.39076800
O     1.80451500  2.72951500  0.36949700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -381.026573942057

Frequencies (cm^{-1}): -567.7404, 40.1512, 146.426, 187.9263, 227.472, 254.0857, 345.0806, 391.6888, 471.2298, 549.6461, 746.7201, 804.7365, 875.3137, 950.5334, 962.3448, 996.452, 1082.0915, 1090.3093, 1171.3538, 1187.5339, 1195.2656, 1380.7596, 1483.9242, 1488.5791, 1499.2125, 1510.1079, 1725.6948, 1892.4715, 2936.1271, 3021.2445, 3066.7101, 3249.1551, 3284.8238

1-Methyoxycyclopropene 1-hydroperoxide (TS-AAAH 2- conformer)

```
C     0.00000000  0.00000000  0.00000000
O    -0.83695400  0.72596800 -0.88839700
H    -3.30481200  0.10089300 -0.36242900
H     0.34740300 -0.87264400 -0.54817800
H    -0.54723500 -0.32199400  0.88956100
H     0.86935000  0.58965500  0.30728700
```

```
C    -1.38142000  1.91262400 -0.37895700
C    -0.73001600  3.21829000 -0.52695600
C    -0.73876400  2.71704800  0.67400500
H    -0.45755600  2.80747100  1.70834900
H    -0.44771700  4.00930800 -1.19880300
O    -2.76971900  1.90662000 -0.55166500
O    -3.32781900  0.83619400  0.26701000
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -381.095367184994

Frequencies (cm^{-1}): 48.0246, 122.478, 180.9771, 232.1753, 265.7047, 313.0066, 390.6751, 455.7738, 545.1679, 564.555, 682.8823, 749.4225, 884.8477, 904.4887, 946.123, 970.7543, 1038.7711, 1089.9838, 1110.8889, 1173.6442, 1208.947, 1266.9571, 1362.5534, 1474.8912, 1493.7315, 1508.4422, 1682.1039, 2997.5821, 3050.8137, 3118.3469, 3236.645, 3277.8632, 3737.6673

IRC:

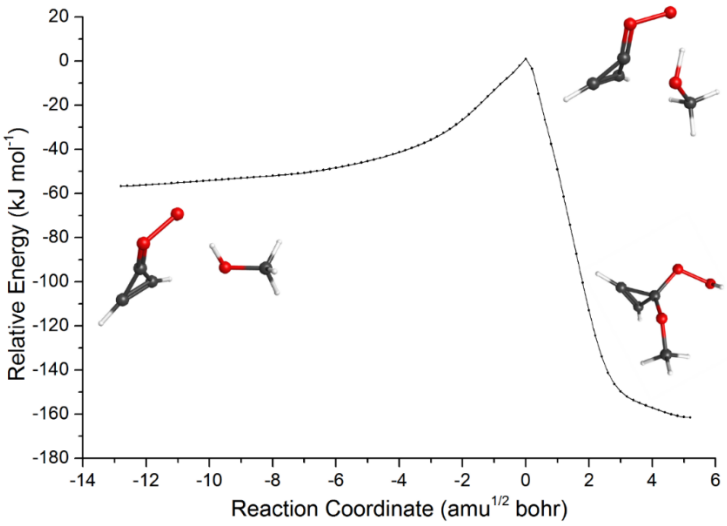


Figure S108: SCI 21 + MeOH TS-AAAH 2 IRC

7.22 sCI 22 + MeOH Reaction

1,3 dioxolane-2-carbonyl oxide (SCI 22):

```
C    0.00000000  0.00000000  0.00000000
O   -1.44079100 -0.01599500 -0.16639500
C   -1.84341100 -1.26409900 -0.08596100
O   -3.02275700 -1.64248800 -0.08449100
O   -4.00773900 -0.57353900 -0.12863700
O   -0.86227000 -2.15981600 -0.00021400
C    0.38705900 -1.46212400 -0.22523200
H    0.71103300 -1.66593600 -1.24468700
H    1.11647000 -1.84126300  0.48356500
H    0.21476800  0.35157600  1.00742300
H    0.41295500  0.68535800 -0.73319600
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -417.039649784178

Frequencies (cm^{-1}): 131.107, 159.3723, 223.8473, 239.5523, 490.2996, 675.0142, 694.1915, 711.9686, 824.508, 884.6819, 914.7891, 974.0527, 1030.1436, 1085.5606, 1153.9076, 1229.4289, 1252.6023, 1268.8437, 1389.3243, 1458.0667, 1524.3951, 1530.4661, 1702.4911, 3073.9995, 3081.6196, 3138.7596, 3152.818

1,3 dioxolane-2-carbonyl oxide + MeOH PRC (for both TS-AAAH 1 and TS-AAAH 2)

```
C    0.00000000  0.00000000  0.00000000
O   -0.85601500  1.16348700  0.14752300
C   -1.03142900  1.67162800 -1.04206000
O   -1.86085900  2.55274100 -1.33923400
O   -2.84640300  2.80181500 -0.28628900
O   -0.22492600  1.19967600 -1.97743100
C    0.69165400  0.27192600 -1.33507200
H    1.65447400  0.76895300 -1.23036000
H    0.78191100 -0.60060300 -1.97379300
H   -0.64829800 -0.87322300 -0.01925200
H    0.67032000 -0.02983000  0.85229300
C   -4.58771900 -0.12266800 -1.32275500
O   -3.41936800  0.15330200 -0.57085900
H   -3.40927400  1.11308600 -0.33790100
H   -4.55224000 -1.16884800 -1.62797400
H   -4.65290800  0.49801000 -2.22258900
H   -5.49736300  0.03041100 -0.73261500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -532.669837185152

Frequencies (cm^{-1}): 37.3406, 59.2215, 86.6096, 105.4578, 141.3926, 151.7848, 196.1099, 218.5035, 241.77, 291.0121, 492.6396, 681.5005, 709.5481, 714.0304, 836.4141, 888.7327, 902.2452, 924.1128, 976.8893, 1024.3893, 1066.5462, 1091.1717, 1145.616, 1153.5615, 1175.3367, 1229.1725, 1253.1781, 1277.8559, 1388.9647, 1462.2378, 1476.0386, 1483.6316, 1494.2941, 1515.9358, 1522.5333, 1526.6503, 1687.3908, 2983.3221, 3025.139, 3075.9724, 3078.3588, 3091.7816, 3146.8449, 3162.9089, 3306.363

1,3 dioxolane-2-carbonyl oxide + MeOH TS-AAAH 1

```
C    0.00000000  0.00000000  0.00000000
O   -1.09600700  0.91127200 -0.21774200
C   -1.78403500  0.43195600 -1.24816800
O   -2.74564700  1.08254000 -1.80431200
O   -3.71474000  1.42636200 -0.74581000
O   -1.07301900 -0.37064800 -2.03074800
C    0.21419500 -0.58602900 -1.39644700
H    0.96442100 -0.05304700 -1.97801800
H    0.42109900 -1.65192200 -1.40041100
H   -0.31174500 -0.74730300  0.72729500
H    0.84069000  0.57522300  0.37414600
C   -3.63304200 -1.75239800 -0.91566400
O   -2.95343900 -0.75722200 -0.16386200
H   -3.52817800  0.19913700 -0.21924700
H   -4.50954000 -2.09703100 -0.36188300
H   -2.96834600 -2.60160600 -1.07981500
H   -3.96415300 -1.36761900 -1.88405900
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -532.663543716704

Frequencies (cm^{-1}): -612.7132, 78.3647, 105.5709, 127.0871, 162.4785, 188.1438, 222.105, 310.5394, 347.2619, 432.3106, 488.6437, 625.6306, 692.8766, 730.3669, 863.0419, 887.5237, 900.9811, 965.9949, 1010.7964, 1033.4503, 1059.5446, 1079.8296, 1151.0093, 1175.7501, 1188.1214, 1222.481, 1244.1616, 1257.8958, 1387.7532, 1433.8934, 1470.6266, 1479.7406, 1493.6627, 1505.6505, 1513.9433, 1522.9797, 1561.8276, 1847.5299, 3004.5083, 3060.466, 3075.6865, 3076.6672, 3081.9069, 3136.582, 3153.4294

2-methyloxy, 1,3 dioxolane, 2-hydroperoxide (TS-AAAH 1 conformer)

```
C    0.00000000  0.00000000  0.00000000
O   -1.33566700 -0.42446600 -0.29866800
```

```
C    -2.20546000   0.19666800   0.57868600
O    -2.75468800  -0.72992500   1.52429900
O    -3.37828300  -1.81773000   0.80853200
O    -1.49087900   1.08812000   1.37307000
C    -0.13366400   0.62610300   1.38303300
H     0.00468000  -0.10340100   2.18270800
H     0.51290700   1.48439000   1.54604700
H     0.32116100   0.72525500  -0.75035500
H     0.65642000  -0.86733800  -0.02298100
C    -4.09006700   1.64532400   0.59159100
O    -3.19490200   0.80921100  -0.15174300
H    -4.23277600  -1.43529200   0.55972700
H    -4.84782500   1.96704900  -0.11711900
H    -3.56514700   2.51292000   0.98987700
H    -4.55737300   1.09816700   1.41163400
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -532.722729508497

Frequencies (cm^{-1}): 44.7492, 98.8525, 127.3573, 158.2447, 178.1621, 188.5424, 258.3343, 283.8156, 432.1335, 455.3325, 515.2662, 608.9562, 671.29, 725.8338, 829.3793, 893.3333, 951.0161, 957.2551, 1014.9334, 1019.0622, 1055.946, 1095.18, 1127.461, 1150.7584, 1175.4268, 1212.2045, 1222.8223, 1236.3263, 1259.633, 1384.3684, 1391.909, 1397.7495, 1473.486, 1489.0833, 1514.9061, 1516.2909, 1529.1506, 3033.281, 3036.725, 3047.3195, 3097.5445, 3103.7097, 3123.6376, 3136.4688, 3726.5481

IRC:

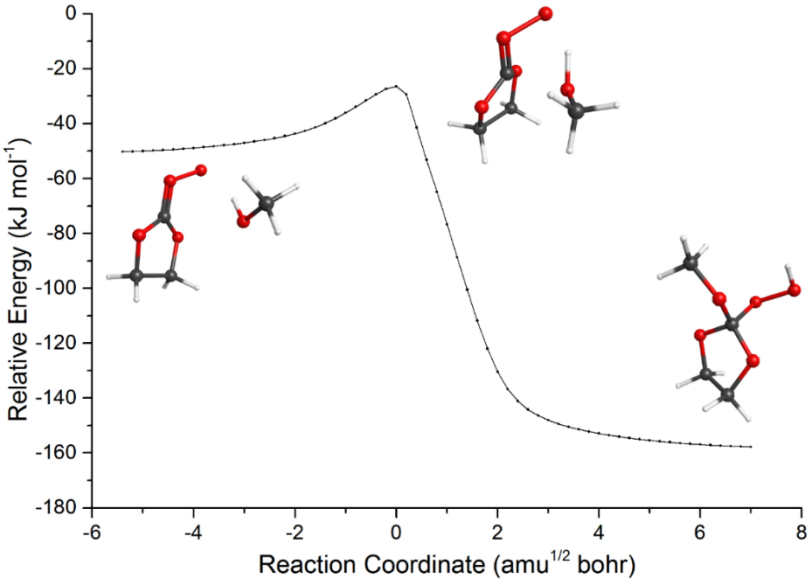


Figure S109: SCI 22 + MeOH TS-AAAH 1 IRC

1,3 dioxolane-2-carbonyl oxide + MeOH TS-AAAH 2:

```
C     0.00000000   0.00000000   0.00000000
O     1.19941300  -0.75476800   0.27785700
C     1.56795400  -1.34368600  -0.86076000
O     2.42182000  -2.30716600  -0.90641600
O     3.67084400  -1.85648900  -0.27707700
O     0.60358000  -1.38423900  -1.76744200
C    -0.55627000  -0.70005500  -1.24028900
H    -1.31050000  -1.45027700  -1.00865000
H    -0.92536400  -0.01915700  -2.00144400
H     0.27006900   1.03751000  -0.18743200
H    -0.64145100  -0.06887700   0.87301500
C     3.02063500   1.26696100  -0.94950300
O     2.89745800  -0.00982000  -1.54132700
H     3.54123200  -0.74972500  -0.96841500
H     2.79887600   1.24610300   0.12316700
H     2.34501500   1.97010600  -1.44263800
H     4.04247300   1.63738400  -1.07252500
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -532.657710199563

Frequencies (cm^{-1}): -708.5404, 104.1625, 116.4468, 148.2383, 163.4438, 194.6267, 223.6175, 277.1467, 352.8379, 409.2509, 485.5175, 624.248, 700.4385, 714.1145, 869.0447, 881.1159, 890.8027, 958.3607,

972.354, 1032.5904, 1060.7618, 1093.1304, 1151.6779, 1174.1315, 1186.7218, 1221.3072, 1242.644, 1254.6162, 1355.6145, 1388.853, 1441.3068, 1474.1012, 1496.4608, 1502.7002, 1521.9053, 1524.0664, 1553.6898, 1896.0645, 2984.7851, 3035.6715, 3052.253, 3074.7816, 3080.4217, 3133.2467, 3148.7978

2-methyloxy, 1,3 dioxolane, 2-hydroperoxide (TS-AAAH 2- conformer):

```
C     0.00000000  0.00000000  0.00000000
O     1.34350900  0.42993800  0.22193700
C     1.93975800  0.50206000 -1.03557500
O     2.38399200 -0.75642400 -1.50859000
O     3.39841700 -1.26939200 -0.61588500
O     0.94673200  0.86751300 -1.94798000
C    -0.33827200  0.63614400 -1.35295300
H    -0.92314400 -0.01811100 -1.99695000
H    -0.84681600  1.59563900 -1.24868100
H    -0.61309800  0.36231400  0.82105400
H    -0.04237200 -1.08950500 -0.04004900
C     2.78238200  2.67662200 -0.57397900
O     3.01540200  1.34388600 -1.03946400
H     4.17950800 -0.78193400 -0.91810900
H     2.53732900  2.68032700  0.48705600
H     1.98255400  3.14822600 -1.14563600
H     3.71186000  3.21317100 -0.74128700
```

DF-HF//DF-LCCSD(T)-F12a Energy (Hartree): -532.726764520097

Frequencies (cm^{-1}): 75.1137, 92.6515, 132.3072, 158.4723, 171.1916, 235.8528, 294.8405, 303.3337, 404.0349, 464.9795, 531.929, 646.3847, 683.1319, 709.3371, 830.3469, 881.615, 944.8451, 954.6628, 1033.603, 1049.5056, 1058.2542, 1083.6142, 1121.2989, 1157.0047, 1175.8244, 1200.2043, 1233.7696, 1237.016, 1261.2801, 1382.2417, 1387.4713, 1399.041, 1476.1123, 1492.1427, 1509.3588, 1519.602, 1531.5914, 3038.4948, 3043.392, 3048.2927, 3096.2565, 3105.2597, 3121.4219, 3138.5936, 3726.0723

IRC:

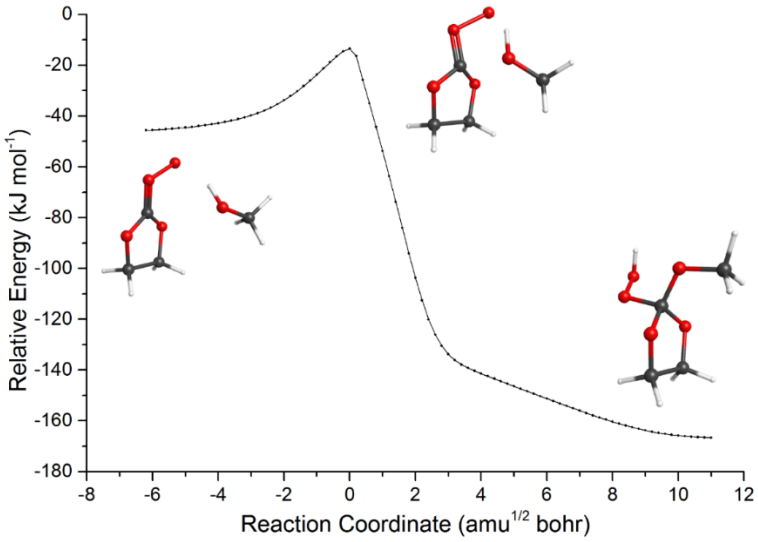


Figure S110: SCI 20 + MeOH TS-AAAH 2 IRC

8.0 Cartesian Co-ordinates for Chapter 5: HFO-sCIs reactions

8.1 HFO derived Criegee intermediates

Compound: sCI 1 (HCHOO)	**Energy (kJ mol^{-1}):** -189.400847568329
Reaction Coordinates: 6 -1.068412 0.202194 -0.000000 8 -0.003231 -0.459294 -0.000000 8 1.179333 0.194958 0.000000 1 -1.021445 1.284352 -0.000000 1 -1.976903 -0.382830 0.000002	**Frequencies (cm^{-1}):** 527.7609,673.7578, 912.8476, 951.0664, 1242.0554, 1402.0013, 1543.5428, 3118.1651, 3267.9600

Compound: sCI 23 (*Syn*-CF_3CHOO)	**Energy (kJ mol^{-1}):** -526.2050097
Reaction Coordinates: 6 0.544326 0.408563 0.000000 6 -0.965669 0.489858 0.000000 8 -1.720767 -0.517005 -0.000000 8 -1.205470 -1.752491 -0.000000 1 -1.466000 1.447260 0.000000 9 1.014961 -0.207422 1.087387 9 1.014961 -0.207422 -1.087387 9 1.014961 1.672420 0.000000	**Frequencies (cm^{-1}):** 83.4264, 179.3385, 247.1426, .2827, 478.5065, 507.3023, ,536.2006, 591.5612, 758.0400, 772.8798, 885.1813, 947.2031, 1151.7894, 1176.1918, 1243.1084, 1364.7774, 1539.7613, ,3220.6741

Compound: sCI 24 (*Anti*-CF_3CHOO)	**Energy (kJ mol^{-1}):** -526.2059784
Reaction Coordinates: 6 -0.814124 -0.010987 0.000000 6 0.599627 -0.529934 0.000001 8 1.532385 0.307937 -0.000000 8 2.803565 -0.122750 -0.000000 1 0.814702 -1.591587 0.000002 9 -0.871266 1.317793 -0.000001 9 -1.465219 -0.472475 -1.084562 9 -1.465219 -0.472472 1.084563	**Frequencies (cm^{-1}):** 53.4225, 186.5103, 191.8874, 388.9843, 394.1412, 416.4183, 552.7580, 560.7356, 699.8777, 883.4653, 889.1822, 988.9465, 1131.2630, 1171.7198, 1270.0033, 1355.9541, 1546.1599, 3188.0668

Compound: sCI 25 (*Syn*-CF_3CFOO)	**Energy (kJ mol^{-1}):** -625.3731138
Reaction Coordinates: 6 0.267347 0.734443 0.000000 6 -0.668190 -0.480912 0.000000 8 -0.317071 -1.670141 0.000000 8 1.031885 -1.966693 0.000000 9 -1.951916 -0.250006 0.000000 9 1.031885 0.735046 1.087938 9 1.031885 0.735046 -1.087938 9 -0.480015 1.843635 0.000000	**Frequencies (cm^{-1}):** 58.8820, 180.2110, 218.4479, 269.2791, 292.9260, ,363.8515, 484.2548, 493.0742, 582.0033, 631.0249, 653.9584, 780.2000, 927.2456, 1158.8972, 1195.1079, 1198.3764, 1398.0465, 1580.9318

Compound: sCI 26 (*Anti*-CF_3CFOO)	**Energy (kJ mol^{-1}):** -625.3783361

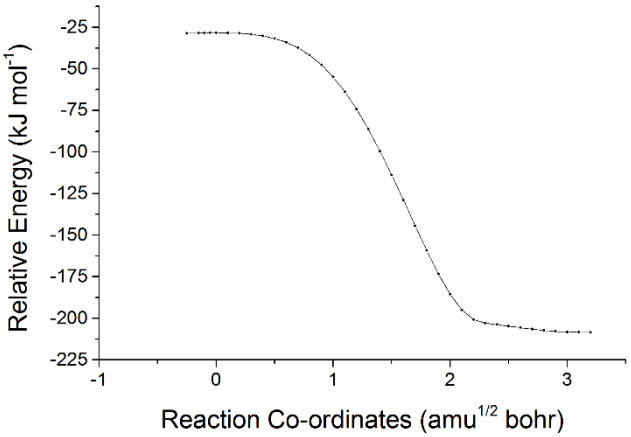
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.277404 -0.919423 0.000000 6 0.018963 0.571292 0.000000 8 1.190937 0.987253 0.000000 8 1.417147 2.337638 0.000000 9 -0.997920 1.369496 0.000000 9 0.847756 -1.621862 0.000000 9 -0.997920 -1.235503 1.084149 9 -0.997920 -1.235503 -1.084149	41.8080, 154.2443, 183.9192, 293.0541, 346.5294, 372.3393, 406.8758, 515.4784, 576.4030, 659.0393, 728.8220, .5490, 906.9387, 1155.2541, 1155.7283, 1229.1869, 1400.7892, 1601.0242

8.2 HFO-sCIs + HCHO

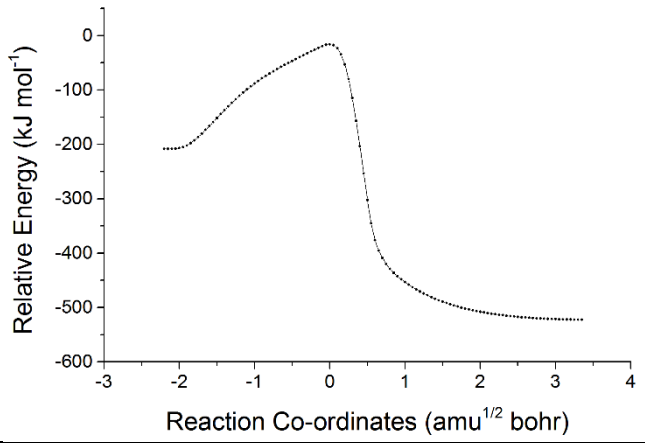
Compound: HCHO	**Energy (kJ mol^{-1}):** -114.386051813463
Reaction Coordinates: 6 -0.000000 -0.526970 -0.000000 8 0.000000 0.673271 0.000000 1 -0.000000 -1.112173 0.938294 1 -0.000000 -1.112173 -0.938294	**Frequencies (cm^{-1}):** 1198.1780, 1262.9587, 1530.2218, 1813.2454, 2885.3911, 2940.0951

8.2.1 sCI 1 + HCHO

Compound: sCI 1 + HCHO PRC	**Energy (kJ mol^{-1}):** -303.798329359066
Reaction Coordinates: 6 -1.568793 0.372025 -0.025055 8 -1.363160 -0.828477 -0.072239 1 -1.657461 0.978246 -0.937211 1 -1.783433 0.887713 0.921406 6 1.125843 -0.947653 0.216022 1 1.548975 -1.796415 -0.304241 1 0.693612 -0.991078 1.204393 8 1.223576 0.146118 -0.385058 8 0.621585 1.229271 0.203528	**Frequencies (cm^{-1}):** 74.8509, 103.5754, 200.3540, 278.7803, 321.9694, 483.9337, 530.6353, 685.8280, 894.8752, 1002.3931, 1157.3881, 1239.1392, 1254.7518, 1413.4948, 1517.9212, 1564.5284, 1716.1748, 2949.5550, 3015.1791, 3137.8091, 3282.9945

Compound: sCI 1 + HCHO TS_c	**Energy (kJ mol^{-1}):** -303.798797734635
Reaction Coordinates: 6 -1.487001 0.353271 0.010278 6 1.049308 -0.925024 0.242888 8 -1.242190 -0.844058 -0.122774 1 -1.676186 0.993769 -0.859690 1 -1.706764 0.792026 0.991823 1 1.451806 -1.797973 -0.253471 1 0.671776 -0.928437 1.253159 8 1.183806 0.153845 -0.385267 8 0.544074 1.236604 0.176688	**Frequencies (cm^{-1}):** -118.7612, 95.7382, 234.5586, 345.4726, 399.7370, 537.6674, 590.3087, 710.8836, ,903.1654, 1013.8378, 1146.8734, 1233.3069, 1247.5743, 1407.0484, 1501.0072, 1558.8347,6 1669.3075, 2963.4503, 3032.3718, 3142.2215, 3285.8554
IRC:  	

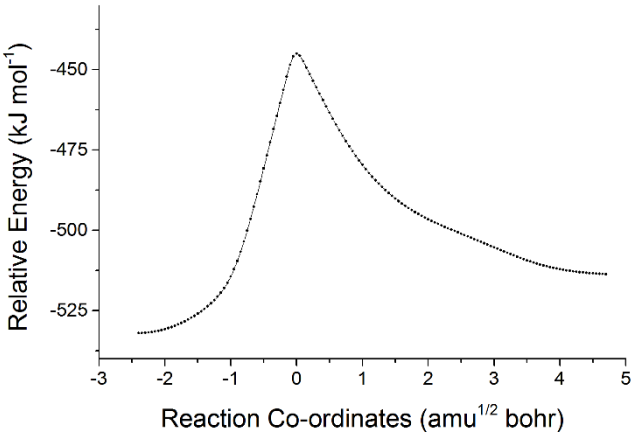
Compound: sCI 1 + HCHO HOZ	**Energy (kJ mol^{-1}):** -303.878537225920
Reaction Coordinates: 6 1.118320 0.321848 -0.133769 8 0.000001 1.185457 -0.000005 1 -1.921112 0.617737 -0.541368 1 -1.444573 0.296995 1.177335 6 -1.118317 0.321850 0.133776 1 1.921105 0.617728 0.541390 1 1.444593 0.296997 -1.177322 8 0.669522 -0.948459 0.290933 8 -0.669527 -0.948454 -0.290938	**Frequencies (cm^{-1}):** 163.2068, 371.3640, 708.1220, 750.0747, 861.2831, 925.9772, 954.1919, 1041.1937, 1086.5608, 1142.2906, 1145.0755, 1218.3662, 1222.1489, 1370.6921, 1414.6761, 1519.1635, 1529.2393, 3014.9743, 3016.9237, 3096.0501, 3097.3415

Compound: sCI 1 + HCHO TS_d	**Energy (kJ mol^{-1}):** -303.807859688040
Reaction Coordinates: 6 -1.204271 0.195038 -0.204006 6 1.013769 0.309599 0.311038 8 -0.063824 1.098505 -0.089969 1 -2.002883 0.746061 0.330078 1 -1.513034 0.164053 -1.270020 1 1.829321 0.907119 0.746096 1 0.499372 -0.213545 1.248177 8 1.327196 -0.694146 -0.413719 8 -0.972093 -0.983297 0.291623	**Frequencies (cm^{-1}):** -963.8912, 228.1363, 313.3548, 468.8414, 547.0783, 739.8412, 811.6421, 907.5403, 946.3363, 992.9338, 1120.5118, 1130.5080, 1233.0628, 1263.7100, 1269.1727, 1337.9092, 1376.8823, 2112.8107, 2855.1673, 2878.1255, 2969.9759
IRC:  	

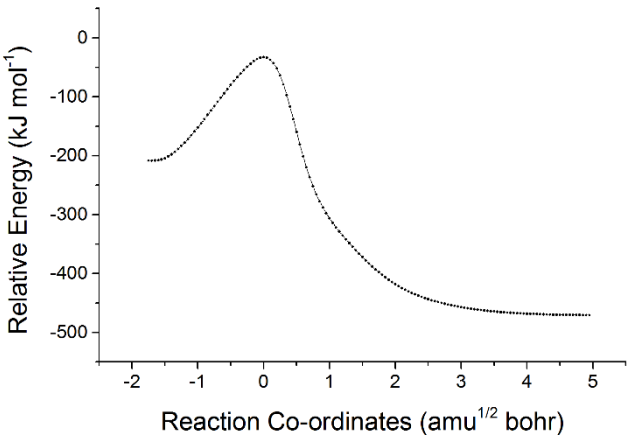
Compound: sCI 1 + HCHO HAE con 1	**Energy (kJ mol^{-1}):** -303.997300763222
Reaction Coordinates: 6 -1.305850 0.289288 -0.231552 6 0.940582 0.108875 0.562488 8 -0.113961 0.892842 -0.041694 1 2.217403 0.120005 -0.894036 1 -1.978441 0.989618 -0.741641 1 0.504100 -0.659409 1.192085 1 1.510830 0.833055 1.143035 8 1.709527 -0.532334 -0.400318 8 -1.603351 -0.819539 0.106380	**Frequencies (cm^{-1}):** 70.4857, 248.4112, 299.0854, 381.9429, 547.6482, 755.4857, 887.0359, 1041.6181, 1059.1008, 1083.6745, 1160.7621, 1288.9470, 1396.6575, 1400.1716, 1435.6149, 1511.3613, 1800.1743, 3033.9528, 3065.1750, 3152.7357, 3803.4239

Compound: sCI 1 + HCHO TS_{ISO}	**Energy (kJ mol^{-1}):** -303.991840303773
Reaction Coordinates: 6 1.312004 0.313671 -0.206358 6 -0.930064 0.023397 0.582096 8 0.087792 0.853126 -0.000989 1 -1.526009 -0.131808 -1.262605 1 1.954963 1.077031 -0.660097 1 -0.464130 -0.834440 1.062866 1 -1.444117 0.655822 1.304341 8 -1.842940 -0.400862 -0.395533 8 1.653606 -0.800891 0.059156	**Frequencies (cm^{-1}):** -422.7115, 38.5836, 260.2890, 315.7944, ,510.8464, 752.0342, 886.7029, 1041.3061, 1062.2173, 1136.1380, 1174.7639, 1275.0176, 1301.7533, 1400.7928, 1454.4948, 1531.3924, 1804.1671, 3042.0345, 3062.5202, 3115.8914, 3834.6789

Compound: sCI 1 + HCHO HAE con 2	**Energy (kJ mol^{-1}):** -304.001807069015
Reaction Coordinates: 6 -1.260600 -0.237487 -0.167386 6 1.023485 -0.390383 0.400595 8 -0.168614 -1.005790 -0.171215 1 0.907472 1.414099 -0.227820 1 -2.108826 -0.788602 -0.589538 1 1.764187 -1.182273 0.386199 1 0.774725 -0.093172 1.420070 8 1.496495 0.660749 -0.360576 8 -1.317239 0.897188 0.233271	**Frequencies (cm^{-1}):** 134.0932, 255.9643, 311.9088, 498.3134, 561.1357, 795.3260, 864.0522, 1045.5382, 1057.3010, 1110.4985, 1185.2944, 1293.0581, 1394.8699, 1405.6822, 1444.0186, 1510.2254, 1767.9081, 3044.7503, 3055.0210, 3155.2797, 3770.5265

Compound: sCI 1 + HCHO TS_{HAE}	**Energy (kJ mol^{-1}):** -303.962565700012
Reaction Coordinates: 6 1.259724 0.228825 -0.065861 6 -1.300930 0.415269 0.217050 8 0.390711 1.135692 -0.108964 1 -0.140029 -1.130261 0.047319 1 2.302132 0.521079 -0.236182 1 -1.881506 1.181054 -0.297803 1 -1.172603 0.572406 1.291527 8 -1.283919 -0.759522 -0.264454 8 1.035612 -1.002275 0.159419	**Frequencies (cm^{-1}):** -1115.5862, 186.3394, 274.1524, 418.1722, 517.4046, 579.7763, 825.7630, 933.1747, 1065.4507, 1221.2134, 1269.0745, 1326.4903, 1369.5579, 1384.3739, 1426.3933, 1614.5353, 1664.1975, 1769.6394, 3013.1948, 3043.6088, 3103.6379
IRC:  	

Compound: sCI 1 + HCHO $C_{FA}1$	**Energy (kJ mol^{-1}):** -303.990619638538
Reaction Coordinates: 6 1.657241 0.078650 -0.000000 8 1.043083 -1.098158 -0.000000 1 0.062756 -0.961278 0.000000 1 2.745848 -0.055528 0.000001 8 1.117502 1.158015 -0.000000 6 -2.029026 0.516294 -0.000000 1 -3.098216 0.781136 -0.000000 1 -1.289414 1.329652 0.000001 8 -1.684368 -0.642813 0.000000	**Frequencies (cm^{-1}):** 79.6236, 129.7900, 169.6478, 170.9258, 222.4930, 278.0783, 683.5053, 929.9644, 1069.2322, 1203.2888, 1228.4469, 1278.6536, 1380.1043, 1433.9700, 1520.6897, 1759.5075, 1791.2246, 2935.6401, 3032.6033, 3035.6839, 3329.9795

Compound: sCI 1 + HCHO TS_{FAc}	**Energy (kJ mol^{-1}):** -303.798809356950
Reaction Coordinates: 6 -1.240479 0.362821 -0.185443 6 1.098625 0.163043 0.257745 8 0.375297 1.190354 -0.047479 1 -1.744598 1.114643 0.430772 1 -1.336379 0.488679 -1.266462 1 1.536373 0.118717 1.267026 1 1.992081 -0.143278 -0.499480 8 0.778126 -0.994917 -0.319869 8 -1.102967 -0.787180 0.321638	**Frequencies (cm^{-1}):** -1096.7712, 206.5170, 256.9022, 324.0747, 431.0549, 572.4996, 727.5382, 839.5537, 918.9246, 1138.6108, 1158.0605, 1191.6131, 1205.9149, 1326.2421, 1374.7565, 1428.0091, 1525.1102, 2292.9905, 2959.8703, 2995.5443, 3072.2430
IRC:  	

Compound: sCI 1 + HCHO $C_{FA}2$	**Energy (kJ mol^{-1}):** -303.977039930179
Reaction Coordinates: 6 -1.065592 -0.087673 -0.000001 8 -0.608544 1.017095 -0.000001 1 -0.449781 -0.999539 -0.000001 8 -2.394409 -0.311317 0.000001 1 -2.569904 -1.260625 0.000001 6 2.137059 0.348295 0.000001 1 2.195113 0.930061 0.935342 1 2.195122 0.930065 -0.935336 8 2.028034 -0.851239 -0.000001	**Frequencies (cm^{-1}):** 62.0233, 85.0729, 96.4283, 104.1922, 151.3635, 200.7762, 548.5041, 664.7080, 1053.7673, 1121.0790, 1195.0673, 1262.7951, 1275.3896, 1425.0166, 1531.7929, 1794.9661, 1835.5258, 2912.6865, 2973.8170, 2995.6876, 3779.8452

Compound:	HCOOH conformer 1	**Energy (kJ mol^{-1}):**	-189.590120303627
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 0.000000 0.421050 -0.000000 8 1.158545 0.117329 -0.000000 8 -1.028178 -0.446131 0.000000 1 -0.659713 -1.343779 0.000000 1 -0.383224 1.447894 -0.000000		628.6127, 676.8905, 1051.6911, 1121.3699, ,1298.0934, 1401.7983, 1811.5029, 3048.9648, 3717.6132	

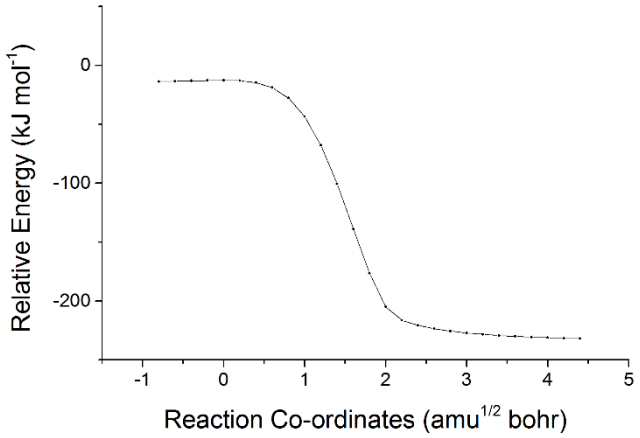
Compound:	HCOOH conformer 2	**Energy (kJ mol^{-1}):**	-189.583325855473
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 0.133997 0.361764 -0.000000 8 1.173188 -0.220201 0.000000 8 -1.056592 -0.278816 -0.000000 1 -1.779073 0.361263 0.000001 1 0.042323 1.460290 -0.000000		530.6018, 659.6880, 1032.5549, 1103.7723, 1268.4932, 1413.8078, 1855.6257, 2962.7301, 3780.4926	

8.2.2 sCIs 23 & 24 + HCHO & sCIs 1 + CF_3CHO

Compound:	sCI 23 + HCHO PRC	**Energy (kJ mol^{-1}):**	-640.600757425560
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 -1.180344 -0.230641 -0.046857 6 -0.299183 0.435311 0.995105 1 -0.446023 0.217189 2.043332 8 0.555870 1.315583 0.742164 8 0.850811 1.621339 -0.538900 9 -1.964927 -1.112890 0.600682 9 -0.513822 -0.882972 -0.993276 9 -1.975264 0.679816 -0.627729 8 2.104802 -1.100010 0.536169 6 2.603324 -0.596540 -0.440591 1 2.258798 -0.835449 -1.459457 1 3.438696 0.118587 -0.362384		37.0708, 60.8826, 81.7946, 97.3619, 111.0942, 164.0783, 188.0260, 210.5000, 265.4560, 327.3318, 475.0201, 506.6223, 536.7568, 585.0303, 757.4736, 803.4917, 880.2936, 928.3002, 1153.7845, 1170.7827, 1191.6829, 1250.4028, 1262.9443, 1368.9269, 1530.1666, 1560.6252, 1782.9473, 2922.5875, 2988.1962, 3218.3068	

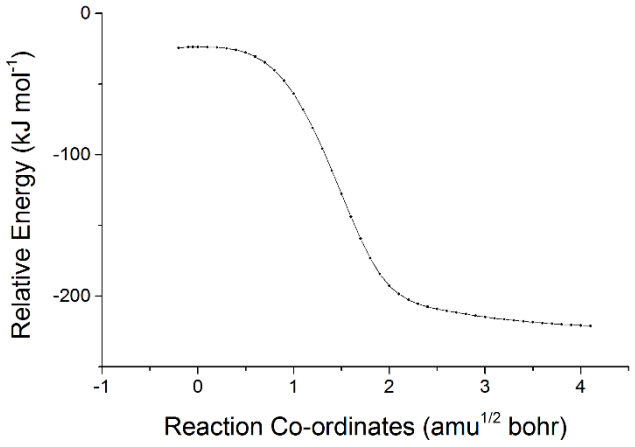
Compound:	sCI 23 + HCHO TS_c	**Energy (kJ mol^{-1}):**	-640.598646446407
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 1.092215 -0.129997 0.058184 6 0.100620 0.466841 -0.934798 1 0.343043 0.361471 -1.984193 8 -0.797561 1.308568 -0.687912 8 -1.272647 1.384786 0.588980 9 1.764815 -1.099970 -0.580750 9 0.611298 -0.619326 1.188676 9 1.973002 0.848592 0.363137 8 -1.513961 -1.198018 -0.587087 6 -2.163773 -0.843793 0.385501 1 -1.799910 -0.986918 1.408525 1 -3.186182 -0.459212 0.270934		-101.5617, 38.4107, 137.2510, 151.3563, 177.4183, 217.1369, 308.7619, 321.1385, 348.7483, 452.6528, 476.9346, 513.6888, 538.4700, 575.6568, 755.0955, 846.8308, 874.2992, 926.7008, 1124.3981, 1158.5445, 1168.3125, 1255.2191, 1280.9832, 1368.3635, 1515.2006, 1562.4061, .6061, 2970.6576, 3052.7393, 3203.3552	

IRC



Compound: sCI 23 + HCHO HOZ1	**Energy (kJ mol^{-1}):** -640.693594205454
Reaction Coordinates: 6 -1.139558 0.021002 0.054719 6 0.170641 0.051083 -0.760444 1 -0.090393 0.101412 -1.820168 8 0.948084 -1.114764 -0.588504 8 1.785506 -0.749925 0.551876 6 2.154623 0.552911 0.174737 8 0.968223 1.133091 -0.357516 1 2.456979 1.080978 1.077043 1 2.936113 0.542263 -0.589467 9 -1.845283 1.141421 -0.185469 9 -0.938327 -0.072135 1.371621 9 -1.886550 -1.027268 -0.333743	**Frequencies (cm^{-1}):** 59.1063, 109.3494, 182.6206, 246.9681, 316.5757, 361.0581, 425.8088, 520.4651, 571.5285, 674.7369, 736.3570, 797.4111, 848.6080, 871.4982, 946.6412, 997.2191, 1056.8708, 1107.0675, 1149.2593, 1160.3118, 1162.8976, 1228.4602, 1290.9247, 1296.5657, 1398.3701, 1404.9809, 1520.9829, 3026.1795, 3063.2864, 3121.7528

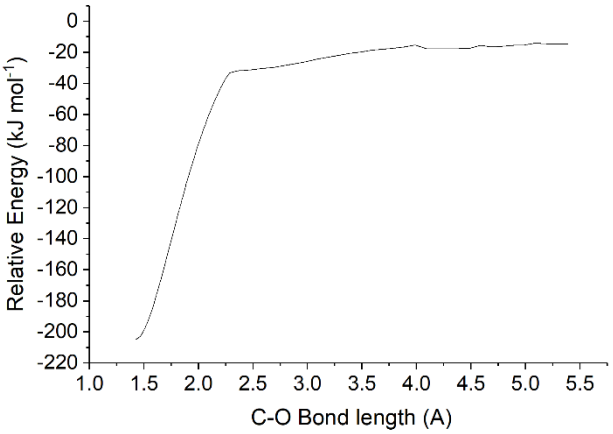
Compound: sCI 24 + HCHO PRC	**Energy (kJ mol^{-1}):** -640.603980608439
Reaction Coordinates: 6 1.395048 0.105593 -0.002788 6 0.022720 -0.321612 -0.476169 1 -0.363411 0.002589 -1.431854 8 -0.599263 -1.140283 0.236215 8 -1.841748 -1.515337 -0.175639 9 1.542932 1.421931 -0.179678 9 2.330250 -0.518267 -0.749247 9 1.608632 -0.193064 1.275855 6 -2.809371 0.706607 0.105628 8 -1.810139 1.383829 -0.036680 1 -3.152938 0.385323 1.099579 1 -3.461164 0.447480 -0.741295	**Frequencies (cm^{-1}):** 26.0215, 58.6615, 71.4215, 113.1524, 179.8264, 198.8805, 262.8157, 292.8331, 389.0975, 416.4647, 420.4978, 428.0257, 552.7682, 565.6375, 701.5734, 881.9017, 894.2454, 960.3389, 1133.9182, 1171.0645, 1189.3448, 1257.3784, 1269.2401, 1357.9965, 1522.7347, 1562.6462, 1734.2093, 2944.3504, 3012.1390, 3219.1546

Compound: sCI 24 + HCHO TS_c	**Energy (kJ mol^{-1}):** -640.602817064141
Reaction Coordinates: 6 1.347878 0.073175 -0.009024 6 -0.042885 -0.314571 -0.470147 1 -0.382351 -0.053128 -1.460716 8 -0.678629 -1.118670 0.253750 8 -1.961632 -1.378830 -0.150523 9 1.599343 1.337368 -0.356012 9 2.249777 -0.714834 -0.632407 9 1.505896 -0.065064 1.303663 6 -2.631041 0.764258 0.033598 8 -1.548350 1.343408 0.050311 1 -3.151648 0.509727 0.964824 1 -3.195983 0.621731 -0.896167	**Frequencies (cm^{-1}):** -108.4983, 34.2541, 80.4906, 101.0591, 190.0208, 216.2135, 336.3818, 353.9170, 404.2459, 441.4964, 451.1272, 553.6226, 559.5445, 576.7438, 703.4921, 876.6809, 909.8247, 958.9078, 1132.4025, 1154.0451, 1193.3540, 1247.9350, 1271.4011, 1352.7332, 1504.1140, 1552.4877, 1673.8982, 2966.5520, 3039.4073, 3229.4170
IRC  	

Compound: sCI 23 + HCHO HOZ2	**Energy (kJ mol^{-1}):** -640.692237225941
Reaction Coordinates: 6 -1.199474 -0.006887 0.025742 6 0.188982 0.075516 -0.632497 1 0.066771 0.219589 -1.709669 8 0.886315 1.153776 -0.023764 8 2.263774 0.688372 -0.073467 9 -1.912002 -0.986844 -0.552341 9 -1.865454 1.147074 -0.144863 9 -1.122709 -0.261077 1.336176 6 2.082671 -0.644790 0.338694 8 0.942805 -1.084525 -0.386997 1 1.899865 -0.705867 1.413986 1 2.958623 -1.210111 0.027110	**Frequencies (cm^{-1}):** 69.3077, 77.4879, 179.4407, 253.9583, 338.8035, 359.3502, 394.3628, 520.8056, 560.9398, 693.6963, 725.0348, 762.4881, 855.7256, 889.6512, 943.1106, 1019.7862, 1053.9849, 1110.1529, 1156.8169, 1164.3491, 1169.6625, 1229.0507, 1279.8213, 1324.1151, 1395.3592, 1417.9899, 1520.2746, 3034.5928, 3042.4603, 3125.6720

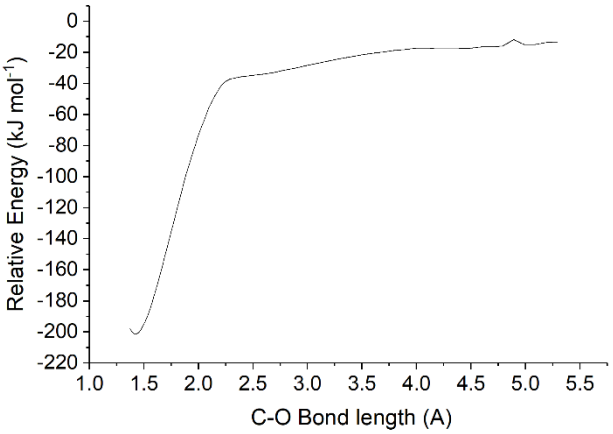
Compound: sCI 1 + CF_3CHO TS_C 3 reaction profile

IRC



Compound: sCI 1 + CF_3CHO TS_C 4 reaction profile

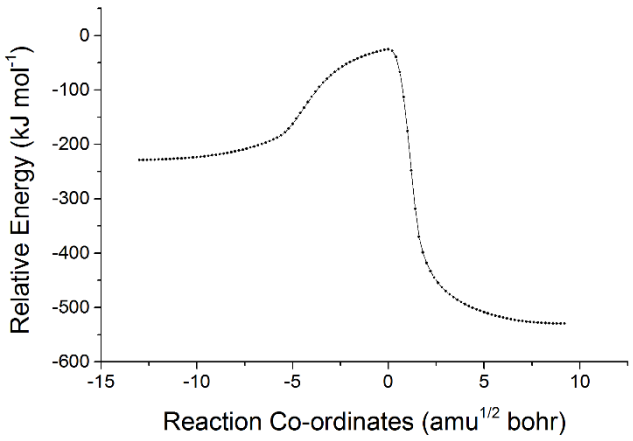
IRC



Compound: sCI 23 + HCHO TS_{HOZ}	**Energy (kJ mol^{-1}):** -640.684269884806
Reaction Coordinates: 6 -1.234099 -0.016283 0.006992 6 0.217213 -0.006609 -0.495282 1 0.218277 -0.049061 -1.592572 8 0.855493 1.160309 -0.027043 8 2.258508 0.764235 0.099653 9 -1.857504 -1.113969 -0.452291 9 -1.882837 1.059394 -0.467529 9 -1.314504 -0.008957 1.336003 8 0.921671 -1.073107 0.066267 6 2.262564 -0.669437 -0.024369 1 2.695489 -0.937726 -0.993919 1 2.820401 -1.098946 0.805786	**Frequencies (cm^{-1}):** -165.8267, 67.5700, 127.7216, 175.6983, 283.1192, 342.4707, 385.5527, 523.0921, 560.2367, 704.2322, 737.7067, 743.3313, 872.9650, 886.7348, 969.5435, 1045.4194, 1080.9912, 1104.8589, 1149.3572, 1169.1195, 1171.0625, 1213.1812, 1288.3676, 1324.0129, 1403.4090, 1440.7109, 1542.0138, 2991.1447, 3001.7444, 3106.4815

Compound: sCI 23 + HCHO TS_d1	**Energy (kJ mol^{-1}):** -640.617420542433
Reaction Coordinates: 6 1.272566 -0.064462 -0.073317 6 -0.244352 0.274927 0.044246 1 -0.645217 0.341103 -1.063275 8 -0.552453 1.411193 0.535921 8 -2.503654 0.476103 -0.643557 9 1.439852 -1.233548 -0.702036 9 1.827864 -0.156384 1.139634 9 1.903380 0.887839 -0.761182 8 -0.981873 -0.842524 0.464269 6 -2.354325 -0.570621 0.105257 1 -2.947279 -0.507834 1.045947 1 -2.686871 -1.511682 -0.380590	**Frequencies (cm^{-1}):** -741.0428, 59.4313, 151.2334, 186.1966, 243.5673, 303.5509, 339.1981, 349.3825, 404.0339, 518.6383, 563.2478, 592.0433, 701.5788, 748.6722, 795.3978, 867.4294, 908.7148, 1011.7064, 1059.6639, 1109.0522, 1182.1362, 1200.4362, 1205.6404, 1237.9073, 1274.6459, 1307.2383, 1361.3928, 2176.3273, 2823.9085, 2857.7175

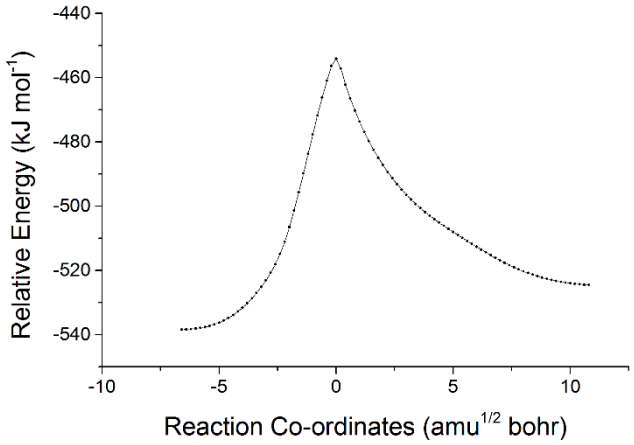
IRC



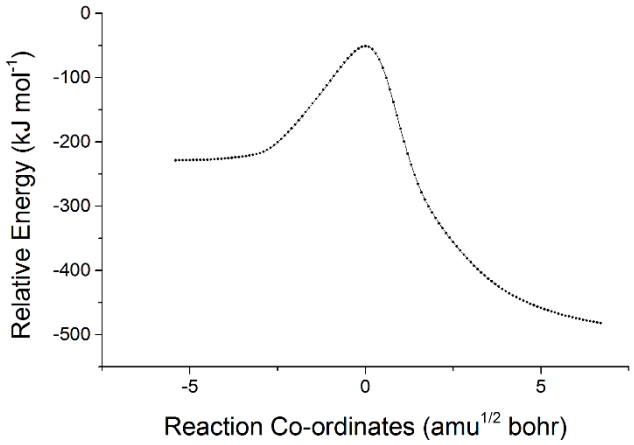
Compound: sCI 23 + HCHO HAE1	**Energy (kJ mol^{-1}):** -640.805561786150
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.351795 -0.125467 0.048198 6 0.065137 0.490331 -0.114630 8 0.286253 1.656338 0.015812 8 0.932103 -0.477171 -0.423884 6 2.335472 -0.103488 -0.537474 8 2.973678 -0.179972 0.685937 1 3.074254 -1.101793 0.946812 1 2.399971 0.923885 -0.880158 1 2.725373 -0.805410 -1.272305 9 -1.357699 -1.041318 1.031295 9 -1.738702 -0.730048 -1.087855 9 -2.240127 0.818198 0.346133	27.9049, 64.9955, 82.2236, 179.2410, 252.1594, 310.6391, 345.4473, 394.3004, 414.0244, 511.8310, 545.7231, 597.1920, 729.1634, 784.3867, 829.9422, 904.5459, 1062.5305, 1093.5179, 1149.6677, 1155.4669, 1212.3045, 1289.3237, 1330.8387, 1400.0656, 1440.7955, 1512.2298, 1841.2052, 3075.9799, 3157.7365, 3800.2458

Compound: sCI 23 + HCHO $TS_{ISO}1$	**Energy (kJ mol^{-1}):** -640.799853308352
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.306299 -0.187066 -0.541446 1 -2.717596 -0.973662 -1.173786 1 -2.373790 0.790343 -1.020955 8 -2.873212 -0.183469 0.739477 1 -3.832746 -0.200502 0.667780 8 -0.929146 -0.531110 -0.379707 6 -0.075965 0.469745 -0.131854 6 1.350154 -0.115599 0.056431 9 2.220727 0.857467 0.311018 9 1.376565 -0.988847 1.073888 9 1.743814 -0.756991 -1.057586 8 -0.316787 1.636664 -0.074482	-238.4497, 25.7190, 72.3081, 88.5166, 183.0110, 252.5813, 326.5163, 348.8901, 412.3888, 509.5526, 542.9971, 591.4858, 730.3949, 782.7179, 829.1229, 963.6820, 1080.2566, 1134.6460, 1154.5610, 1155.6226, 1212.5796, 1256.2745, 1300.2406, 1335.7964, 1469.5455, 1523.2246, 1846.9871, 3041.7344, 3095.0383, 3824.0172

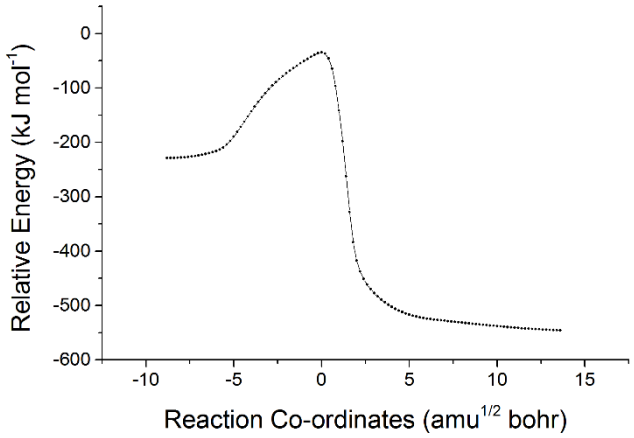
Compound: sCI 23 + HCHO HAE2	**Energy (kJ mol^{-1}):** -640.808924257914
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.318124 -0.533342 -0.393417 1 -2.737399 -1.532535 -0.416846 1 -2.393672 -0.038330 -1.361679 8 -2.916957 0.172141 0.624254 1 -2.679712 1.103745 0.538181 8 -0.888763 -0.765465 -0.148492 6 -0.130277 0.319304 -0.178029 6 1.358012 -0.057160 0.056207 9 2.122069 1.031756 0.040807 9 1.510068 -0.668874 1.240348 9 1.786173 -0.891063 -0.906048 8 -0.495740 1.449316 -0.356285	27.6747, 80.3699, 121.4909, 183.6917, 250.5901, 295.7323, 345.1689, 415.1064, 509.5916, 513.2878, 551.7353, 590.8439, 739.6659, 792.6490, 838.9950, 890.4196, 1055.1402, 1117.6863, 1154.7276, 1163.8789, 1213.1588, 1290.4440, 1345.6009, 1406.7222, 1448.6631, 1511.0362, 1811.0926, 3062.8440, 3165.5278, 3776.0480

Compound: sCI 23 + HCHO $TS_{HAE}1$	**Energy (kJ mol^{-1}):** -640.770283337633
Reaction Coordinates: 6 -1.390799 0.035220 0.021329 6 0.155415 -0.046897 -0.116251 1 1.833446 -1.112235 -0.029863 8 0.626879 -1.209964 -0.281780 8 2.801207 -0.543215 0.375049 9 -1.988022 -0.775715 -0.858875 9 -1.746400 -0.348928 1.259495 9 -1.836261 1.276977 -0.177237 8 0.797982 1.019752 -0.026542 6 2.702880 0.589884 -0.173390 1 3.096326 1.459636 0.350032 1 2.592859 0.679766 -1.254562	**Frequencies (cm^{-1}):** -1089.5421, 16.5601, 76.9026, 165.4483, 216.2266, 266.7990, 281.1986, 388.8310, 462.6379, 475.7872, 517.5003, 574.2078, 636.4659, 747.7625, 804.0394, 858.0309, 881.8098, 1156.5163, 1189.1043, 1208.1041, 1220.3110, 1246.2111, 1347.3573, 1438.7791, 1465.4423, 1624.4152, 1668.6753, 1790.7038, 3045.2640, 3141.5807
IRC  	

Compound: sCI 23 + HCHO $C_{TFA}1$	**Energy (kJ mol^{-1}):** -640.799194296748
Reaction Coordinates: 6 -1.584811 0.005077 -0.000001 6 -0.039654 0.156627 0.000008 1 1.529652 -0.913874 0.000007 8 0.540782 -1.026051 0.000005 8 3.222675 -0.659518 0.000004 9 -1.992953 -0.669392 -1.087888 9 -1.992964 -0.669470 1.087833 9 -2.176496 1.197977 0.000039 8 0.498638 1.231972 0.000014 6 3.647165 0.473450 -0.000009 1 4.731211 0.662243 -0.000012 1 2.967885 1.337445 -0.000019	**Frequencies (cm^{-1}):** 25.6546, 47.4526, 85.6725, 89.5655, 138.7878, 212.8202, 239.2894, 272.2450, 275.9329, 398.0737, 430.5026, 516.2915, 588.3812, 699.8772, 781.4965, 807.0049, 948.7741, 1152.7095, 1171.4562, 1205.8043, 1228.0063, 1276.9303, 1322.5883, 1468.8858, 1522.6090, 1770.4123, 1819.6128, 2945.5541, 3040.2391, 3222.9658

Compound: sCI 23 + HCHO $TS_{acid}1$	**Energy (kJ mol^{-1}):** -640.610730401605
Reaction Coordinates: 6 1.170040 -0.019333 0.102506 6 -0.168113 -0.057013 -0.702440 1 0.095200 0.410473 -1.787063 8 -0.833645 1.094628 -0.827126 8 -1.972031 0.668468 0.724614 9 1.933853 -1.065833 -0.239568 9 0.934323 -0.078480 1.416071 9 1.854340 1.102900 -0.157453 8 -0.842555 -1.144501 -0.647246 6 -2.345900 -0.451047 0.296177 1 -2.344359 -1.284700 1.006253 1 -3.003801 -0.537460 -0.570039	**Frequencies (cm^{-1}):** -1053.5436, 42.5106, 105.4209, 173.6081, 261.0965, 263.0094, 289.2795, 345.4982, 404.0330, 428.2578, 517.2237, 537.4321, 592.1376, 704.0861, 797.1483, 818.3344, 854.2981, 933.9543, 1132.9398, 1155.0775, 1183.1777, 1194.8084, 1196.7304, 1273.4821, 1394.2535, 1446.8064, 1542.9920, 2285.7600, 3003.4676, 3093.2029
IRC  	

Compound: sCI 23 + HCHO $C_{TFA}2$	**Energy (kJ mol^{-1}):** -640.787589964388
Reaction Coordinates: 6 1.019299 -0.360811 -0.053058 6 0.148131 0.922496 -0.173713 8 0.046381 1.641340 0.947305 1 0.368706 1.141827 1.710470 8 -0.304737 1.263154 -1.223148 9 2.273904 -0.073288 -0.444518 9 0.557232 -1.344920 -0.812178 9 1.087654 -0.796104 1.225627 8 -2.080165 -0.612552 0.614197 6 -2.894107 -0.391330 -0.244657 1 -2.637248 0.185901 -1.148649 1 -3.932339 -0.756588 -0.160453	**Frequencies (cm^{-1}):** 43.6805, 46.0995, 76.9727, 88.5261, 90.8361, 152.1740, 182.0909, 250.5153, 254.9155, 383.7001, 426.9844, 506.3784, 531.5898, 586.9922, 689.0061, 762.0313, 796.3404, 1125.2518, 1139.2762, 1210.1226, 1212.7643, 1246.2164, 1270.1461, 1372.0470, 1527.1554, 1799.1525, 1869.7527, 2909.7687, 2982.7885, 3755.1592

Compound: sCI 23 + HCHO TS_d2	**Energy (kJ mol^{-1}):** -640.621055369406
Reaction Coordinates: 6 -0.175640 0.329999 -0.502393 1 -0.058554 0.493890 -1.591676 6 1.274700 -0.031924 0.005777 9 1.738207 -1.102156 -0.647013 9 2.091775 0.995729 -0.230496 9 1.276257 -0.294315 1.313791 8 -0.688512 1.334729 0.131328 8 -0.918574 -0.908852 -0.312853 6 -2.105447 -0.552757 0.321201 1 -2.608572 -1.415811 0.787748 8 -2.842231 0.328488 -0.233668 1 -1.656171 0.021768 1.251429	**Frequencies (cm^{-1}):** -858.3901, 83.4451, 100.7020, 167.0216, 224.4556, 310.1539, 342.4178, 408.5183, 472.7327, 531.3920, 566.5172, 584.1015, 720.7180, 750.4830, 808.8318, 848.8824, 940.9329, 988.9430, 1105.4595, 1136.6271, 1147.7638, 1181.9117, 1219.2248, 1243.8147, 1252.5114, 1271.6928, 1375.0411, 2178.8550, 2883.0314, 2954.8922
IRC  	

Compound: sCI 23 + HCHO HAE3	**Energy (kJ mol^{-1}):** -640.813164616868
Reaction Coordinates: 6 -0.189522 0.476776 -0.240249 1 -0.577133 0.286665 -1.237829 6 1.154475 -0.250359 -0.066579 9 1.008237 -1.579445 -0.146258 9 2.013485 0.132641 -1.021670 9 1.710486 0.040828 1.127511 8 -0.061070 1.841415 -0.086936 1 0.325339 2.036387 0.776578 8 -1.067326 -0.079665 0.744616 6 -2.334230 -0.377776 0.357102 1 -2.884504 -0.748554 1.228277 8 -2.776342 -0.263320 -0.745795	**Frequencies (cm^{-1}):** 32.0458, 66.2195, 177.5694, 205.0507, 255.5542, 262.8436, 365.1985, 385.3922, 425.7036, 513.8521, 562.9730, 589.7024, 680.8692, 764.7864, 881.3630, , 959.4360, 1038.3529, 1099.5497, 1146.6269, 1158.8844, 1191.1342, 1265.9866, 1318.5849, 1370.9634, 1396.6574, 1449.4686, 1809.0497, 3057.9653, 3129.6457, 3768.2098

Compound: sCI 23 + HCHO $TS_{ISO}2$	**Energy (kJ mol^{-1}):** -640.807843829511
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.158204 0.531709 -0.275737 1 -0.562091 0.254605 -1.249995 6 1.125250 -0.280012 -0.029274 9 0.857357 -1.595448 -0.127519 9 2.045912 0.026063 -0.954538 9 1.649418 -0.050709 1.179213 8 0.151353 1.885728 -0.204465 1 -0.525151 2.338407 0.308813 8 -1.086252 0.178143 0.746633 6 -2.303982 -0.305716 0.373145 1 -2.874678 -0.526092 1.281221 8 -2.688933 -0.459116 -0.745074	-339.0386, 21.8885, 66.0356, 174.9537, 209.7879, 258.4835, 271.7906, 375.9960, 408.9945, 504.7021, 546.2406, 581.1835, 686.3237, 766.7458, 880.0458, 961.8218, 1037.9249, 1108.4232, 1140.8063, 1167.3180, 1179.8049, 1245.5598, 1311.0747, 1381.8595, 1398.2379, 1447.5863, 1812.9194, 3061.1220, 3082.6758, 3827.1680

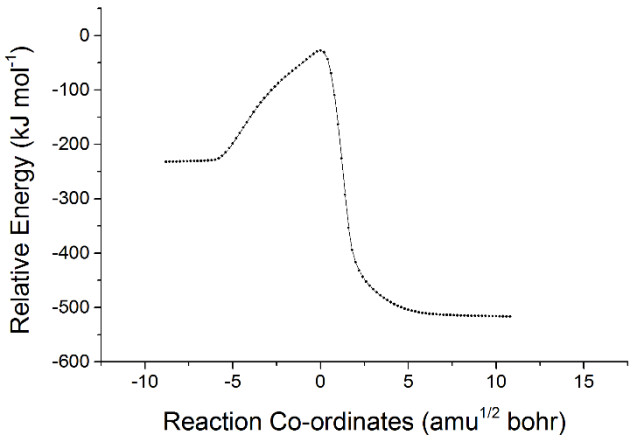
Compound: sCI 23 + HCHO HAE5	**Energy (kJ mol^{-1}):** -640.814946031998
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.210661 0.309903 -0.247637 1 -0.430875 0.333422 -1.316440 6 1.255880 -0.101420 -0.059852 9 1.476777 -1.299065 -0.627801 9 2.055084 0.793281 -0.660280 9 1.600789 -0.177441 1.228334 8 -0.407314 1.523418 0.368428 1 -1.252566 1.879199 0.066418 8 -0.991056 -0.750088 0.345904 6 -2.314706 -0.652497 0.145899 1 -2.822176 -1.505794 0.607070 8 -2.860544 0.239956 -0.445556	67.4596, 75.6599, 159.7185, 229.0168, 251.3286, 282.3992, 355.7306, 403.4892, 457.7356, 527.4247, 560.9981, 577.8060, 696.8742, 787.0476, 887.3511, 953.7355, 1043.7123, 1129.5545, 1144.6425, 1176.4830, 1194.2838, 1253.9800, 1297.3140, 1377.7165, 1392.9043, 1480.8655, 1775.7436, 3064.0576, 3066.2607, 3773.3065

Compound: sCI 23 + HCHO $TS_{ISO}3$	**Energy (kJ mol^{-1}):** -640.804184792221
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.073278 0.304727 -0.670768 1 0.145021 0.312637 -1.742577 6 1.228980 -0.082193 0.065831 9 1.719098 -1.237879 -0.414811 9 2.152502 0.869287 -0.121552 9 1.029377 -0.227967 1.382204 8 -0.506133 1.534381 -0.234289 1 -1.419321 1.457247 0.096643 8 -0.969506 -0.814841 -0.472175 6 -2.201526 -0.704448 0.034236 1 -2.648110 -1.702810 0.087808 8 -2.763291 0.304641 0.377683	-120.2227, 72.1141, 163.1147, 205.5213, 279.6381, 290.2422, 338.0677, 391.7004, 464.5542, 508.5861, 544.2558, 572.1653, 707.8013, 809.6028, 847.6336, 904.6825, 1041.7221, 1151.3840, 1158.4978, 1180.9676, 1190.4618, 1269.3497, 1350.4665, 1397.6865, 1413.3643, 1458.0097, 1760.0678, 3036.0700, 3060.7974, 3562.0744

Compound: sCI 23 + HCHO HAE6	**Energy (kJ mol^{-1}):** -640.810954254638
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.023422 0.519662 -0.759457 1 0.400592 0.711002 -1.742809 6 1.089680 -0.149560 0.081852 9 1.464574 -1.316150 -0.468800 9 2.162028 0.656306 0.113136 9 0.712418 -0.388332 1.346300 8 -0.451637 1.712395 -0.239187 8 -1.072358 -0.448844 -1.004296 6 -2.066917 -0.604329 -0.113028 1 -2.765359 -1.357094 -0.494272 8 -2.195222 -0.019867 0.928208 1 -0.928721 1.535550 0.587345	41.6872, 104.5853, 181.4384, 230.9965, 246.0566, 278.7974, 363.6505, 415.0763, 499.4583, 530.9290, 571.2800, 580.2686, 703.3542, 796.4718, 852.6964, 921.4691, 1041.5112, 1135.0504, 1154.7981, 1157.9586, 1177.1062, 1277.2267, 1350.7516, 1389.9819, 1406.1744, 1453.7478, 1778.4832, 3055.5168, 3113.8394, 3681.8234

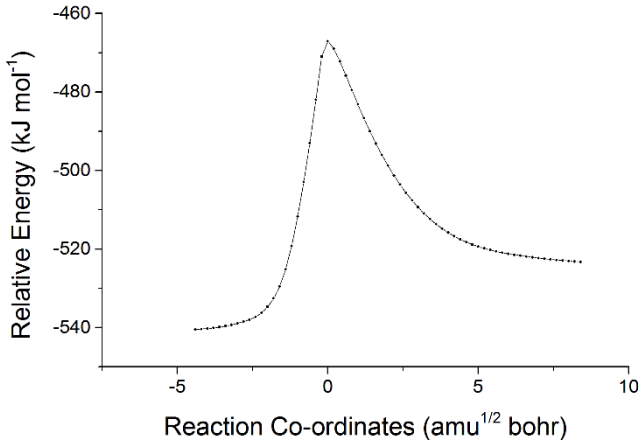
Compound: sCI 23 + HCHO TS_d3	**Energy (kJ mol^{-1}):** -640.616512703843
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.102613 0.190000 -0.770855 1 -0.221783 0.041157 -1.817708 6 -1.189442 -0.051158 0.089343 9 -0.942064 0.021767 1.393584 9 -2.103225 0.872153 -0.231028 9 -1.703562 -1.260393 -0.183258 8 0.671612 1.336675 -0.574015 8 1.026313 -0.941670 -0.577476 6 2.201564 -0.395027 -0.087848 1 3.079946 -1.035607 -0.266433 8 2.157626 0.272677 0.997020 1 2.348680 0.488346 -0.877614	-1048.6305, 61.4215, 108.2979, 187.4575, 233.9898, 294.4733, 349.9156, 393.7248, 454.9065, 519.6814, 543.1833, 575.9719, 711.6622, 736.8896, 814.5896, 855.4579, 938.4998, 990.7274, 1096.1528, 1126.2765, 1171.0636, 1177.9754, 1221.2983, 1244.8104, 1256.5281, 1292.2984, 1372.3378, 2085.0301, 2895.7780, 2964.750

IRC

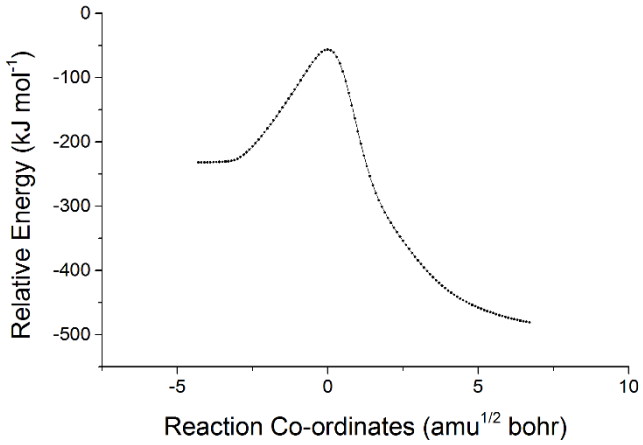


Compound: sCI 23 + HCHO HAE4	**Energy (kJ mol^{-1}):** -640.802893876772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.003320 0.869526 -0.446611 1 -0.448004 1.351622 -1.313680 6 -0.990751 -0.244810 -0.023382 9 -0.907543 -0.608257 1.249326 9 -2.241268 0.226824 -0.231581 9 -0.836126 -1.331722 -0.797407 8 0.156092 1.730646 0.621894 1 0.442813 2.592697 0.303624 8 1.246046 0.388794 -0.977262 6 2.085126 -0.380418 -0.232513 1 2.989831 -0.555784 -0.827072 8 1.884565 -0.798931 0.864007	45.2715, 100.4461, 159.7963, 195.2888, 256.9147, 262.5438, 317.4227, 378.9325, 414.6407, 510.0905, 550.3725, 586.8127, 671.2922, 776.2965, 868.9183, 962.7327, 1037.1402, 1097.2875, 1122.7443, 1153.0702, 1173.1465, 1241.1347, 1311.4807, 1397.6599, 1415.5469, 1461.4654, 1825.1669, 3037.6121, 3078.2371, 3813.5831

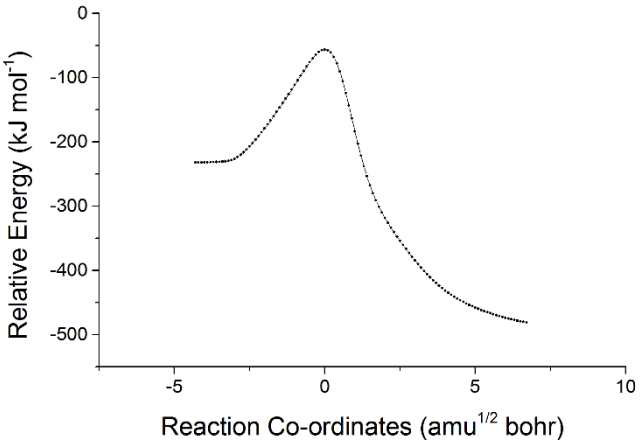
Compound: sCI 23 + HCHO $TS_{ISO}4$	**Energy (kJ mol^{-1}):** -640.799602135995
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.008981 0.703216 -0.618432 1 0.454897 1.055477 -1.544508 6 1.044954 -0.226075 0.029517 9 1.450361 -1.148558 -0.855586 9 2.120492 0.537396 0.353339 9 0.648222 -0.849616 1.135229 8 -0.386453 1.757944 0.201981 1 0.360995 2.058173 0.730998 8 -1.152087 0.002061 -1.068513 6 -2.125534 -0.449922 -0.219502 1 -2.923603 -0.860758 -0.849254 8 -2.127285 -0.418657 0.968585	-205.8349, 29.6258, 111.6347, 163.0098, 198.8716, 233.8819, 261.6935, 365.4356, 414.8042, 501.7893, 544.4509, 579.2414, 686.6904, 777.6938, 869.5887, 961.1872, 1032.4184, 1105.0513, 1120.2350, 1153.8295, 1180.0968, 1249.2081, 1329.0742, 1390.0135, 1408.1359, 1439.4732, 1830.9429, 3032.2077, 3040.2313, 3805.9390

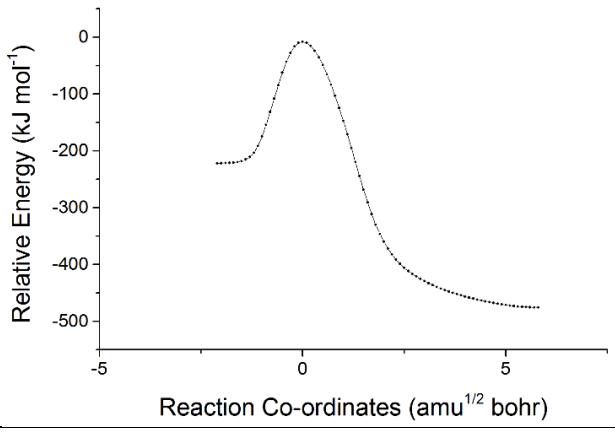
Compound: sCI 23 + HCHO $TS_{HAE}2$	**Energy (kJ mol^{-1}):** -640.777964091842
Reaction Coordinates: 6 -1.152459 0.080578 0.088526 6 -0.033283 -0.462620 -0.831746 1 -0.299276 -0.321810 -1.883881 8 0.573899 -1.523208 -0.483750 8 2.298411 -0.380018 0.678641 9 -1.608559 1.271322 -0.327484 9 -0.751636 0.201253 1.362196 9 -2.178307 -0.787312 0.053382 8 1.065071 0.900315 -0.699501 6 2.074660 0.682226 0.028917 1 2.814064 1.484922 0.095223 1 1.499183 -1.108300 0.318517	**Frequencies (cm^{-1}):** -968.8390, 66.1525, 81.9851, 177.5996, 246.6260, 280.8294, 330.3906, 389.7532, 484.2083, 522.6232, 557.7775, 587.2552, 662.2032, 745.8993, 846.9394, 864.7260, 1062.9738, 1129.9689, 1171.0954, 1194.3591, 1240.7771, 1274.2240, 1359.3244, 1379.3200, 1386.7151, 1574.1782, 1699.5035, 1801.5823, 3041.8683, 3078.8532
IRC  	

Compound: sCI 23 + HCHO $C_{FAc}1$	**Energy (kJ mol^{-1}):** -640.799644233095
Reaction Coordinates: 6 1.829574 -0.075226 0.000000 6 0.291807 0.035526 -0.000003 8 -0.263422 1.100263 -0.000005 1 -0.249851 -0.921563 -0.000003 9 2.218400 -0.762929 -1.089059 9 2.432490 1.107775 -0.000003 9 2.218396 -0.762921 1.089067 1 -2.123558 1.071582 -0.000002 8 -3.099430 0.950319 0.000002 6 -3.378418 -0.349903 0.000002 1 -4.462694 -0.509946 0.000007 8 -2.567803 -1.243054 -0.000003	**Frequencies (cm^{-1}):** 28.8611, 44.0666, 71.4606, 106.0397, 119.5735, 145.4401, 190.5235, 279.0593, 330.0197, 433.6041, 524.6309, 528.5168, 671.6616, 704.5942, 839.6375, 867.8719, 1012.6684, 1066.0493, 1162.4944, 1180.2903, 1189.8676, 1287.0851, 1365.2464, 1402.9839, 1421.8376, 1773.3347, 1819.2331, 3016.2653, 3046.6481, 3453.4462

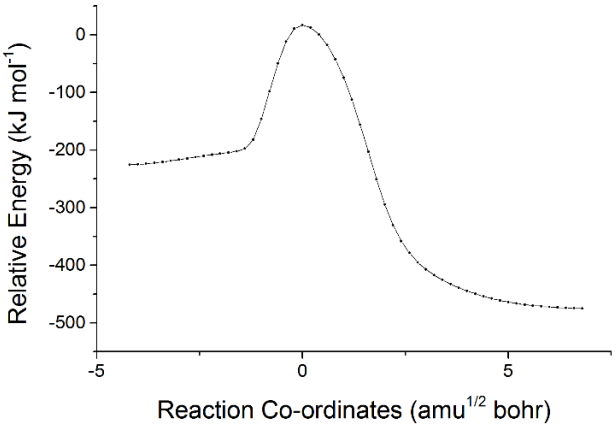
Compound: sCI 23 + HCHO $TS_{FAc}1$	**Energy (kJ mol^{-1}):** -640.612916191139
Reaction Coordinates: 6 -1.240405 -0.026036 0.011886 6 0.135836 0.407482 -0.547764 1 0.137618 0.408999 -1.642472 8 0.718010 1.333292 0.105212 8 2.531811 0.535366 -0.129761 9 -1.702755 -1.106895 -0.631309 9 -2.115923 0.974405 -0.195571 9 -1.203698 -0.285322 1.319510 8 0.991060 -1.056635 -0.286017 6 2.064870 -0.626086 0.301543 1 3.149347 -0.774754 -0.253715 1 2.225567 -0.902282 1.353046	**Frequencies (cm^{-1}):** -1193.8039, 72.1271, 92.5885, 172.7720, 246.7119, 259.0645, 304.4696, 372.7167, 439.4271, 457.7900, 523.2859, 566.3051, 662.7034, 705.8703, 756.4539, 845.5288, 868.5412, 1116.5453, 1148.5230, 1163.0003, 1187.5554, 1221.3952, 1249.2538, 1315.7469, 1334.6176, 1406.7356, 1461.4554, 2235.1404, 2988.7376, 3028.7966
IRC  	

Compound: sCI 23 + HCHO $C_{FAc}2$	**Energy (kJ mol^{-1}):** -640.788851617549
Reaction Coordinates: 6 1.761049 -0.285003 0.062007 6 0.767135 0.875943 -0.175926 1 -0.257265 0.540397 -0.401807 8 1.105685 2.020870 -0.112233 9 1.319382 -1.051507 1.080043 9 2.990040 0.134105 0.349675 9 1.818020 -1.060276 -1.039329 8 -2.419881 -0.169238 -0.879313 6 -3.495306 -0.228361 -0.363768 8 -3.693042 0.103780 0.926100 1 -4.622004 -0.005565 1.165569 1 -4.407068 -0.554496 -0.887567	**Frequencies (cm^{-1}):** 7.7036, 15.0143, 16.8036, 26.8905, 62.3992, 79.8049, 94.8453, 252.0524, 314.0173, 421.4039, 518.3137, 525.3090, 541.7266, 664.0237, 700.2285, 829.9758, 995.0095, 1037.5429, 1118.4110, 1152.2179, 1173.2951, 1271.6813, 1282.9539, 1414.6775, 1423.2612, 1831.9042, 1845.8547, 2982.1286, 2998.3238, 3779.6741

Compound: sCI 23 + HCHO $TS_{FAc}2$	**Energy (kJ mol^{-1}):** -640.615657587046
Reaction Coordinates: 6 1.147981 -0.047437 0.071635 6 -0.076256 0.257681 -0.819982 1 0.131984 -0.008703 -1.863370 8 -0.731916 1.334815 -0.635515 8 -1.928481 0.546508 0.772565 9 1.667176 -1.252307 -0.222732 9 0.876371 -0.014318 1.378858 9 2.094288 0.876690 -0.181581 8 -1.080636 -1.067320 -0.500936 6 -2.141677 -0.496699 -0.009589 1 -2.458690 -0.736594 1.153285 1 -3.065839 -0.538569 -0.602108	**Frequencies (cm^{-1}):** -1223.3404, 55.2869, 120.1231, 182.4610, 242.8627, 279.4588, 308.6175, 372.9038, 441.0465, 453.2497, 518.5714, 571.7535, 649.2592, 714.2083, 781.7622, 841.9288, 847.1269, 1080.7267, 1144.2891, 1156.3786, 1162.0579, 1222.3706, 1266.8167, 1291.5830, 1322.0916, 1407.5412, 1473.0139, 2243.0956, 2991.9693, 3009.3838
IRC  	

Compound: sCI 23 + HCHO $TS_{ester}1$	**Energy (kJ mol^{-1}):** -640.591726379101
Reaction Coordinates: 6 1.366331 -0.026686 0.061260 6 -0.368759 0.156879 -0.654823 1 -0.095006 0.135080 -1.722017 8 -0.528243 -0.990651 -0.039830 8 -2.562658 -0.772364 -0.186019 9 1.910254 1.083396 -0.410810 9 1.342257 -0.001711 1.364600 9 2.005600 -1.065334 -0.417362 6 -2.540376 0.329368 0.410312 8 -0.975599 1.192560 -0.211818 1 -2.239606 0.402513 1.457551 1 -3.199567 1.121523 0.037456	**Frequencies (cm^{-1}):** -560.5388, 50.0694, 60.3894, 102.9234, 178.5244, 242.8272, 256.1040, 306.1896, 352.1444, 491.3535, 533.1564, 542.4147, 573.0182, 711.7424, 738.2562, 847.6028, 946.0872, 1055.5919, 1141.1780, 1188.2539, 1222.2839, 1262.1485, 1301.4676, 1344.3947, 1391.0679, 1441.0526, 1534.6863, 2949.1530, 2992.2289, 3074.1389
IRC  	

Compound: sCI 23 + HCHO $C_{ester}1$	**Energy (kJ mol^{-1}):** -640.785087532247
Reaction Coordinates: 6 1.791858 0.065785 -0.000001 8 0.650662 0.840112 -0.000017 6 -0.593997 0.236702 -0.000007 1 -1.352802 1.022550 -0.000021 8 -0.791968 -0.935019 0.000015 9 1.871240 -0.706996 -1.084234 9 2.825281 0.904836 -0.000020 9 1.871241 -0.706947 1.084267 6 -4.178424 -0.338090 -0.000012 8 -3.745980 0.785560 0.000010 1 -3.510320 -1.215360 -0.000071 1 -5.265067 -0.536821 0.000027	**Frequencies (cm^{-1}):** 17.6764, 39.3605, 53.9006, 79.8186, 93.9123, 111.7895, 112.6025, 188.4592, 231.1980, 373.5513, 441.8426, 547.8735, 581.2838, 619.1427, 818.3698, 840.7698, 1056.6360, 1094.8676, 1160.5880, 1205.7308, 1212.1275, 1237.8546, 1270.3234, 1396.9949, 1529.3276, 1796.6426, 1829.5309, 2903.8149, 2979.3096, 3101.5598

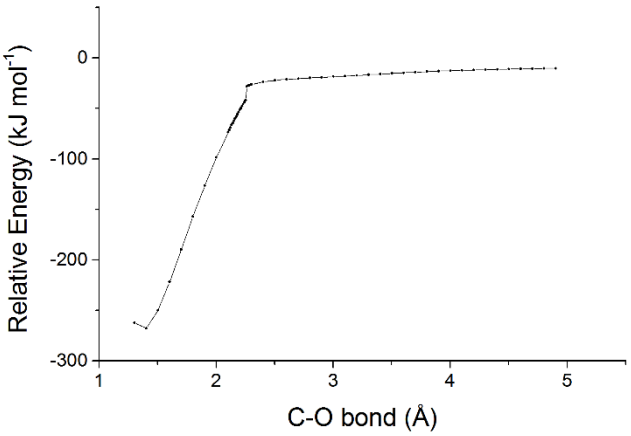
Compound: sCI 23 + HCHO $TS_{ester}2$	**Energy (kJ mol^{-1}):** -640.587782961932
Reaction Coordinates: 6 1.378359 0.010001 0.025154 6 -0.332347 -0.141342 -0.462417 1 -0.200721 -0.278102 -1.556026 8 -0.824975 -1.139154 0.189235 8 -2.605340 0.761834 0.178537 9 1.471795 0.194651 1.310528 9 1.966170 0.961699 -0.661715 9 1.884549 -1.158456 -0.319820 6 -2.709063 -0.441339 -0.112929 8 -0.558469 1.084594 -0.065633 1 -3.097189 -1.143606 0.633883 1 -2.716139 -0.781448 -1.154760	**Frequencies (cm^{-1}):** -462.6014, 72.7718, 82.3414, 102.8373, 171.3199, 249.8559, 274.1585, 312.0720, 324.4221, 443.0121, 521.3093, 547.7848, 576.1725, 709.5628, 721.9533, 744.0114, 933.7447, 1091.5664, 1150.9995, 1197.9039, 1221.0053, 1231.3293, 1303.8615, 1330.7661, 1377.2627, 1441.3485, 1573.5282, 2855.4590, 2970.3282, 3047.9176
IRC  	

Compound: CF_3COOH conformer 2	**Energy (kJ mol^{-1}):** -526.391647939292
Reaction Coordinates: 6 -0.581404 -0.010401 -0.000000 6 0.970727 -0.156509 -0.000004 8 1.477110 -1.232961 0.000000 8 1.654341 0.993148 -0.000001 1 1.057725 1.754791 -0.000017 9 -1.102989 -0.583142 -1.084628 9 -1.102975 -0.583095 1.084656 9 -0.954622 1.295701 -0.000023	**Frequencies (cm^{-1}):** 21.6602, 251.5689, 256.7023, 383.9419, 424.0892, 504.2317, 558.0545, 581.8488, 686.6362, 774.0185, 789.5230, 1111.2671, 1173.1962, 1190.7699, 1238.1250, 1367.2329, ,1882.0972, 3753.0385

Compound: CF_3CHO	**Energy (kJ mol^{-1}):** -451.199957828211
Reaction Coordinates: 6 0.015009 0.360282 0.000000 6 0.501814 -1.106406 -0.000000 8 -0.245475 -2.035870 -0.000000 1 1.601864 -1.198064 -0.000000 9 0.501814 0.987869 1.088491 9 0.501814 0.987869 -1.088491 9 -1.307962 0.464459 0.000000	**Frequencies (cm^{-1}):** 73.5798, 250.7650, 307.2813, 422.6928, 518.9491, 524.0490, 701.8523, 834.5377, 974.2730, 1150.4161, 1174.8562, 1288.1325, 1403.3576, 1849.8517, 2955.8187

Compound: CF_3OCHO	**Energy (kJ mol^{-1}):** -526.392169685219
Reaction Coordinates: 6 -0.663849 -0.000032 0.000000 8 0.336896 0.952890 -0.000000 6 1.661196 0.558397 0.000000 8 2.058027 -0.558385 0.000000 1 2.265245 1.470480 0.000000 9 -0.613300 -0.773286 1.084140 9 -0.613300 -0.773286 -1.084140 9 -1.818813 0.660272 0.000000	**Frequencies (cm^{-1}):** 88.2784, 182.4643, 213.8832, 372.9073, 440.5306, 548.4446, 580.4343, 618.6761, 819.4841, 841.6604, 1029.7431, ,1099.7328, 1158.7538, 1210.5947, 1240.5018, 1402.5579, 1846.9478, 3073.3668

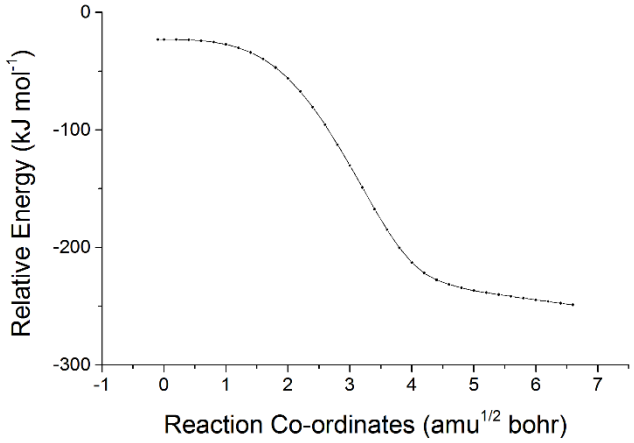
8.2.3 sCIs 25 & 26 + HCHO & sCIs 1 + CF_3CFO

Compound: sCI 25 + HCHO TS_c reaction profile
IRC 

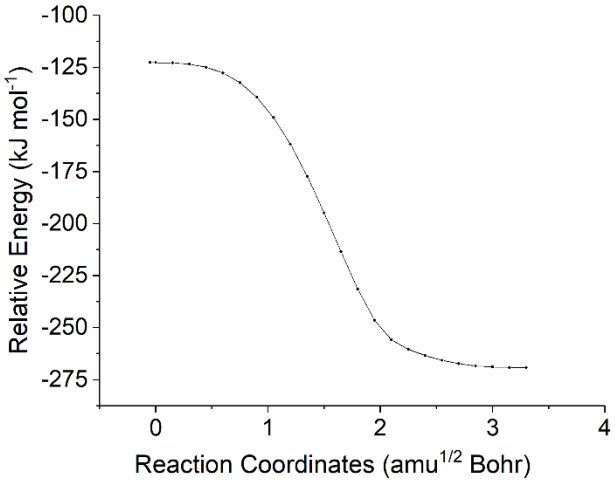
Compound: sCI 25 + HCHO HOZ1	**Energy (kJ mol^{-1}):** -739.880971561098
Reaction Coordinates: 6 -1.203229 -0.230964 0.058463 6 0.191425 0.440783 -0.055823 9 -0.018442 1.768072 -0.284796 8 0.923264 -0.051022 -1.159256 8 2.011888 -0.814233 -0.568390 9 -1.873473 0.255806 1.109021 9 -1.065362 -1.550484 0.213301 9 -1.918007 -0.002321 -1.047544 8 0.930952 0.217053 1.072410 6 2.246328 -0.074884 0.601161 1 2.755836 -0.715948 1.315224 1 2.785743 0.852302 0.394021	**Frequencies (cm^{-1}):** 62.9168, 82.3412, 181.5539, 225.3051, 306.3116, 333.8341, 372.3751, 383.1249, 472.7730, 537.6227, 578.2342, 616.4528, 733.4968, 748.0603, 840.5352, 900.2599, 961.3323, 1051.7447, 1075.2302, 1084.3749, 1160.0607, 1174.0468, 1194.6284, 1204.5660, 1240.5871, 1353.3296, 1400.3061, 1519.3524, 3039.2896, 3147.1681

Compound: sCI 26 + HCHO PRC	**Energy (kJ mol^{-1}):** -739.777926184174
Reaction Coordinates: 6 -1.414853 0.141074 -0.112497 6 -0.050978 -0.450704 0.236511 9 0.273257 -0.457980 1.482950 8 0.616211 -1.031007 -0.636363	**Frequencies (cm^{-1}):** 34.8048, 60.5055, 70.4194, 101.2900, 143.9768, 186.7900, 200.3901, 237.6640, 298.5269, 339.1001, 362.6188, 384.0722,

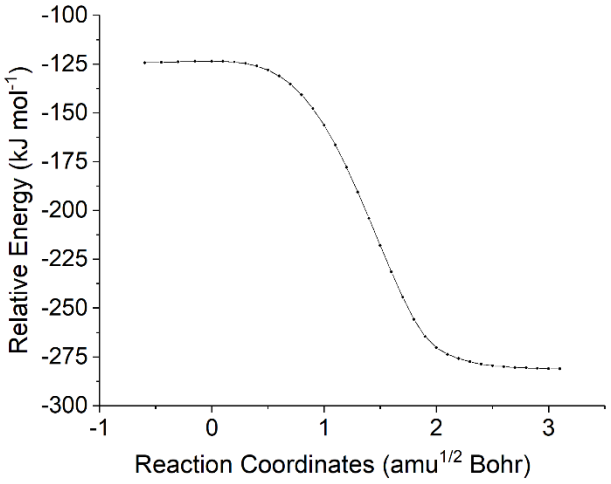
8 1.855522 -1.524854 -0.274925 9 -1.545297 1.342529 0.441524 9 -2.373565 -0.660000 0.384471 9 -1.564546 0.229935 -1.426569 6 2.716861 0.890240 -0.070701 8 1.640783 1.447690 -0.108533 1 3.315311 0.728201 -0.979729 1 3.169732 0.563154 0.877031	406.9206, 514.5633, 577.3863, 663.2692, 730.6738, 857.5480, 900.9980, 1138.3690, 1178.3830, 1181.7442, 1238.6573, 1260.7686, 1402.6054, 1526.8058, 1612.0198, 1752.6652, 2940.4081, 3008.9838

Compound: sCI 26 + HCHO TS_c	**Energy (kJ mol^{-1}):** -739.778430516598
Reaction Coordinates: 6 -1.380202 0.101938 -0.105985 6 0.026431 -0.396275 0.231970 9 0.339614 -0.408275 1.484467 8 0.674169 -1.022580 -0.631521 8 1.973753 -1.364286 -0.283260 9 -1.617791 1.251789 0.515572 9 -2.273681 -0.806175 0.325723 9 -1.521302 0.255771 -1.414694 6 2.529514 0.925062 -0.042405 8 1.408494 1.394738 -0.179406 1 3.221657 0.854342 -0.891297 1 2.931003 0.660345 0.943705	**Frequencies (cm^{-1}):** -118.4252, 38.2811, 89.8377, 110.0542, 181.1767, 201.7179, 229.7311, 297.2903, 325.3079, 373.7338, 408.0919, 414.9295, 476.0417, 518.7753, 577.7736, 650.4742, 730.7338, 849.8975, 909.3393, 1133.4831, 1156.2947, 1183.8163, 1241.0371, 1252.0155, 1396.4643, 1511.2865, 1586.8143, 1697.9348, 2967.7444, 3042.2769
IRC  	

Compound: sCI 1 + CF_3CFO PRC 3	**Energy (kJ mol^{-1}):** -739.813259682201
Reaction Coordinates: 6 1.276276 -0.317441 0.042768 6 0.199237 0.765686 0.278781 9 0.332320 1.754487 -0.609756 8 -0.466774 0.863601 1.257424 9 1.452943 -0.610239 -1.240654 9 2.442962 0.159259 0.528183 9 0.975427 -1.429876 0.713343 6 -2.711550 -0.451865 0.655072 1 -2.030034 -1.117147 1.167434 1 -3.638928 -0.080588 1.070988 8 -2.468023 -0.081048 -0.512669 8 -1.283662 -0.487955 -1.072029	**Frequencies (cm^{-1}):** 42.13, 63.96, 88.06, 113.40, 161.90, 192.84, 220.11, 240.50, 279.50, 379.83, 428.50, 513.34, 528.59, 586.64, 680.60, 693.20, 716.22, 802.10, 885.19, 1024.72, 1084.45, 1147.22, 1223.53, 1243.79, 1311.45, 1417.81, 1571.35, 1851.85, 3127.16, 3272.45

Compound: sCl 1 + CF_3CHO TS_c 3	**Energy (kJ mol^{-1}):** -739.811613027458
Reaction Coordinates: 6 1.245988 -0.265523 -0.092261 6 0.041332 0.700989 -0.145855 9 0.189726 1.675069 0.774721 8 -0.632687 0.863682 -1.129472 9 0.969226 -1.399460 -0.736156 9 2.281569 0.329362 -0.721769 9 1.631765 -0.547889 1.150351 6 -2.741525 0.035486 -0.376479 1 -2.703817 1.033485 0.033747 1 -3.404323 -0.266334 -1.177649 8 -2.081522 -0.894047 0.143083 8 -1.137941 -0.482961 1.064781	**Frequencies (cm^{-1}):** -109.92, 56.94, 80.14, 142.31, 211.44, 220.36, 269.82, 308.99, 347.33, 383.64, 438.27, 518.42, 539.95, 587.75, 681.43, 700.45, 719.16, 802.82, 898.27, 1048.01, 1067.15, 1146.40, 1218.82, 1236.65, 1296.61, 1415.35, 1570.32, 1749.53, 3135.01, 3279.84
IRC  	

Compound: sCl 1 + CF_3CFO PRC 4	**Energy (kJ mol^{-1}):** -739.812611750193
Reaction Coordinates: 6 1.260836 -0.292596 -0.100143 6 0.149504 0.780864 -0.149444 9 0.297955 1.652770 0.857863 8 -0.528324 1.011186 -1.101148 9 0.919770 -1.358554 -0.820669 9 2.367461 0.250369 -0.655394 9 1.568501 -0.670948 1.136250 6 -2.843813 0.077420 -0.381769 1 -2.757537 1.070839 0.035688 1 -3.523078 -0.196672 -1.178448 8 -2.165570 -0.862809 0.084248 8 -1.243822 -0.539755 1.050455	**Frequencies (cm^{-1}):** 47.51, 65.26, 85.39, 118.69, 174.40, 200.92, 245.37, 260.90, 295.89, 379.05, 431.01, 513.18, 531.84, 586.90, 683.81, 689.53, 708.55, 800.11, 888.72, 1029.39, 1075.49, 1142.75, 1227.75, 1241.45, 1305.29, 1418.19, 1572.94, 1830.56, 3129.42, 3274.44

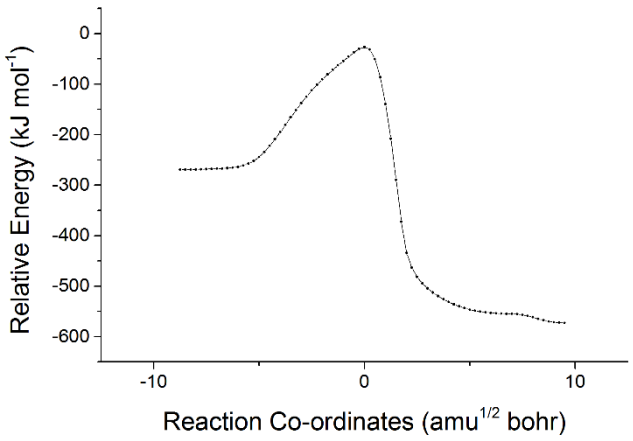
Compound: sCI 26 + HCHO TS_c 4	**Energy (kJ mol^{-1}):** -739.810121917775
Reaction Coordinates: 6 -1.248348 -0.270044 0.006638 6 -0.008169 0.583650 -0.339239 9 -0.144618 1.819566 0.181718 8 0.652411 0.405323 -1.339539 9 -1.571793 -0.215886 1.298125 9 -2.295289 0.186594 -0.706355 9 -1.043079 -1.547385 -0.334192 6 2.510833 -0.639402 -0.503616 1 1.860205 -1.459838 -0.765152 1 3.419149 -0.395132 -1.040673 8 2.340293 0.000196 0.562465 8 1.093266 -0.202550 1.135756	**Frequencies (cm^{-1}):** -183.41, 56.54, 69.23, 156.11, 217.15, 232.18, 267.46, 317.85, 359.89, 391.03, 438.72, 523.41, 544.08, 588.04, 680.37, 717.37, 735.62, 813.89, 897.93, 1063.92, 1073.84, 1155.76, 1205.38, 1234.21, 1299.76, 1411.54, 1567.26, 1700.60, 3135.05, 3279.77
IRC  	

Compound: sCI 25 + HCHO HOZ2	**Energy (kJ mol^{-1}):** -739.882612577417
Reaction Coordinates: 6 1.226910 -0.202398 -0.060082 6 -0.201622 0.381734 0.127609 9 -0.062041 1.673083 0.536046 8 -0.874081 0.296507 -1.089563 8 -2.266214 0.162553 -0.664667 9 1.914395 -0.099267 1.079534 9 1.884341 0.455130 -1.019776 9 1.155217 -1.494768 -0.399219 6 -2.112229 -0.756332 0.387029 8 -0.929811 -0.323497 1.059019 1 -1.972248 -1.775555 0.020385 1 -2.972454 -0.654571 1.044696	**Frequencies (cm^{-1}):** 64.4536, 102.3338, 183.0668, 231.2002, 294.0750, 331.7999, 368.8521, 380.9341, 498.1395, 541.8807, 578.3703, 614.4270, 736.4144, 747.4253, 853.1992, 888.9747, 962.5108, 1062.4176, 1072.9408, 1103.2970, 1140.8250, 1158.2995, 1199.1282, 1201.9356, 1230.5616, 1346.8978, 1405.6107, 1520.8092, 3040.2533, 3134.6001

Compound: sCI 25 + HCHO TS_{HOZ}	**Energy (kJ mol^{-1}):** -739.875860313659
Reaction Coordinates: 6 1.265369 -0.175561 0.037602 6 -0.208538 0.310764 -0.045038 9 -0.184141 1.676299 -0.198393 8 -0.829394 -0.290458 -1.120223 8 -2.230537 -0.415601 -0.725606 9 1.884369 0.424204 1.057845 9 1.910458 0.124204 -1.093056 9 1.313647 -1.495448 0.223619 8 -0.898614 -0.037440 1.082003 6 -2.251377 -0.184335 0.692050 1 -2.668140 -1.050180 1.204313 1 -2.815225 0.729644 0.888491	**Frequencies (cm^{-1}):** -189.6719, 62.0184, 109.2801, 182.8716, 230.0115, 331.1898, 348.7338, 374.9499, 499.8881, 542.7314, 582.2789, 610.0967, 746.4942, 754.1945, 869.7451, 901.9045, 968.8900, 1048.1702, 1086.4867, 1121.6619, 1139.7391, 1146.8914, 1196.4040, 1206.6516, 1208.5915, 1362.0792, 1415.8068, 1546.9949, 3037.1675, 3106.9218

Compound: sCI 25 + HCHO TS_d	**Energy (kJ mol^{-1}):** -739.782964789564
Reaction Coordinates: 6 -1.132888 -0.348496 0.049909 6 0.088137 0.601384 -0.200781 9 -0.351809 1.880118 0.009060 8 0.692141 0.446831 -1.329195 8 2.166824 -1.086986 -0.341132 9 -1.665464 -0.132582 1.258465 9 -2.068538 -0.112927 -0.873457 9 -0.765110 -1.629932 -0.029165 8 1.040273 0.404491 0.955358 6 2.194450 -0.076899 0.433864 1 3.083877 0.021690 1.088126 1 2.482319 0.765599 -0.350458	**Frequencies (cm^{-1}):** -1092.6757, 10.7391, 58.7066, 102.7274, 208.6094, 221.0911, 289.6020, 325.9773, 353.6172, 364.6832, 462.4753, 511.2091, 536.9760, 584.6930, 630.5246, 690.8930, 747.1988, 814.9985, 891.8665, 954.1079, 1052.8209, 1130.4231, 1189.0187, 1191.1713, 1196.9907, 1221.1659, 1306.7988, 1394.4501, 2143.4453, 2907.5597

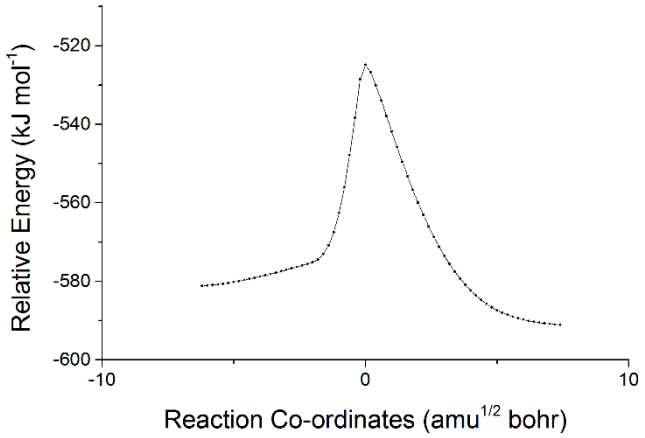
IRC



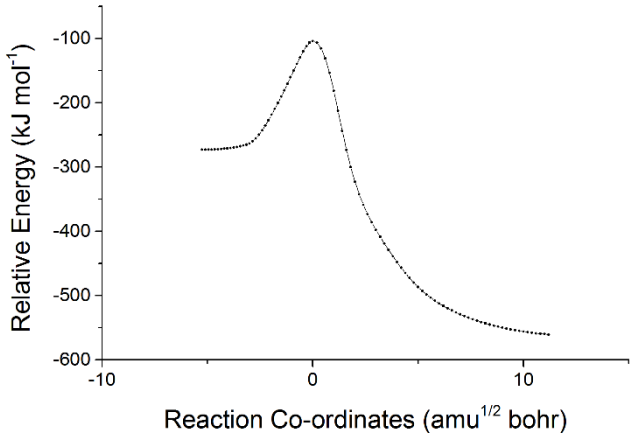
Compound: sCI 25 + HCHO HAE Con 1	**Energy (kJ mol^{-1}):** -739.996820249036
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.027344 0.687582 0.061851 9 0.541121 1.825651 -0.379093 6 1.069431 -0.424089 -0.008015 9 1.545648 -0.560058 -1.249390 9 0.546169 -1.601185 0.374737 9 2.079687 -0.122821 0.807936 8 -0.492323 0.894840 1.311132 1 -1.196959 0.244012 1.495796 8 -1.029442 0.369800 -0.917077 6 -2.150050 -0.303772 -0.587385 1 -2.754555 -0.439892 -1.488583 8 -2.455027 -0.694230 0.506741	57.1808, 70.9230, 175.4045, 217.9644, 261.4777, 273.1843, 344.6606, 348.2922, 389.4253, 465.3067, 496.8327, 576.1035, 582.0878, 591.6309, 692.0873, 767.3125, 831.8341, 957.2695, 1041.7683, 1089.3072, 1164.7213, 1187.9694, 1210.3953, 1227.3088, 1340.8463, 1404.0025, 1408.7922, 1775.9420, 3078.0550, 3558.3955

Compound: sCI 25 + HCHO TS_{ISO}	**Energy (kJ mol^{-1}):** -739.995345880234
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.180838 -0.342869 -0.047973 6 0.073704 0.584064 0.009736 9 -0.311472 1.726564 0.635169 8 0.533091 0.864102 -1.223076 8 2.708270 -0.408426 -0.546306 9 -0.834243 -1.531697 -0.567266 9 -2.119928 0.203241 -0.820694 9 -1.692200 -0.548962 1.169557 8 0.994616 -0.042609 0.911524 6 2.210140 -0.487251 0.545545 1 2.693131 -0.941839 1.415039 1 1.421598 0.471337 -1.346912	-65.3287, 65.3295, 166.1356, 213.5199, 249.6288, 294.2800, 334.9333, 360.6191, 367.4474, 473.8145, 495.1819, 570.1397, 578.3899, 600.4688, 687.7175, 766.2511, 829.2022, 951.9805, 1042.0443, 1086.6002, 1174.1938, 1187.2994, 1210.9436, 1233.8137, 1329.3611, 1409.5539, 1441.6080, 1769.3460, 3080.5580, 3478.084

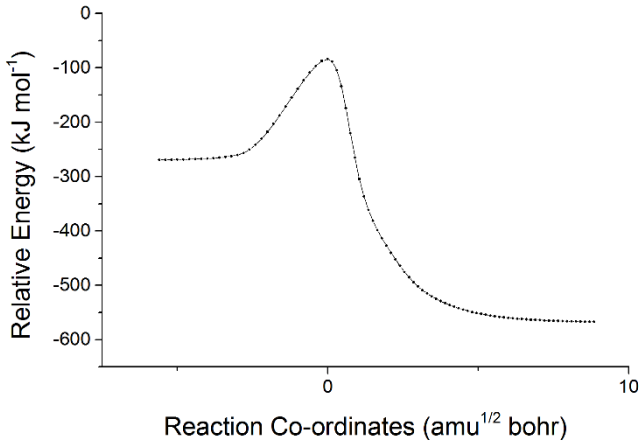
Compound: sCI 25 + HCHO HAE Con 2	**Energy (kJ mol^{-1}):** -740.000308948885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.321852 -0.149789 -0.076490 6 -0.155453 0.309802 0.082835 9 -0.271021 0.919507 1.304423 8 -0.467139 1.141710 -0.926994 8 -2.894484 0.204685 -0.202411 9 1.670431 -0.952740 0.933231 9 2.129042 0.912548 -0.076403 9 1.484130 -0.813728 -1.225184 8 -0.932051 -0.884704 0.150989 6 -2.272728 -0.797419 0.017660 1 -2.706482 -1.794969 0.133869 1 -1.419383 1.335588 -0.875184	62.9145, 78.9746, 159.2883, 218.4675, 240.9289, 261.5800, 319.6150, 363.1625, 387.2717, 494.0228, 520.8418, 570.2369, 584.1607, 606.8505, 657.1655, 769.9403, 843.4823, 972.8608, 1041.0624, 1049.4737, 1157.4872, 1199.4818, 1205.8249, 1227.3689, 1264.5355, 1400.2948, 1476.3678, 1784.9247, 3074.5473, 3642.2040

Compound: sCI 25 + HCHO $TS_{HAE}1$	**Energy (kJ mol^{-1}):** -739.973401978791
Reaction Coordinates: 6 -1.270961 0.225027 -0.120025 6 0.067462 -0.548936 0.046984 9 -0.045608 -1.375286 1.118974 8 0.616065 -1.007043 -0.985121 8 2.721721 -0.011133 -0.566773 9 -1.706195 0.736593 1.034153 9 -2.198727 -0.617761 -0.589049 9 -1.119164 1.223240 -0.997924 8 1.021045 0.649180 0.745659 6 2.215773 0.724389 0.322488 1 2.840018 1.495011 0.779358 1 1.842939 -0.646990 -0.921553	**Frequencies (cm^{-1}):** -949.5685, 39.2733, 64.5013, 169.6876, 218.9110, 259.7737, 315.1775, 356.2053, 360.5612, 421.2820, 485.2187, 541.0347, 583.6573, 625.6704, 695.3956, 773.3250, 878.5740, 885.8521, 1061.8765, 1064.7041, 1178.3447, 1184.4422, 1203.2622, 1306.9569, 1376.1017, 1392.3137, 1618.0324, 1702.9903, 1832.9846, 3099.3367
IRC  	

Compound: sCI 25 + HCHO $C_{FAc}3$	**Energy (kJ mol^{-1}):** -739.998047248532
Reaction Coordinates: 6 -1.303574 -0.423757 -0.134810 6 -0.542531 0.923451 -0.061129 9 -0.880671 1.585261 1.039484 8 0.177014 1.361022 -0.887458 9 -1.346035 -1.037976 1.041452 9 -0.738419 -1.221730 -1.034678 9 -2.564929 -0.160186 -0.526656 8 1.707875 -0.538008 0.986448 6 2.746001 -0.483644 0.380256 8 2.938640 0.151744 -0.778891 1 2.105506 0.574602 -1.052806 1 3.677370 -0.957283 0.709707	**Frequencies (cm^{-1}):** 19.1597, 41.5247, 46.2241, 60.3739, 103.4226, 115.2644, 137.3165, 232.0005, 242.2931, 378.9404, 421.5547, 511.4081, 586.5512, 650.9862, 693.5929, 730.3301, 759.1088, 805.5547, 1060.7112, 1102.4056, 1154.7082, 1162.0222, 1234.4325, 1313.3144, 1332.7441, 1412.3901, 1787.5158, 1911.7446, 3053.1846, 3652.1981

Compound: sCI 25 + HCHO $TS_{FAc}1$	**Energy (kJ mol^{-1}):** -739.806907643778
Reaction Coordinates: 6 1.249403 -0.207960 -0.071445 6 -0.136173 0.515847 -0.043915 9 -0.036599 1.614349 0.743981 8 -0.722589 0.624809 -1.149411 8 -2.550474 0.172171 -0.451244 9 1.736422 -0.392010 1.156046 9 2.116045 0.545375 -0.758823 9 1.144722 -1.394462 -0.677279 8 -0.973738 -0.526973 0.935336 6 -2.022844 -0.827505 0.223626 1 -3.122417 -0.555871 0.681826 1 -2.090814 -1.845743 -0.184181	**Frequencies (cm^{-1}):** -1180.7629, 71.5676, 94.3298, 177.0207, 221.5961, 286.7658, 296.2595, 310.7880, 364.2419, 418.3103, 467.9715, 471.7714, 541.7660, 587.4465, 665.9389, 704.6313, 756.7313, 833.3443, 888.0859, 1062.5610, 1150.5311, 1182.8067, 1202.5667, 1226.2364, 1259.7834, 1305.1679, 1394.7117, 1473.7019, 2271.2614, 2992.2183
IRC  	

Compound: sCI 25 + HCHO $C_{FAc}1$	**Energy (kJ mol^{-1}):** -739.988628614865
Reaction Coordinates: 6 -1.483755 -0.338849 -0.052076 6 -0.609282 0.901099 0.255281 9 -0.273207 1.517624 -0.882979 8 -0.344831 1.310813 1.324133 9 -1.077788 -0.992867 -1.137908 9 -2.745012 0.090180 -0.267307 9 -1.493370 -1.169297 0.984494 8 1.652661 -0.858738 0.114745 6 2.838184 -0.717960 0.124003 8 3.429826 0.431611 -0.250386 1 4.389305 0.358859 -0.171998 1 3.542958 -1.504848 0.434112	**Frequencies (cm^{-1}):** 12.2529, 20.2627, 35.6667, 44.4359, 61.7051, 76.2215, 106.1653, 231.3434, 242.0643, 378.2535, 420.8184, 511.7076, 538.9062, 585.0890, 663.4870, 689.6856, 755.8780, 800.1773, 1037.2738, 1083.9196, 1119.7911, 1149.5036, 1229.3486, 1271.2585, 1311.0063, 1415.9550, 1846.2374, 1934.9597, 2981.0252, 3779.8872

Compound: sCI 23 + HCHO $TS_{FAc}2$	**Energy (kJ mol^{-1}):** -739.799988971889
Reaction Coordinates: 6 -1.263159 -0.231854 0.043601 6 0.102664 0.427301 -0.293785 9 0.021464 1.768105 -0.050184 8 0.710354 0.068060 -1.326239 8 2.392624 -0.674104 -0.554776 9 -1.708869 0.127474 1.248179 9 -1.156407 -1.558841 -0.000709 9 -2.163586 0.156430 -0.871899 8 1.020614 -0.082642 1.079098 6 2.216518 -0.013896 0.573236 1 2.952503 -0.932840 0.826383 1 2.789200 0.914505 0.722162	**Frequencies (cm^{-1}):** -1104.2800, 62.1223, 68.0935, 171.2913, 216.9350, 272.6382, 279.8117, 307.6771, 350.9695, 387.9892, 427.3649, 484.5099, 540.8308, 585.7682, 660.9810, 703.0031, 750.5784, 812.8046, 884.6414, 1047.5704, 1160.2951, 1176.9495, 1212.6657, 1233.5197, 1260.8937, 1309.0540, 1400.2571, 1491.3314, 2343.7280, 2968.5175
IRC  	

Compound: sCI 25 + HCHO $C_{FAc}2$	**Energy (kJ mol^{-1}):** -739.988569845236
Reaction Coordinates: 6 1.210441 -0.586106 -0.060428 6 0.951717 0.878761 0.367628 9 1.170879 1.701187 -0.662919 8 0.687562 1.243968 1.452601 9 0.766535 -0.844231 -1.288894 9 0.643623 -1.427640 0.797277 9 2.543536 -0.792621 -0.043619 8 -3.160120 -0.849352 0.341988 6 -2.883208 0.325688 -0.253731 8 -1.765750 0.680545 -0.478184 1 -3.774505 0.918577 -0.511101 1 -4.113886 -0.960173 0.442444	**Frequencies (cm^{-1}):** 9.2098, 19.1505, 33.4684, 43.5209, 59.6264, 74.8819, 104.5050, 231.1540, 242.2426, 378.5483, 420.8136, 511.9706, 538.9994, 585.0978, 662.8509, 689.9521, 757.8900, 800.6257, 1037.2046, 1085.4595, 1119.5570, 1150.2551, 1227.3961, 1271.4277, 1311.4866, 1416.1844, 1846.9631, 1934.9215, 2980.6069, 3779.7123

Compound: sCI 25 + HCHO $TS_{ester}1$	**Energy (kJ mol^{-1}):** -739.781535601567

Reaction Coordinates:

```
6 -1.422805 -0.213581 0.086132
6 0.359595 0.380720 -0.081407
9 0.191519 1.620006 -0.668748
8 0.538537 -0.583618 -0.907970
8 2.469527 -0.856868 -0.466226
9 -1.926600 0.722605 0.853416
9 -1.399451 -1.367685 0.681583
9 -2.034024 -0.242012 -1.065347
8 0.871900 0.395574 1.076719
6 2.664197 0.007717 0.427705
1 3.007473 -0.336057 1.408659
1 2.863899 1.049987 0.168430
```

Frequencies (cm^{-1}):

```
-588.2564, 60.7916, 99.0798,
108.1427, 164.7614, 193.2517,
230.6891, 255.7045, 306.6388,
317.2887, 487.2591, 534.9642,
554.2207, 567.5308, 621.5868,
676.4830, 756.5990, 807.2190,
898.5517, 976.0160, 1150.8830,
1197.0207, 1251.1035, 1261.5896,
1330.9552, 1395.3279, 1473.9622,
1554.1570, 2995.2314, 3082.5091
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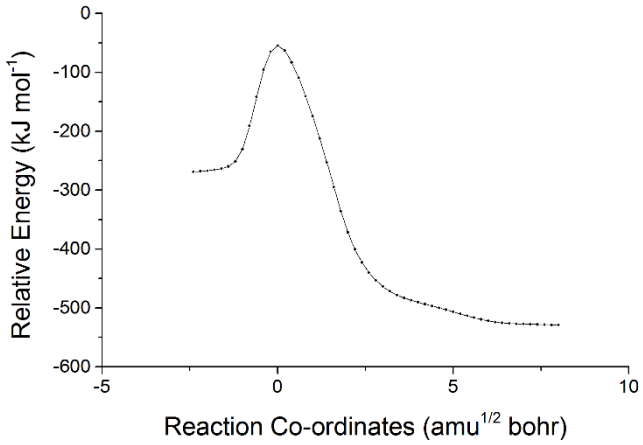
IRC



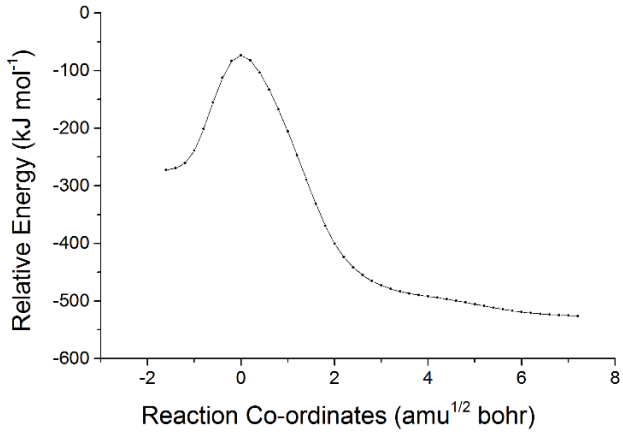
Compound: sCI 25 + HCHO $C_{ester}1$	**Energy (kJ mol^{-1}):** -739.977318615772

Reaction Coordinates:

```
6 -1.438091 -0.328538 -0.053297
9 -2.123748 0.239571 0.936736
9 -2.280767 -0.693219 -1.009719
9 -0.817177 -1.406218 0.414875
8 -0.556511 0.567248 -0.640931
6 0.433924 1.093616 0.117396
9 1.086785 1.935488 -0.663881
8 0.673618 0.909472 1.257292
8 2.281535 -0.867481 -0.682601
6 2.928435 -1.225038 0.266485
1 3.752697 -1.952181 0.162579
1 2.726723 -0.842568 1.281745
```

Frequencies (cm^{-1}):

```
31.7264, 43.5110, 60.0890, 78.1354,
102.3299, 117.0928, 149.9059,
165.4967, 179.4153, 378.1240,
403.6030, 427.4693, 550.9837,
609.0345, 669.9364, 737.6815,
757.5186, 879.5778, 1023.6817,
1149.5186, 1207.6212, 1215.8080,
1240.9116, 1267.7803, 1278.8360,
1527.3657, 1803.0161, 1911.4485,
2906.0910, 2974.0356
```

Compound: sCI 25 + HCHO $TS_{ester}2$	**Energy (kJ mol^{-1}):** -739.786202678286
Reaction Coordinates: 6 1.396175 -0.267274 0.002936 6 -0.388780 0.495260 0.047108 9 -0.090167 1.814698 -0.114078 8 -0.540319 -0.195561 -1.022155 8 -2.553430 -0.185580 -0.752387 9 1.934085 0.381624 1.010036 9 1.284892 -1.539686 0.259211 9 2.044179 -0.022649 -1.101464 6 -2.469377 -0.623178 0.426331 8 -0.970239 0.192826 1.133098 1 -2.121480 -1.639456 0.624488 1 -3.151636 -0.188761 1.165464	**Frequencies (cm^{-1}):** -594.8467, 54.8487, 91.2012, 121.2305, 171.7936, 201.1541, 241.4115, 246.9698, 297.8808, 328.8755, 519.5294, 529.9244, 550.6988, 593.3187, 627.0561, 672.7171, 743.0208, 879.0350, 937.2457, 970.3107, 1143.5766, 1189.1849, 1256.0499, 1280.3139, 1328.2734, 1378.7216, 1490.3402, 1533.3773, 2992.9535, 3075.6329
IRC  	

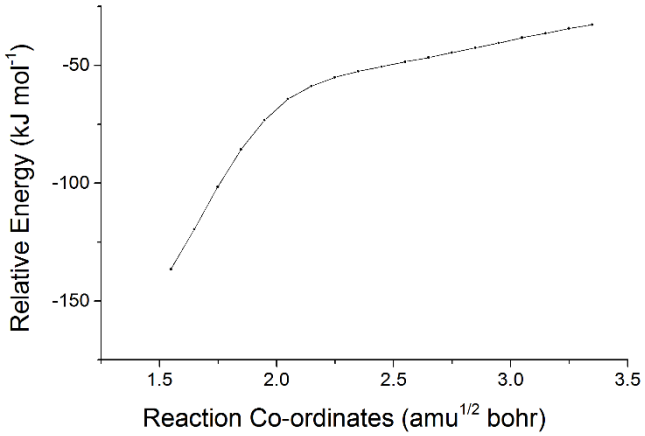
Compound: CF_3CFO	**Energy (kJ mol^{-1}):** -451.199957828211
Reaction Coordinates: 6 -0.590884 0.016760 -0.000000 6 0.950258 0.161191 -0.000000 8 1.560686 1.164510 0.000000 9 1.511346 -1.053957 -0.000000 9 -0.986585 -0.656718 1.087722 9 -1.165035 1.213645 -0.000003 9 -0.986585 -0.656723 -1.087719	**Frequencies (cm^{-1}):** 43.7845, 226.0109, 238.7949, 378.7825, 419.3861,1. 512.0808, 584.7772, 688.3344, 765.2522, 800.0823, 1086.2930, 1167.3575, 1222.6180, ,1305.3726, 1935.9581

Compound: CF_3OCFO	**Energy (kJ mol^{-1}):** -526.392169685219
Reaction Coordinates: 6 0.985021 -0.064022 0.000000 9 1.142265 0.688671 1.083247 9 1.895578 -1.026215 -0.000000 9 1.142264 0.688671 -1.083247 8 -0.249812 -0.707922 0.000001 6 -1.372203 0.051286 0.000000 9 -2.386217 -0.800803 -0.000000 8 -1.477929 1.223361 -0.000000	**Frequencies (cm^{-1}):** 75.3080, 177.0143, 376.9655, 401.4174, 427.2777, 550.7688, 610.1072, 668.4452, 737.8881, 774.4134, 880.1638, 1021.3954, 1141.4172, 1225.8672, 1237.8952, 1275.4731, 1923.5619

8.3 sCI Reactions with SO_2

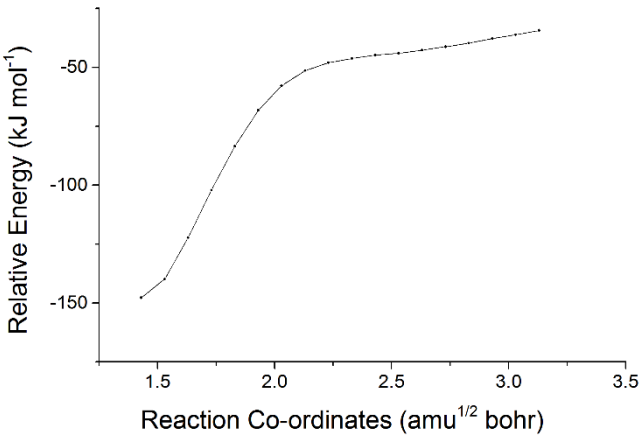
Compound: SO_2	**Energy (kJ mol^{-1}):** -548.08584429715
Reaction Coordinates: 16 0.000000 0.000000 0.372669 8 0.000000 1.245290 -0.372669 8 -0.000000 -1.245290 -0.372669	**Frequencies (cm^{-1}):** 513.3417, 1156.5416, 1337.5576

8.3.1 sCI 1 + SO_2

Compound: sCI 1 + SO_2 $TS_{Cyc}1$ reaction profile
IRC 

Compound: sCI 1 + SO_2 SOZ1	**Energy (kJ mol^{-1}):** -737.54758505440
Reaction Coordinates: 6 1.382069 -0.646247 0.414243 1 1.138310 -0.656463 1.477779 8 1.589137 0.652527 -0.058367 8 0.269739 1.234086 0.029932 16 -0.903903 0.016549 -0.430359 8 0.274519 -1.149994 -0.346833 8 -1.787516 -0.049041 0.719351 1 2.264694 -1.231458 0.169849	**Frequencies (cm^{-1}):** 122.2352, 300.3218, 365.2906, 429.7004, 512.9059, 611.8820, 691.2164, 714.2195, 868.9158, 923.9394, 1046.7403, 1148.9215, 1243.2803, 1247.7933, 1377.9775, 1505.9329, 3052.1770, 3146.1962

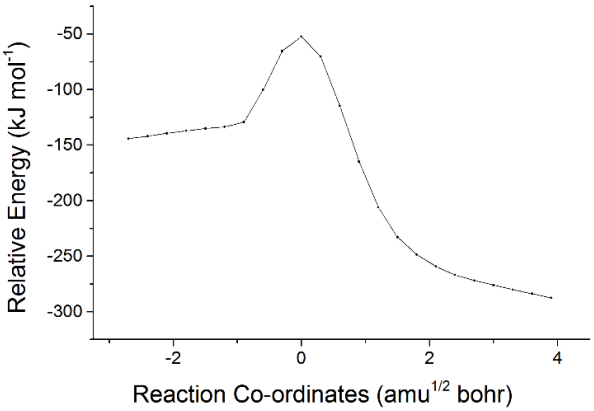
Compound: sCI 1 + SO_2 $TS_{Cyc}2$ reaction profile
IRC



Compound: sCl 1 + SO_2 SOZ2	**Energy (kJ mol^{-1}):** -737.54937458407
Reaction Coordinates: 6 -1.556878 -0.547909 0.071274 1 -2.103692 -0.542148 -0.874056 8 -1.293568 0.748906 0.523130 8 -0.267816 1.181102 -0.421646 16 0.909912 -0.063250 -0.409928 8 -0.292974 -1.188917 -0.119714 8 1.727057 -0.003975 0.785128 1 -2.095215 -1.055326 0.870085	**Frequencies (cm^{-1}):** 132.0686, 287.7793, 374.3085, 447.0565, 519.4221, 630.6105, 667.5639, 714.3830, 835.9980, 947.7173, 1040.2338, 1133.8437, 1234.1709, 1258.4403, 1386.7702, 1504.2540, 3036.7579, 3124.0647

Compound: sCl 1 + SO_2 TS_{hoz}	**Energy (kJ mol^{-1}):** -737.54937458407
Reaction Coordinates: 6 1.386780 -0.692255 0.278605 1 1.274693 -1.092237 1.287451 8 1.397845 0.745999 0.369330 8 0.212787 1.242656 -0.331163 16 -0.931332 0.018255 -0.381583 8 0.303256 -1.082345 -0.546129 8 -1.538487 -0.158847 0.927095 1 2.302725 -1.026016 -0.206819	**Frequencies (cm^{-1}):** -179.8160, 159.1954, 353.4794, 451.0161, 572.8258, 671.8872, 697.3124, 723.2182, 833.2018, 938.3023, 1040.7095, 1126.7846, 1197.2006, 1241.8372, 1393.0334, 1531.9412, 3041.7383, 3108.8411

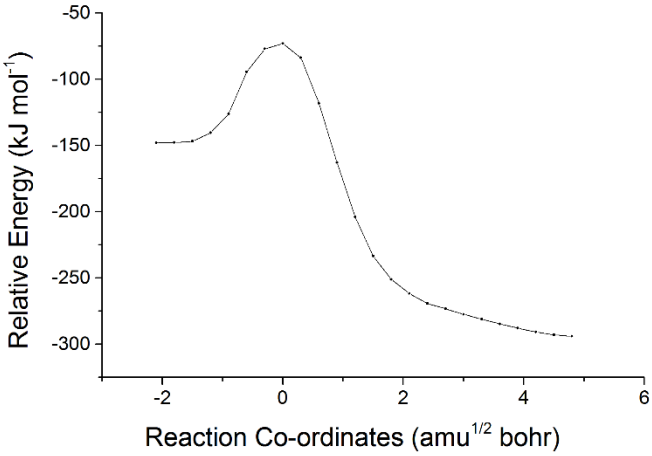
Compound: sCl 1 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -737.51404208200
Reaction Coordinates: 6 1.501312 -0.650356 0.305770 1 1.174843 -1.145000 1.224048 8 1.700162 0.635117 0.346011 8 -0.052180 1.317998 -0.225692 16 -0.881951 0.066084 -0.304427 8 0.227311 -0.967082 -0.711171 8 -1.665008 -0.337595 0.852781 1 2.246226 -1.197717 -0.283267	**Frequencies (cm^{-1}):** -559.6034, 124.6928, 185.5359, 320.2554, 418.0848, 482.2966, 535.8077, 616.2304, 804.3402, 960.9313, 1009.8710, 1160.8091, 1224.0481, 1249.8633, 1310.5436, 1506.3998, 2983.3701, 3065.2443
IRC	

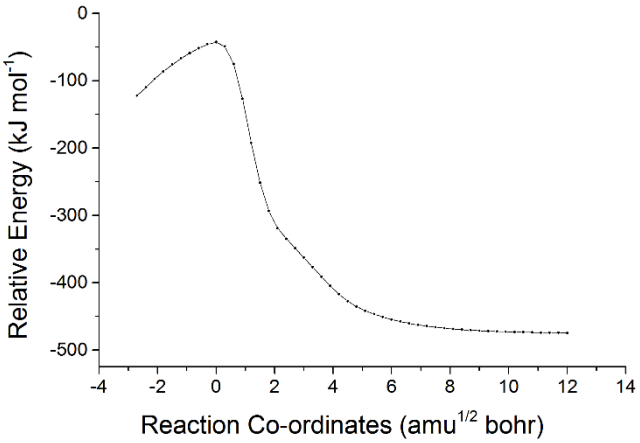
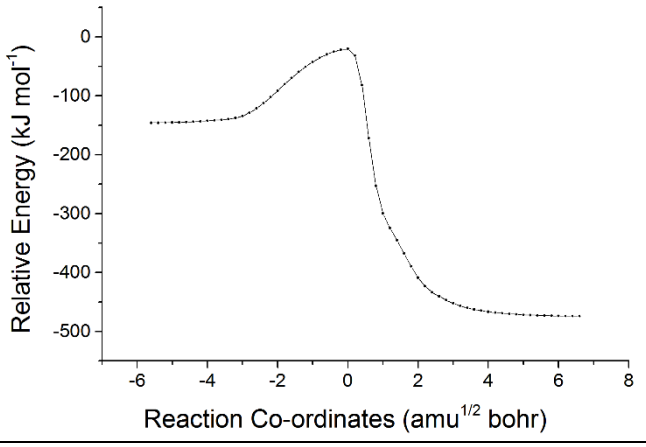


Compound: sCl 1 + SO_2 $Cso_3$1	**Energy (kJ mol^{-1}):** -737.62562027792
Reaction Coordinates: 6 2.341652 0.110229 -0.000001 1 3.391734 -0.210515 0.000002 1 2.117654 1.185058 -0.000005 8 1.456406 -0.714452 0.000001 8 -1.068999 -0.553788 1.247214 16 -0.728472 0.078182 0.000000 8 -0.306356 1.461227 -0.000032 8 -1.069019 -0.553840 -1.247182	**Frequencies (cm^{-1}):** 57.7179, 151.3388, 177.0498, 181.1805, 298.8735, 366.7314, 474.7464, 514.5355, 515.9279, 1039.7032, 1215.7655, 1262.8801, 1342.6023, 1367.2268, 1508.6567, 1769.9047, 2969.2137, 3063.1764

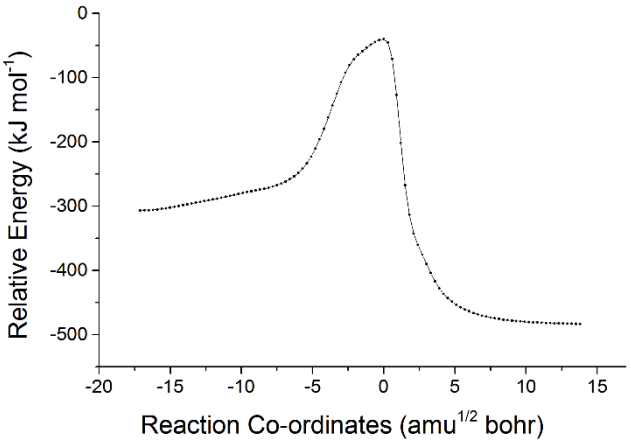
Compound: sCl 1 + SO_2 $TSso_3$2	**Energy (kJ mol^{-1}):** -737.52348576070
Reaction Coordinates: 6 1.675324 -0.427293 0.002391 1 2.138285 -0.364549 -0.986984 8 1.512196 0.659717 0.679127 8 -0.065910 1.221055 -0.501149 16 -0.865776 -0.027908 -0.316199 8 -1.784157 -0.175642 0.798381 8 0.285073 -1.128409 -0.300800 1 2.084584 -1.238935 0.627351	**Frequencies (cm^{-1}):** -443.3199, 143.9413, 241.7856, 303.0127, 428.7202, 491.0293, 511.7264, 656.5097, 759.3473, 969.7000, 1000.6678, 1124.3188, 1249.0727, 1270.1735, 1322.2826, 1438.5225, 2937.7277, 3037.1136

IRC



Compound: sCI 1 + SO_2 $TS_{acid}1$	**Energy (kJ mol^{-1}):** -737.49389238926
Reaction Coordinates: 6 1.629372 -0.345072 -0.136515 1 2.240069 -0.218982 -1.044043 8 1.512066 0.699746 0.661067 8 -0.200944 1.243956 -0.386806 16 -0.992011 -0.032259 -0.373489 8 0.632019 -1.195266 -0.210455 8 -1.755655 -0.317004 0.823119 1 2.355981 -0.645892 0.743562	**Frequencies (cm^{-1}):** -832.8318, 133.5888, 195.8912, 247.3174, 358.5430, 385.4304, 432.5792, 505.1556, 704.0409, 802.4629, 986.7936, 1136.3870, 1204.3920, 1276.1307, 1298.1726, 1376.3094, 2452.6451, 2962.2799
IRC  	
Compound: sCI 1 + SO_2 $TS_{acid}2$	**Energy (kJ mol^{-1}):** -737.50143644919
Reaction Coordinates: 6 1.405536 -0.555411 0.316090 1 1.245825 -0.987224 1.317976 8 1.705258 0.735066 0.276800 8 -0.214092 1.312346 -0.104809 16 -1.027584 0.071542 -0.362876 8 0.694356 -1.055207 -0.664845 8 -1.658572 -0.514248 0.807833 1 2.546705 -0.648638 0.071658	**Frequencies (cm^{-1}):** -731.4789, 123.8317, 184.0541, 234.6166, 338.4323, 409.5670, 426.8130, 509.2331, 691.9101, 790.8737, 971.3345, 1128.3870, 1220.4001, 1255.4461, 1285.1249, 1375.6071, 2501.8042, 2945.3882
IRC  	

Compound: sCl 1 + SO_2 $C_{acid}1$	**Energy (kJ mol^{-1}):** -737.67576753941
Reaction Coordinates: 6 -2.324179 -0.010590 -0.355769 1 -3.146885 0.039791 1.368678 8 -1.344757 -0.030178 -1.041439 8 1.571462 -1.228815 0.473015 16 1.508648 -0.009039 -0.313940 8 -2.260866 0.029061 0.985361 8 1.571843 1.253882 0.401687 1 -3.347860 -0.023224 -0.760015	**Frequencies (cm^{-1}):** 21.5880, 28.3617, 29.0618, 78.5591, 96.3446, 133.8663, 517.6701, 540.0397, 665.5994, 1037.9677, 1126.1208, 1156.9469, 1270.4993, 1328.5625, 1414.4276, 1835.1316, 2984.2698, 3780.5005

Compound: sCl 1 + SO_2 $TS_{acid}3$	**Energy (kJ mol^{-1}):** -737.50120403903
Reaction Coordinates: 6 1.709591 0.242649 -0.179014 1 2.146751 1.259339 0.231095 8 1.783991 -0.584592 0.760050 8 -0.399436 -1.312706 -0.358881 16 -1.001669 0.023142 -0.323319 8 0.603396 1.091388 -0.319156 8 -1.810743 0.415679 0.812871 1 2.204744 0.036341 -1.142972	**Frequencies (cm^{-1}):** -678.6198, 109.1496, 138.7703, 218.4693, 272.9500, 341.8787, 378.3924, 500.2041, 662.2154, 704.1694, 924.9739, 1094.5164, 1142.6219, 1294.3151, 1318.3949, 1468.5642, 2392.1632, 2938.2548
IRC  	

Compound: sCl 1 + SO_2 $C_{acid}2$	**Energy (kJ mol^{-1}):** -737.68599404256
Reaction Coordinates: 6 2.153108 0.466614 -0.030781 8 1.189385 1.145996 0.230713 8 2.145949 -0.843591 -0.256551 1 1.232434 -1.183415 -0.184780 1 3.169916 0.865614 -0.112439 8 -2.084303 0.668245 -0.679832 16 -1.347910 -0.002589 0.371589 8 -0.720335 -1.275707 0.022731	**Frequencies (cm^{-1}):** 31.4878, 68.9111, 113.5839, 137.3046, 162.6219, 182.6245, 519.2643, 661.9957, 774.6861, 1064.2063, 1148.5395, 1178.5391, 1313.9712, 1351.0209, 1416.0962, 1763.6747, 3056.0992, 3574.5704

Compound: SO_3	**Energy (kJ mol^{-1}):** -623.22229804288
Reaction Coordinates:	**Frequencies (cm^{-1}):**

16 0.000000 -0.000000 0.000000 8 0.246828 -1.418352 0.000000 8 -1.351743 0.495417 0.000000 8 1.104915 0.922936 -0.000000	475.6389, 507.9530, 507.9566, 1044.8229, 1363.4683, 1363.4939

8.3.2 sCIs 23 & 24 + SO_2

Compound: sCI 23 + SO_2 PRC1	**Energy (kJ mol^{-1}):** -1074.30049656118
Reaction Coordinates: 6 -1.680849 -0.330936 0.008724 6 -1.137494 0.933439 0.662474 8 -0.286665 1.695181 0.151214 8 0.351463 1.317116 -0.987851 1 -1.567548 1.282222 1.592022 9 -2.292584 -0.014933 -1.139885 9 -0.764980 -1.257811 -0.222516 9 -2.603039 -0.837675 0.848126 16 2.325088 0.008750 0.066354 8 1.581156 -0.072555 1.323138 8 2.381748 -1.195175 -0.743052	**Frequencies (cm^{-1}):** 29.2239, 48.4725, 62.4815, 91.7570, 100.6754, 174.7347, 180.0268, 226.5884, 268.6855, 328.0287, 471.8117, 505.2088, 516.6429, 535.2394, 580.3347, 756.1669, 830.0680, 877.0832, 910.6656, 1135.9560, 1154.7572, 1181.4849, 1253.8791, 1308.2990, 1367.8966, 1568.4158, 3206.0587

Compound: sCI 23 + SO_2 $TS_{Cyc}1$	**Energy (kJ mol^{-1}):** -1074.29932649603
Reaction Coordinates: 6 -1.567535 -0.331819 -0.021801 6 -0.988288 0.893200 0.685292 8 -0.211136 1.738966 0.185226 8 0.497696 1.392847 -0.932081 1 -1.437201 1.192710 1.623913 9 -2.387958 0.121866 -0.988788 9 -0.705693 -1.173798 -0.552521 9 -2.314631 -0.984971 0.884328 16 2.173682 -0.031753 0.130690 8 1.283290 -0.181356 1.294872 8 2.263619 -1.165560 -0.770900	**Frequencies (cm^{-1}):** -44.3238, 45.4533, 84.8741, 109.5867, 127.1715, 192.3251, 213.1513, 285.4045, 305.8816, 334.5709, 462.8314, 505.3981, 515.4080, 535.7839, 572.3408, 754.0951, 843.8360, 874.8355, 916.4321, 1106.9795, 1146.0291, 1161.5810, 1276.1099, 1295.7925, 1367.9148, 1566.9924, 3200.2906

Compound: sCI 23 + SO_2 SOZ1	**Energy (kJ mol^{-1}):** -1074.35461788075
Reaction Coordinates: 6 1.509783 -0.211551 0.070085 6 0.472691 0.607230 -0.732729 8 -0.097190 1.667245 -0.006489 8 -1.133556 1.051570 0.784769 1 0.991158 1.063821 -1.576545 9 2.487991 0.611495 0.483098 9 1.000662 -0.831871 1.132375 9 2.057394 -1.134082 -0.739936 16 -1.965027 -0.084757 -0.232373 8 -0.582831 -0.198334 -1.205133 8 -2.106424 -1.256938 0.600670	**Frequencies (cm^{-1}):** 44.2404, 70.6265, 157.2900, 209.8630, 255.8569, 303.1416, 343.8475, 400.9612, 422.9259, 510.4862, 527.3151, 561.9128, 628.6370, 670.6377, 673.0996, 794.4516, 871.0570, 895.9295, 1002.9074, 1065.5800, 1165.6786, 1168.0381, 1268.0762, 1290.8391, 1306.0599, 1396.4551, 3091.8167

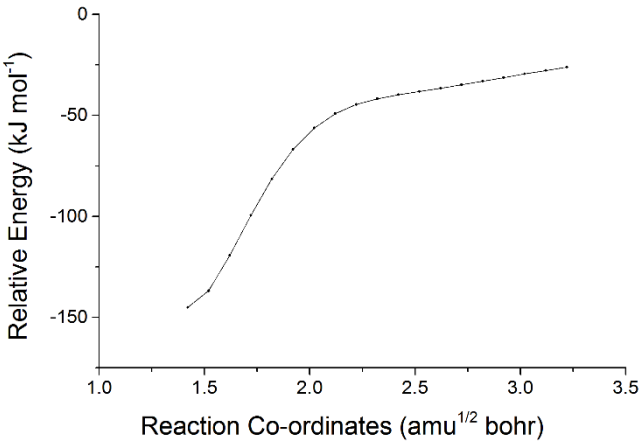
Compound: sCI 23 + SO_2 PRC2	**Energy (kJ mol^{-1}):** -1074.29958900339
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.884175 -0.194669 -0.056099 6 -1.045646 0.530654 0.987311 8 -0.092184 1.297137 0.725886 8 0.348291 1.408367 -0.552527 1 -1.314868 0.467760 2.033230 9 -2.513437 0.695230 -0.833304 9 -1.191282 -1.028633 -0.819448 9 -2.815482 -0.900882 0.610603 16 2.275655 -0.411951 -0.361018 8 1.470431 -1.130483 0.624267 8 3.419101 0.326993 0.144266	24.6678, 6.0920, 55.9841, 81.8352, 103.1086, 146.9604, 190.9617, 214.3366, 264.9684, 327.1424, 474.3552, 505.0058, 518.9497, 534.9524, 582.8485, 756.8278, 825.7794, 877.5626, 913.2445, 1139.9864, 1156.8720, 1179.9236, 1250.4563, 1309.9265, 1368.0173, 1568.8053, 3207.4250

Compound: sCI 23 + SO_2 $TS_{Cyc}2$	**Energy (kJ mol^{-1}):** -1074.29940211685
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.767970 -0.200627 -0.050972 6 -0.892727 0.535501 0.961344 8 -0.010909 1.378492 0.685315 8 0.437785 1.465943 -0.599539 1 -1.147977 0.467376 2.011078 9 -2.588927 0.704888 -0.612708 9 -1.135920 -0.854988 -1.007771 9 -2.520183 -1.071524 0.642652 16 2.118402 -0.439758 -0.360278 8 1.208848 -1.095346 0.588120 8 3.292152 0.195178 0.212553	-31.0837, 46.6099, 55.9795, 106.4244, 127.9574, 150.6068, 212.6447, 267.3147, 290.7125, 327.6061, 469.3283, 504.8931, 519.0325, 534.8190, 577.3396, 755.5527, 838.7640, 874.0912, 912.2329, 1120.7541, 1149.9620, 1164.0053, 1271.7624, 1294.7358, 1367.7513, 1573.1131, 3202.7905

Compound: sCI 23 + SO_2 SOZ2	**Energy (kJ mol^{-1}):** -1074.36037274421
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.660626 -0.102587 0.034820 6 0.359614 0.028112 -0.791388 8 -0.261150 1.276678 -0.666093 8 -1.040876 1.153037 0.563436 1 0.609532 -0.077818 -1.848446 9 2.505897 0.881224 -0.304427 9 1.452955 -0.048177 1.353799 9 2.248145 -1.276966 -0.250026 16 -1.869280 -0.327151 0.446264 8 -0.560881 -0.969187 -0.405574 8 -2.972776 -0.241233 -0.485078	48.0706, 78.6188, 141.0420, 202.3361, 257.8851, 294.1922, 383.5957, 399.3418, 467.0707, 518.5585, 545.0363, 578.2684, 638.3053, 663.9512, 690.5619, 788.0789, 833.9486, 863.3242, 1009.0424, 1064.5929, 1159.6992, 1175.8721, 1265.5730, 1282.5502, 1289.6916, 1391.5748, 3085.6763

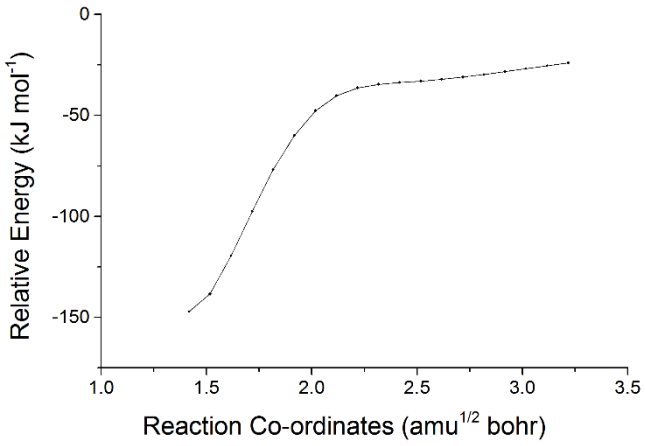
Compound: sCI 24 + SO_2 $TS_{Cyc}1$ reaction profile
IRC


0
-50
-100
-150
Relative Energy (kJ mol-1)
1.0
1.5
2.0
2.5
3.0
3.5
Reaction Co-ordinates (amu1/2 bohr)

Compound: sCI 23 + SO_2 SOZ3	**Energy (kJ mol^{-1}):** -1074.35773058988
Reaction Coordinates: 6 1.702452 -0.118431 0.047577 6 0.387703 0.424608 -0.543796 8 -0.198834 1.268729 0.409836 8 -1.564676 1.367343 -0.075039 16 -2.078769 -0.251684 -0.317001 8 -0.511096 -0.644797 -0.784013 8 -2.332760 -0.913456 0.942857 1 0.594851 0.949559 -1.480180 9 2.537742 0.903356 0.291605 9 2.283775 -0.929409 -0.847908 9 1.509979 -0.794193 1.176345	**Frequencies (cm^{-1}):** 51.6628, 66.2206, 165.4099, 188.0028, 271.1719, 303.6911, 367.9778, 380.8930, 444.9106, 520.1523, 532.6612, 559.3600, 636.8891, 685.6619, 705.9521, 715.0671, 872.6268, 881.7316, , 1019.6375, 1089.4928, 1170.7546, 1177.1922, 1265.7594, 1283.3818, 1342.3435, 1410.2857, 3050.3375

Compound: sCI 24 + SO_2 $TS_{Cyc}2$ reaction profile

IRC

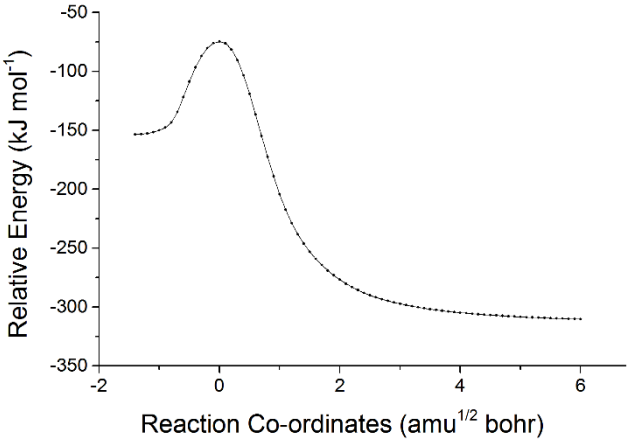


Compound: sCI 23 + SO_2 SOZ4	**Energy (kJ mol^{-1}):** -1074.35489019767
Reaction Coordinates: 6 1.779444 -0.130676 -0.041084 6 0.306102 0.102417 -0.412299 8 -0.074918 1.371532 0.041590 8 -1.506844 1.335170 -0.093337 16 -2.072519 -0.245121 0.411857 8 -0.508107 -0.825571 0.290510 8 -2.873972 -0.681963 -0.712054 1 0.169485 -0.002257 -1.491093 9 1.987951 -0.045424 1.272100 9 2.154784 -1.347066 -0.458012 9 2.544850 0.781422 -0.657643	**Frequencies (cm^{-1}):** 51.7553, 81.6765, 142.5523, 164.0122, 266.7253, 320.0954, 323.3741, 385.3553, 427.9052, 524.1165, 526.5158, 558.0106, 610.8184, 685.2486, 717.4421, 729.0240, 887.8522, 932.4643, 996.8673, 1088.8626, 1172.7260, 1183.7142, 1259.5769, 1278.4975, 1332.3607, 1420.1472, 3063.9397

Compound: sCI 23 + SO_2 $TS_{SOZ}1$	**Energy (kJ mol^{-1}):** -1074.35121769837
Reaction Coordinates: 6 -1.525315 -0.164536 -0.056157 6 -0.430735 0.665276 0.657307 8 0.145384 1.597292 -0.246252 8 1.535307 1.215057 -0.487627 1 -0.910361 1.222606 1.465011 9 -2.054881 -1.045162 0.807896 9 -2.503007 0.669459 -0.452593 9 -1.076416 -0.825045 -1.120134 16 1.940963 -0.260886 0.233548 8 0.581371 -0.131710 1.211230 8 1.775436 -1.336408 -0.718004	**Frequencies (cm^{-1}):** -144.3866, 50.6273, 105.2007, 181.7474, 205.0582, 309.4378, 330.6954, 397.4601, 417.8668, 517.0891, 558.6261, 567.8528, 652.0541, 679.3330, 685.5999, 785.9350, 842.6908, 854.7400, 1010.1829, 1080.4706, 1162.5741, 1171.6860, 1266.5673, 1295.1893, 1303.7839, 1404.6539, 3062.0777

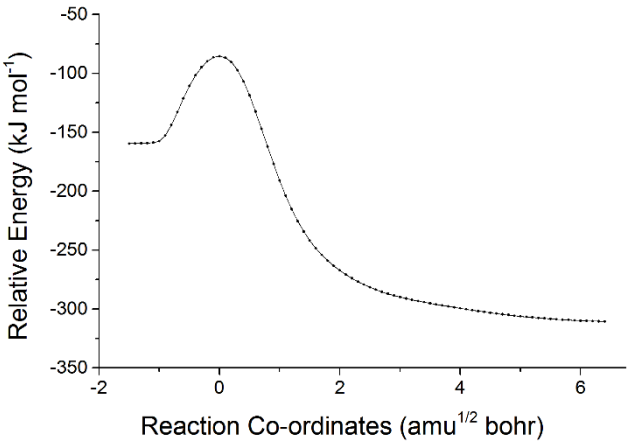
Compound: sCI 23 + SO_2 $TS_{SOZ}2$	**Energy (kJ mol^{-1}):** -1074.35365432423
Reaction Coordinates: 6 1.748937 -0.114434 -0.024259 6 0.274018 -0.031580 -0.460387 8 -0.153842 1.321783 -0.344886 8 -1.482972 1.313361 0.269186 1 0.176216 -0.373303 -1.494543 9 2.486196 0.699763 -0.793583 9 1.915846 0.233503 1.250191 9 2.194913 -1.368014 -0.190779 16 -2.072430 -0.261113 0.390273 8 -0.498174 -0.817146 0.413770 8 -2.680969 -0.650508 -0.867371	**Frequencies (cm^{-1}):** -101.5726, 62.6211, 99.9642, 155.2252, 220.0687, 319.4128, 339.1073, 379.8420, 449.1546, 518.6561, 554.8601, 588.8998, 669.4501, 686.7225, 717.7112, 738.3950, 859.8401, 869.9778, 1010.8214, 1073.4618, 1171.8732, 1176.4586, 1252.2470, 1280.7008, 1331.7885, 1416.1239, 3048.0420

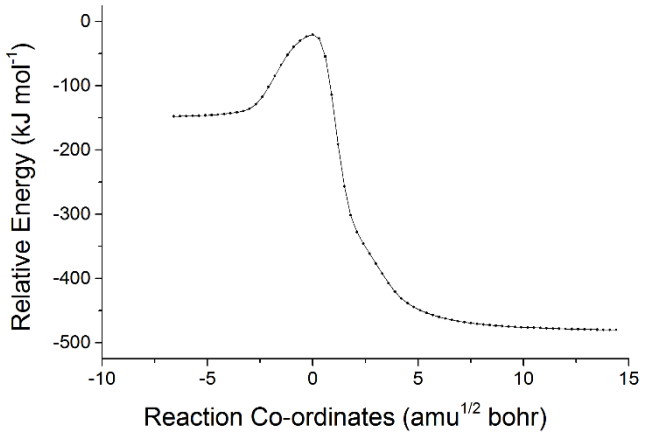
Compound: sCI 23 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -1074.33512300027
Reaction Coordinates: 6 -1.681073 0.106352 0.052263 6 -0.432132 -0.144608 -0.832003 8 0.079204 -1.329812 -0.848233 8 1.230573 -1.027724 0.793877 1 -0.614523 0.241506 -1.849452 9 -2.117836 1.366947 -0.108056 9 -1.449414 -0.096900 1.350768 9 -2.655367 -0.725443 -0.342431 16 1.847120 0.256751 0.351536 8 0.609315 0.938962 -0.387725 8 3.048831 0.290896 -0.457819	**Frequencies (cm^{-1}):** -441.1456, 46.9288, 90.8543, 126.8517, 191.0219, 253.8848, 286.2551, 330.2239, 420.2077, 443.1656, 502.5533, 517.3251, 538.3314, 574.7456, 694.5466, 749.8890, 789.9627, 844.1961, 994.5220, 1091.1145, 1149.2041, 1185.0667, 1223.4300, 1266.6729, 1269.7930, 1382.1165, 2946.7385
IRC	



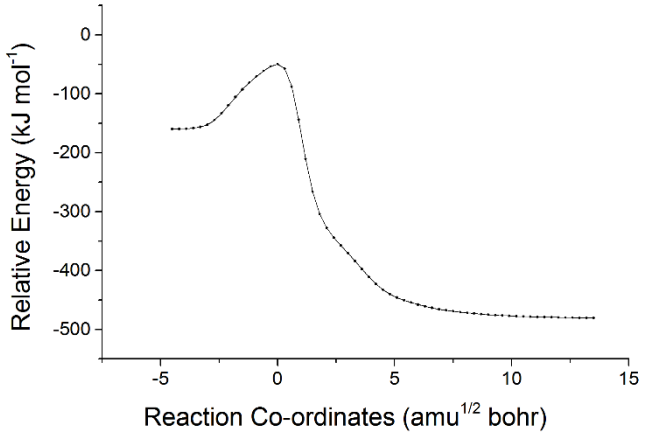
Compound: sCl 23 + SO_2 $CSO_3$1	**Energy (kJ mol^{-1}):** -1074.43431110038
Reaction Coordinates: 6 -2.359197 0.002975 -0.000000 6 -0.844225 -0.282288 -0.000001 8 -0.032595 0.601469 -0.000001 8 2.641537 0.592391 -1.247684 1 -0.574830 -1.348409 -0.000002 9 -2.904523 -0.565307 1.089032 9 -2.636321 1.298767 -0.000005 9 -2.904526 -0.565316 -1.089025 16 2.370290 -0.068647 0.000000 8 1.984410 -1.460059 -0.000014 8 2.641529 0.592367 1.247698	**Frequencies (cm^{-1}):** 20.1907, 42.5260, 69.5071, 81.9062, 83.0338, 166.6485, 171.1706, 294.3903, 329.2156, 434.3420, 463.1476, 509.8777, 511.3396, 527.5328, 529.7630, 706.9608, 846.3766, 999.3410, 1043.9802, 1163.3722, 1181.5146, 1289.2590, 1351.4924, 1373.8588, 1399.6574, 1819.7549, 3013.7213

Compound: sCl 23 + SO_2 $TSSO_3$2	**Energy (kJ mol^{-1}):** -1074.32997089072
Reaction Coordinates: 6 1.728009 -0.125183 0.034650 6 0.441912 0.660406 -0.396289 8 -0.050099 1.358879 0.576907 8 -1.915066 1.267761 -0.144913 1 0.611404 1.151115 -1.360112 9 2.138415 -0.915789 -0.963504 9 1.529476 -0.858648 1.121655 9 2.695958 0.767152 0.278919 16 -1.992157 -0.223075 -0.273980 8 -0.517223 -0.532291 -0.772050 8 -2.396494 -1.060311 0.837555	**Frequencies (cm^{-1}):** -441.5083, 56.4485, 72.5008, 161.8351, 186.0835, 266.6349, 292.1361, 317.1228, 403.2586, 441.0609, 507.0897, 515.8940, 530.1940, 567.2088, 679.8117, 737.2216, 794.7079, 840.8249, 975.2500, 1151.3726, 1175.2529, 1210.0695, 1257.0745, 1277.7910, 1303.9932, 1360.3222, 3030.9695
IRC	

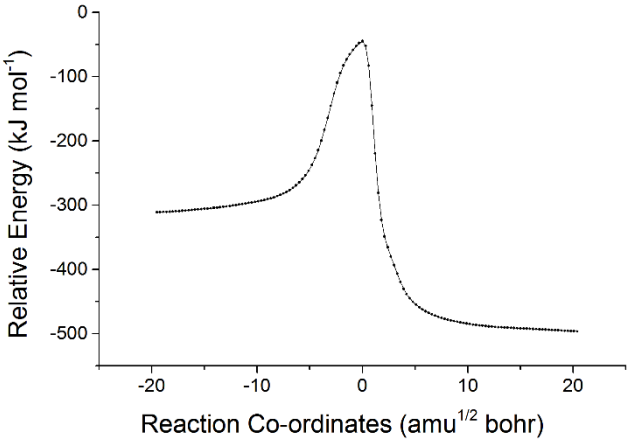

-50
-100
-150
-200
-250
-300
-350
-2
0
2
4
6
Relative Energy (kJ mol-1)
Reaction Co-ordinates (amu1/2 bohr)

Compound: sCI 23 + SO_2 $TS_{acid}1$	**Energy (kJ mol^{-1}):** -1074.30007800359
Reaction Coordinates: 6 -1.505222 -0.239235 -0.072830 6 -0.468416 0.779170 0.532436 8 -0.117868 1.770499 -0.267234 8 1.675590 0.954167 -0.770812 1 -1.112337 1.616668 1.033243 9 -2.586837 0.431945 -0.501419 9 -0.984302 -0.900871 -1.104109 9 -1.892435 -1.114031 0.857215 16 2.020959 -0.176837 0.163869 8 0.396458 0.320788 1.397348 8 1.769694 -1.517986 -0.319049	**Frequencies (cm^{-1}):** -688.6455, 34.5698, 102.7656, 106.7723, 153.6091, 184.0275, 240.9328, 282.9228, 334.7932, 384.6055, 428.8683, 438.7417, 490.1544, 522.3457, 589.2997, 694.3193, 792.1899, 813.5240, 883.2912, 961.6328, 1139.4703, 1187.9310, 1206.3680, 1248.5025, 1281.7435, 1340.6893, 2496.1816
IRC  	

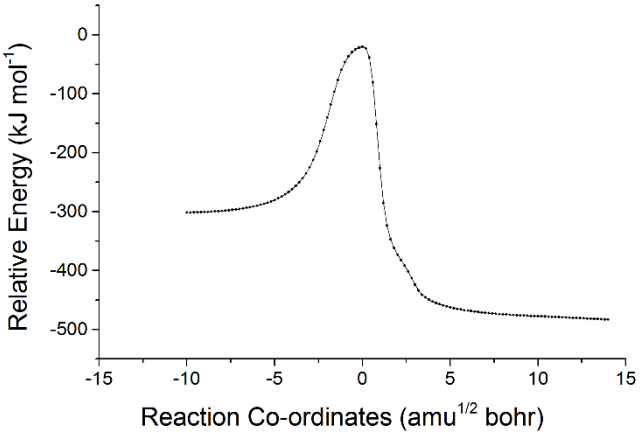
Compound: sCI 23 + SO_2 $C_{acid}1$	**Energy (kJ mol^{-1}):** -1074.48261883124
Reaction Coordinates: 6 2.244544 -0.262546 -0.114768 6 0.894474 0.357660 0.356378 8 0.884820 1.682848 0.496233 1 1.738515 2.069558 0.254068 8 -0.046837 -0.341178 0.576054 9 2.072883 -0.954956 -1.237657 9 3.167254 0.703181 -0.353907 9 2.733065 -1.071123 0.825914 8 -2.852061 0.915641 -0.944483 16 -3.036633 0.092495 0.238408 8 -3.454086 -1.284071 0.043772	**Frequencies (cm^{-1}):** 10.4592, 11.1773, 14.8872, 26.3993, 43.1879, 67.6075, 108.1088, 252.6177, 259.5524, 385.2853, 426.5345, 505.0798, 516.9555, 571.0955, 584.3263, 688.8721, 776.4952, 793.7122, 1118.9072, 1157.7687, 1179.0938, 1197.1657, 1239.8601, 1332.5658, 1372.3901, 1868.7735, 3746.5623

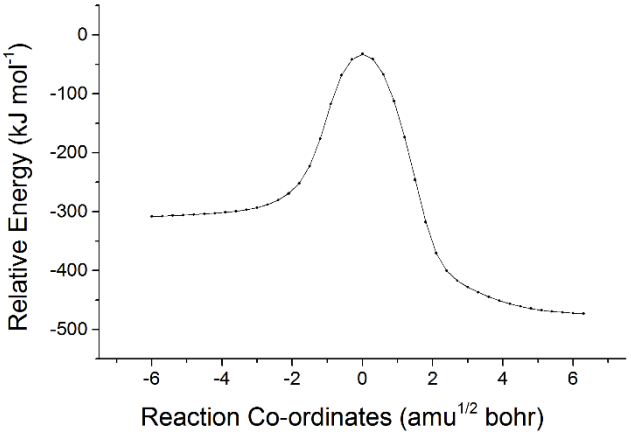
Compound: sCI 23 + SO_2 $TS_{acid}2$	**Energy (kJ mol^{-1}):** -1074.31032548775
Reaction Coordinates: 6 1.719219 -0.101523 0.094679 6 0.407056 0.052457 -0.744778 8 -0.078855 1.275075 -0.892810 8 -1.295967 1.040241 0.709241 1 0.733771 0.348845 -1.848093 9 2.545062 0.924515 -0.130028 9 1.435752 -0.149389 1.398708 9 2.343233 -1.234436 -0.248524 16 -1.963491 -0.284174 0.456166 8 -0.410283 -0.954650 -0.706844 8 -3.088894 -0.282400 -0.451010	**Frequencies (cm^{-1}):** -887.2658, 41.0240, 81.3727, 118.9355, 184.5431, 234.3204, 260.7966, 266.7216, 358.3049, 388.3995, 428.5897, 449.4796, 503.2875, 521.6048, 590.2512, 700.7906, 797.3061, 818.5908, 886.7907, 979.8302, 1149.4563, 1190.2700, 1204.9755, 1265.7669, 1286.7673, 1378.7296, 2403.5005
IRC  	

Compound: sCI 23 + SO_2 $C_{acid}2$	**Energy (kJ mol^{-1}):** -1074.48289929713
Reaction Coordinates: 6 -2.331526 -0.166516 0.000018 6 -0.825440 0.234423 -0.000032 8 -0.574098 1.541614 -0.000171 1 -1.391387 2.060194 -0.000217 8 0.021437 -0.606313 0.000049 9 -3.128764 0.930676 -0.000075 9 -2.620147 -0.883912 -1.084761 9 -2.620128 -0.883715 1.084931 8 3.209723 0.291203 -1.242572 16 3.045037 -0.442475 0.000064 8 3.209681 0.291561 1.242495	**Frequencies (cm^{-1}):** 7.9403, 13.7672, 18.1848, 27.8477, 46.3445, 67.3022, 109.4827, 252.8838, 259.5677, 385.3358, 427.0890, 505.0127, 517.1221, 570.0799, 584.6192, 689.1895, 776.5047, 793.8786, 1121.8089, 1157.6692, 1181.6738, 1193.8914, 1238.5964, 1331.6294, 1373.0344, 1866.6247, 3747.6477

Compound: sCI 23 + SO_2 $TS_{acid}3$	**Energy (kJ mol^{-1}):** -1074.30934048683
Reaction Coordinates: 6 1.728380 -0.129799 0.105668 6 0.489885 0.281918 -0.767563 8 0.192326 1.481797 -0.897550 8 -1.440532 0.892288 0.995355 1 0.630922 -0.217479 -1.837251 9 2.700575 0.766552 -0.040366 9 1.387182 -0.198364 1.394931 9 2.192927 -1.331188 -0.272209 16 -1.958439 -0.308316 0.343069 8 -0.484910 -0.738650 -0.812091 8 -3.158338 -0.247332 -0.463424	**Frequencies (cm^{-1}):** -761.9918, 33.0059, 71.7498, 91.8382, 131.5788, 187.0189, 244.1248, 277.6319, 321.4680, 337.8402, 400.8382, 428.6618, 502.3980, 517.5784, 579.7048, 670.5444, 751.5279, 779.8846, 845.4066, 977.9521, 1103.1089, 1170.8089, 1210.1752, 1223.9501, 1306.7573, 1516.0627, 2325.4651
IRC  	

Compound: sCI 23 + SO_2 $C_{acid}3$	**Energy (kJ mol^{-1}):** -1074.49220772753
Reaction Coordinates: 6 -2.428819 -0.098941 0.012849 6 -0.878113 -0.026969 0.000391 8 -0.182944 -1.004912 0.003846 8 -0.475453 1.235062 -0.015518 1 0.504113 1.254826 -0.019547 9 -2.838189 -1.364577 0.029163 9 -2.919259 0.521800 1.097360 9 -2.934592 0.498452 -1.078159 8 4.423124 -0.352641 0.234115 16 3.030917 -0.280874 -0.155708 8 2.369168 1.009183 0.027076	**Frequencies (cm^{-1}):** 10.4595, 19.9218, 36.7816, 47.8233, 71.4015, 92.8783, 126.1916, 252.5346, 254.4247, 391.1867, 425.0695, 513.8513, 528.8470, 586.4652, 685.4860, 746.0666, 799.0625, 820.6465, 1146.8988, 1155.9481, 1162.3236, 1204.1614, 1278.1810, 1321.4712, 1436.3382, 1826.7385, 3524.3309

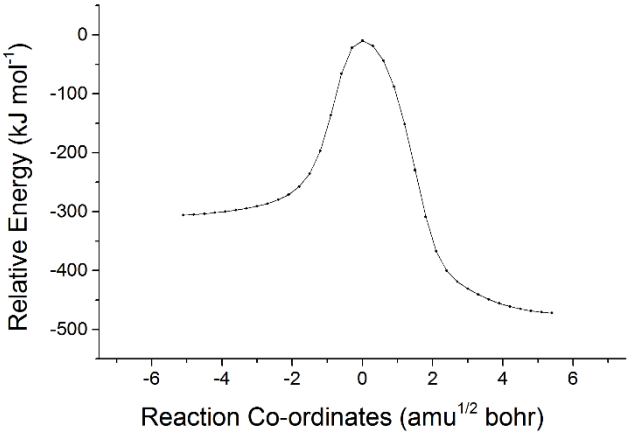
Compound: sCI 23 + SO_2 $TS_{acid}4$	**Energy (kJ mol^{-1}):** -1074.30138997618
Reaction Coordinates: 6 -1.497821 -0.271097 -0.082599 6 -0.562574 0.861364 0.490426 8 -0.446143 1.902397 -0.203525 8 1.828179 -1.522474 -0.221845 1 -1.022648 1.154923 1.518209 9 -2.676354 0.257539 -0.419533 9 -0.945041 -0.819783 -1.166104 9 -1.704821 -1.230321 0.826601 16 1.970706 -0.132616 0.164348 8 0.481865 0.391824 1.297929 8 1.859808 0.923056 -0.842985	**Frequencies (cm^{-1}):** -441.0022, 40.1146, 58.8253, 78.2172, 101.2594, 185.7786, 238.6275, 279.3428, 340.8934, 369.1801, 377.0582, 423.5238, 486.6397, 521.1562, 576.1011, 669.4742, 749.4600, 776.2415, 832.2168, 969.7756, 1090.0897, 1173.6587, 1199.9138, 1221.0713, 1289.3918, 1448.7891, 2476.7645
IRC  	

Compound: sCI 23 + SO_2 $TS_{ester}1$	**Energy (kJ mol^{-1}):** -1074.29521365977
Reaction Coordinates: 6 1.907634 -0.201494 0.010597 6 0.319341 0.835769 -0.322223 8 0.148875 1.494348 0.703135 8 -2.502454 -1.154144 0.790211 1 0.629705 1.306123 -1.270803 9 2.172713 -0.929108 -1.038725 9 1.743607 -0.892227 1.092480 9 2.793668 0.748959 0.157964 16 -2.141148 -0.275051 -0.307714 8 -0.302258 -0.389701 -0.530099 8 -2.359547 1.167052 -0.193433	**Frequencies (cm^{-1}):** -376.2534, 55.8878, 58.7232, 88.2166, 111.0868, 182.5976, 209.2988, 250.7035, 260.5697, 343.0394, 358.6689, 446.6899, 496.5903, 539.0026, 555.7381, 669.7221, 704.3805, 880.2197, 1005.9261, 1070.1386, 1094.6664, 1279.1533, 1284.1591, 1334.0598, 1347.3691, 1524.3376, 2933.3175
IRC  	

Compound: sCI 23 + SO_2 $C_{ester}1$	**Energy (kJ mol^{-1}):** -1074.48491076640
Reaction Coordinates: 6 2.489750 0.054945 0.021225 9 3.664742 -0.422508 0.415892 9 2.317397 1.265565 0.546732 9 2.488990 0.153804 -1.306848 8 1.530686 -0.840754 0.468921 6 0.204279 -0.610540 0.208814 8 -0.236492 0.320211 -0.389198 1 -0.374555 -1.429350 0.644969 8 -3.528716 1.114411 0.585437 16 -3.176166 0.069126 -0.356488 8 -2.916869 -1.258222 0.181918	**Frequencies (cm^{-1}):** 22.5722, 27.3868, 43.6691, 55.6613, 78.4418, 103.8095, 131.6737, 206.5524, 230.6056, 377.5828, 442.6376, 518.2029, 551.5669, 581.7440, 619.2136, 823.7137, 847.0023, 1047.8936, 1116.4729, 1154.9553, 1161.2201, 1215.7607, 1246.9872, 1327.6292, 1404.2327, 1818.7131, 3085.7404

Compound: sCI 23 + SO_2 $TS_{ester}2$	**Energy (kJ mol^{-1}):** -1074.28858393056
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.927643 -0.162049 0.052578 6 0.254333 0.308269 -0.576751 8 0.244085 1.551032 -0.533290 8 -2.324640 1.192076 0.341498 1 0.269447 -0.211321 -1.550195 9 2.037732 -1.464759 0.024301 9 2.091976 0.333440 1.240500 9 2.728281 0.388857 -0.827102 16 -2.169287 -0.261877 0.335354 8 -0.324575 -0.456447 0.437230 8 -2.641696 -1.010886 -0.821653	-370.1730, 16.1198, 59.0942, 67.3353, 109.0338, 167.2670, 226.5308, 246.5961, 279.0198, 325.4507, 365.6545, 468.5518, 508.7152, 543.8417, 559.1264, 664.1420, 698.8355, 866.9331, 984.6277, 1087.8560, 1112.9125, 1263.7941, 1268.3799, 1320.8891, 1351.4615, 1470.4502, 2929.3623

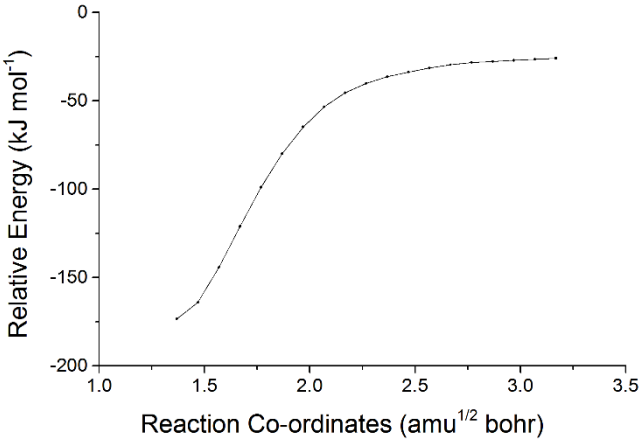
IRC



8.3.3 sCIs 25 & 26 + SO_2

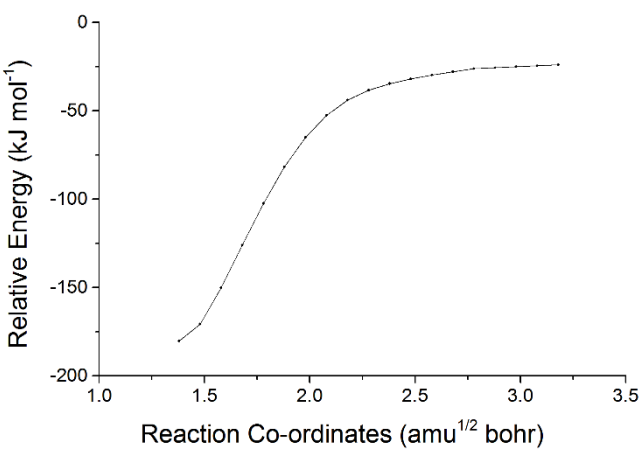
Compound: sCI 25 + SO_2 $TS_{Cyc}1$ reaction profile

IRC



Compound: sCI 25 + SO_2 SOZ1	**Energy (kJ mol^{-1}):** -1173.53663043677
Reaction Coordinates: 6 1.554889 -0.444082 0.043971 6 0.418853 0.592260 -0.202881 8 -0.143415 1.061194 1.019003 8 -1.305516 0.258857 1.272495 9 0.975223 1.683375 -0.767063 9 2.520008 0.104416 0.786549 9 1.071205 -1.509809 0.684478 9 2.079728 -0.839043 -1.119604 16 -2.122305 0.153740 -0.233675 8 -0.568098 0.060591 -0.987590 8 -2.695603 -1.168061 -0.249779	**Frequencies (cm^{-1}):** 45.0068, 58.5952, 129.6858, 213.5561, 224.3170, 262.4941, 314.9923, 344.4554, 355.5024, 424.7648, 458.8257, 504.6762, 546.0177, 566.3235, 595.6943, 678.9116, 700.9905, 741.4844, 823.3340, 959.3827, 1049.1246, 1089.6695, 1186.4706, 1198.4167, 1209.5305, 1289.7024, 1326.0809

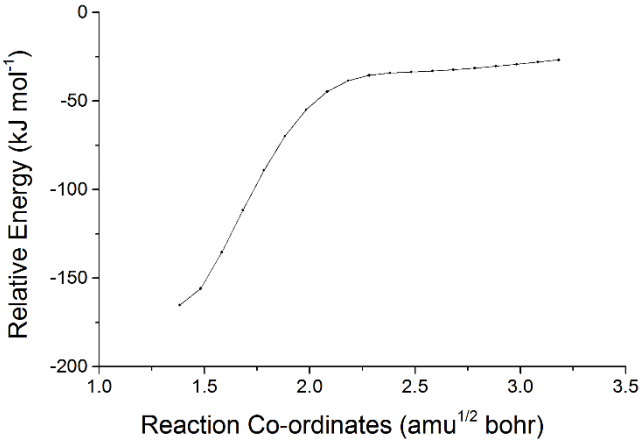
Compound: sCI 25 + SO_2 $TS_{Cyc}2$ reaction profile



Compound: sCI 25 + SO_2 SOZ2	**Energy (kJ mol^{-1}):** -1173.54107480780
Reaction Coordinates: 6 1.700331 -0.154031 -0.148664 6 0.290126 0.421615 0.178222 8 -0.275947 -0.212825 1.306963 8 -1.295685 -1.117905 0.824562 16 -2.064144 -0.354469 -0.480549 8 -0.540673 0.263838 -0.911824 8 -2.887610 0.744374 -0.032400 9 0.443800 1.719711 0.510316 9 2.513062 0.005565 0.897738 9 1.602657 -1.457920 -0.424287 9 2.227468 0.471104 -1.204541	**Frequencies (cm^{-1}):** 52.0720, 62.2597, 115.6779, 186.1203, 220.2380, 287.1115, 337.0379, 366.2857, 370.7109, 444.9691, 462.2021, 513.7914, 556.2475, 589.4587, 603.7358, 673.9915, 707.4480, 739.9283, 823.3987, 922.4626, 1057.9091, 1076.2351, 1166.6656, 1200.6382, 1206.7401, 1278.0201, 1326.4546

Compound: sCI 26 + SO_2 $TS_{Cyc}1$ reaction profile

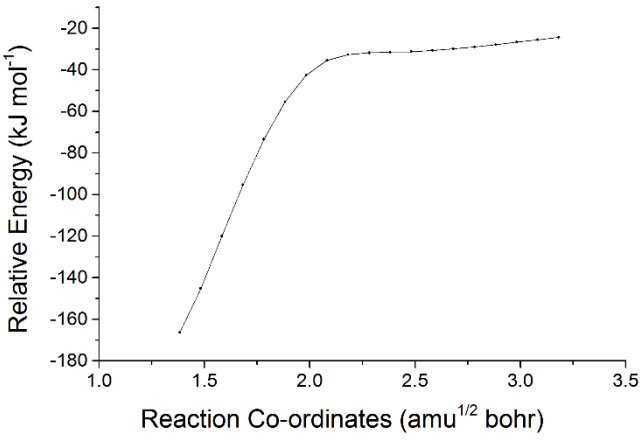
IRC



Compound: sCI 25 + SO_2 SOZ3	**Energy (kJ mol^{-1}):** -1173.53937137970
Reaction Coordinates: 6 1.624021 -0.369006 -0.066746 6 0.353772 0.513907 0.141124 8 -0.226344 0.719616 -1.101301 8 -1.613861 1.041606 -0.800585 9 0.743711 1.684853 0.707724 9 2.468636 0.238292 -0.904194 9 2.233981 -0.549345 1.105701 9 1.290437 -1.554870 -0.569920 16 -2.139784 -0.085078 0.360085 8 -0.552474 -0.117628 0.973985 8 -2.389958 -1.378411 -0.229779	**Frequencies (cm^{-1}):** 53.3878, 68.0440, 151.6147, 187.7091, 228.6704, 288.5831, 322.0043, 349.3383, 381.0432, 412.5424, 495.2303, 532.1745, 559.7927, 593.1859, 611.7228, 650.3890, 708.1821, 748.7677, 862.8946, 872.8553, 1070.9764, 1093.4081, 1121.3912, 1203.8397, 1217.8460, 1280.2051, 1321.1927

Compound: sCI 26 + SO_2 $TS_{Cyc}2$ reaction profile

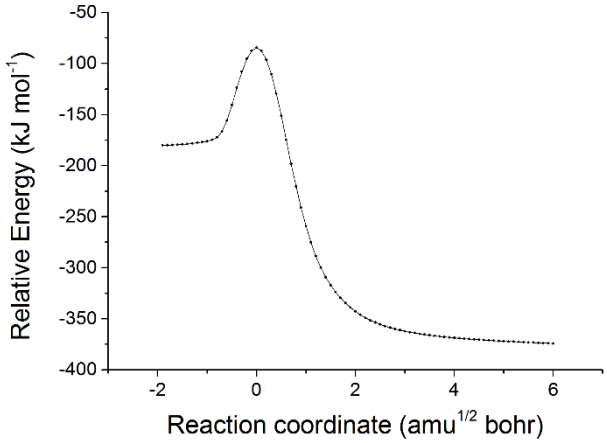
IRC



Compound: sCI 25 + SO_2 SOZ4	**Energy (kJ mol^{-1}):** -1173.54521761536
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.778298 -0.133786 0.148059 6 -0.307417 0.102434 -0.310864 8 0.091734 1.343827 0.168329 8 1.533488 1.319434 0.113336 9 -0.271368 0.056396 -1.665292 9 -2.562575 0.837897 -0.323002 9 -2.209507 -1.304759 -0.320778 9 -1.855159 -0.145465 1.479357 16 2.090638 -0.266878 0.539013 8 0.523530 -0.863798 0.224799 8 2.995195 -0.616770 -0.528957	46.1589, 65.1210, 128.8650, 147.8182, 225.6994, 278.1023, 308.3286, 360.6921, 370.7065, 423.8983, 479.7653, 525.5699, 543.1417, 567.8888, 613.8405, 640.0293, 691.9122, 750.1205, 872.2915, 924.5181, 1078.2136, 1091.8311, 1117.2803, 1207.6709, 1212.2055, 1282.2160, 1335.4386

Compound: sCI 25 + SO_2 $TS_{HOZ}1$	**Energy (kJ mol^{-1}):** -1173.53388111950
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.605497 0.411392 -0.090610 6 -0.406323 -0.535798 0.221133 8 0.108691 -1.057032 -0.980044 8 1.495851 -0.681514 -1.126061 9 -0.891300 -1.580363 0.940705 9 -2.141387 0.867559 1.044041 9 -1.185318 1.446912 -0.818228 9 -2.543014 -0.248470 -0.774978 16 2.149123 -0.051263 0.324664 8 0.557708 0.130605 0.922345 8 2.654514 1.257428 -0.003943	-159.4294, 20.7987, 61.5444, 186.1793, 208.8163, 252.6619, 309.6699, 337.1985, 356.3283, 412.3298, 461.4061, 513.1769, 554.4058, 572.6469, 597.5426, 650.9426, 700.4405, 744.3853, 849.4978, 939.8015, 1061.2802, 1087.6116, 1158.9090, 1201.5767, 1212.2239, 1288.0152, 1318.8162

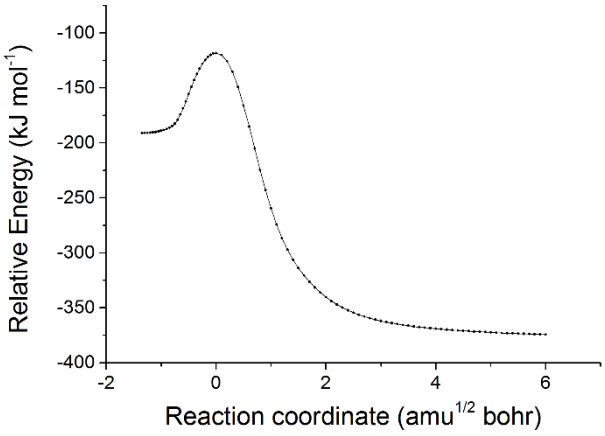
Compound: sCI 25 + SO_2 $TS_{HOZ}2$	**Energy (kJ mol^{-1}):** -1173.53931994965
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.762539 -0.012924 -0.172343 6 -0.279093 0.160238 0.279076 8 0.134175 -1.014808 0.898621 8 1.502083 -1.304033 0.481358 9 -0.233441 1.196656 1.158317 9 -2.208773 1.122235 -0.711780 9 -1.857571 -0.987962 -1.076651 9 -2.522903 -0.320903 0.880330 16 2.110800 -0.109799 -0.563686 8 0.517626 0.412641 -0.816737 8 2.831265 0.879033 0.202589	-73.1102, 60.9569, 89.3910, 152.7468, 210.2652, 280.6427, 305.0765, 360.0640, 369.2964, 423.3978, 478.9291, 527.1686, 549.7716, 587.5226, 604.3232, 669.3209, 698.7581, 748.6942, 858.8646, 895.0221, 1069.7381, 1085.3498, 1119.4200, 1206.0798, 1212.6063, 1280.9879, 1324.0728

Compound: sCI 25 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -1173.50370754569
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.668664 -0.237000 -0.168337 6 -0.413921 0.543417 0.338601 8 0.072233 0.141382 1.476579 8 3.097138 0.560455 -0.262500 9 -0.662681 1.866634 0.289683 9 -1.413638 -1.547102 -0.141910 9 -2.696874 0.019967 0.647230 9 -2.010279 0.093547 -1.420071 16 1.984108 -0.352264 -0.343062 8 0.640213 0.337422 -0.821845 8 1.415545 -1.051721 0.869394	-607.2684, 31.0897, 62.5197, 107.9680, 179.7528, 222.9153, 286.2726, 331.5185, 356.5920, 359.3231, 416.2636, 459.0275, 516.0829, 524.9626, 555.8419, 589.5866, 657.4417, 730.7599, 799.7264, 891.7564, 939.3861, 1099.1259, 1187.0108, 1199.5459, 1221.4319, 1289.6165, 1338.8248
IRC  	

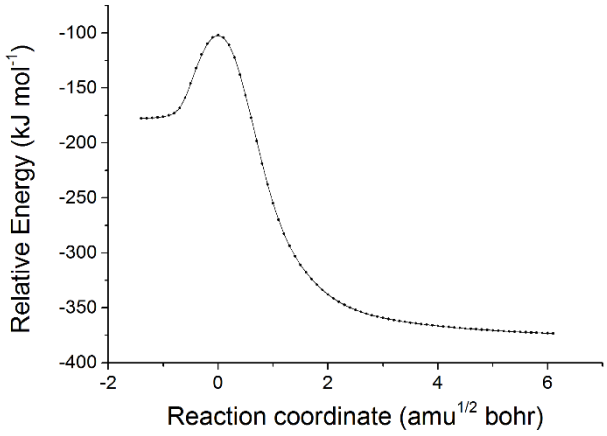
Compound: sC4 + SO_2 $C_{SO_3}1$	**Energy (kJ mol^{-1}):** -1173.62784782028
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.480382 -0.197438 -0.000000 6 0.990324 0.225637 0.000003 8 0.063167 -0.503181 0.000008 8 -2.590732 0.669827 -1.245757 9 0.890156 1.550175 0.000000 9 3.086529 0.290825 1.087804 9 2.581707 -1.519403 0.000001 9 3.086524 0.290823 -1.087808 16 -2.691450 -0.044144 -0.000001 8 -2.590737 0.669888 1.245720 8 -2.952357 -1.458369 0.000033	10.6507, 20.4972, 25.4670, 42.7300, 56.9356, 89.3577, 107.8055, 231.8421, 243.1069, 383.0292, 423.8821, 467.4804, 509.3791, 509.7174, 513.3808, 586.9497, 694.4524, 769.1260, 806.4467, 1047.9805, 1106.0690, 1173.2322, 1229.7700, 1312.0304, 1364.8420, 1369.6582, 1912.9001

Compound: sCI 25 + SO_2 $TS_{SO_3}2$	**Energy (kJ mol^{-1}):** -1173.51911565224
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.641991 -0.377135 0.066413 6 0.404346 0.615056 0.020625 8 -0.092071 0.826587 1.179483 8 -1.946170 1.079105 0.567999 9 0.765621 1.706244 -0.698967 9 2.081261 -0.628174 -1.164642 9 2.621593 0.200698 0.760119 9 1.298166 -1.516645 0.654253 16 -2.052978 -0.132169 -0.311558 8 -0.570151 -0.129146 -0.905302 8 -2.432874 -1.423038 0.221049	-454.1605, 58.6418, 74.9140, 139.1367, 193.4154, 225.2846, 294.4132, 309.7366, 334.7464, 376.4847, 434.5312, 460.9770, 527.9330, 545.8351, 554.8277, 580.4535, 666.8636, 739.8676, 800.0289, 902.6551, 974.8452, 1057.3650, 1180.4144, 1203.0018, 1225.8099, 1268.3720, 1310.7709

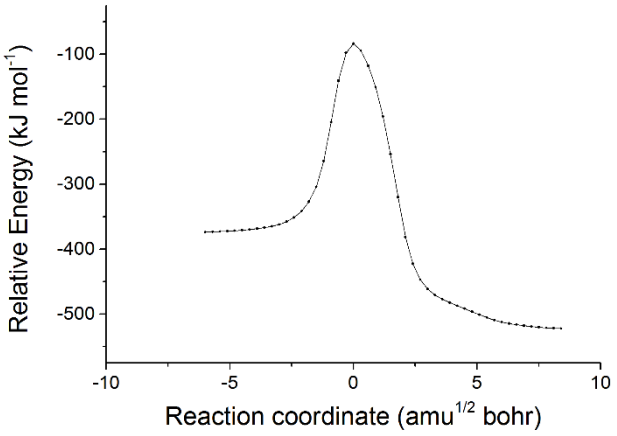
IRC



Compound: sCI 25 + SO_2 TS$SO_3$3	**Energy (kJ mol^{-1}):** -1173.51026243837
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.780248 -0.026481 -0.181348 6 -0.330964 0.078455 0.433961 8 0.018791 -0.951516 1.110358 8 1.770743 -1.335123 0.367013 9 -0.228904 1.275837 1.075993 9 -2.059986 1.043211 -0.922984 9 -1.873485 -1.118473 -0.933310 9 -2.663251 -0.100650 0.814656 16 2.057744 -0.116000 -0.470885 8 0.547504 0.247348 -0.835633 8 2.809712 0.994895 0.071922	-517.8014, 60.7850, 75.0296, 117.7628, 168.3618, 223.2707, 288.8933, 321.0568, 357.7665, 401.9041, 413.9117, 439.8401, 510.8812, 541.3957, 552.9248, 588.5194, 646.5623, 741.3055, 796.7976, 905.0981, 950.8611, 1049.9909, 1201.1346, 1203.7136, 1221.8266, 1267.7164, 1289.7390
IRC	

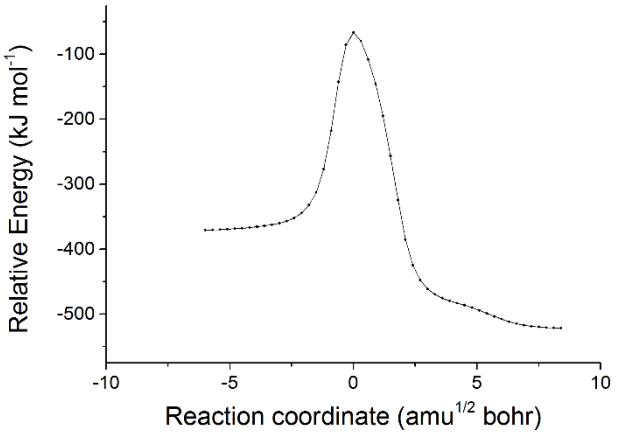


Compound: sCI 25 + SO_2 $TS_{ester}1$	**Energy (kJ mol^{-1}):** -1173.49144000029
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.813541 -0.425632 0.042717 6 0.274173 0.730620 0.067894 8 0.066864 0.917325 1.254961 8 -2.497059 -1.481374 0.252421 9 0.702671 1.753524 -0.724793 9 2.118193 -0.700091 -1.194231 9 1.518967 -1.476391 0.744034 9 2.726344 0.316466 0.605889 16 -2.171217 -0.197071 -0.337911 8 -0.408018 -0.192280 -0.697802 8 -2.334586 1.041535 0.423522	-432.3408, 52.1672, 65.8122, 74.4737, 101.0197, 173.4216, 204.0668, 237.4051, 246.1582, 261.4374, 324.8358, 399.0983, 480.5209, 522.8040, 543.1451, 550.5618, 617.6896, 642.3351, 750.8306, 865.2657, 965.8175, 1056.6910, 1092.7159, 1283.7314, 1295.9325, 1334.5393, 1561.5094
IRC	



Compound: sCI 25 + SO_2 $C_{ester}1$	**Energy (kJ mol^{-1}):** -1173.67282156150
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.246873 -0.570136 0.101837 8 1.940832 0.791280 0.167279 6 0.721378 1.198058 -0.243863 8 -0.171463 0.557311 -0.672656 9 0.693301 2.509378 -0.080159 9 1.426723 -1.287616 0.858143 9 2.198158 -1.015942 -1.147950 9 3.482804 -0.683183 0.560926 16 -3.222589 -0.092447 -0.196467 8 -3.110889 0.436899 1.151248 8 -3.215600 -1.534503 -0.361245	4.0162, 9.3991, 10.7021, 33.6407, 46.7280, 80.6640, 87.7644, 108.0431, 178.9699, 377.6690, 401.8068, 427.2020, 516.1418, 551.9297, 609.9868, 669.3564, 739.3163, 777.5055, 882.0199, 1027.4147, 1136.8106, 1158.2408, 1231.0917, 1248.0268, 1282.9061, 1335.0611, 1909.4847

Compound: sCI 25 + SO_2 $TS_{ester}2$	**Energy (kJ mol^{-1}):** -1173.48550327144
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.928820 -0.043969 -0.274499 9 -2.756202 0.164973 0.713137 9 -2.017816 0.864366 -1.198659 9 -2.036458 -1.257296 -0.737470 6 -0.230013 0.172164 0.564537 8 -0.217642 1.305626 1.000133 9 -0.229429 -0.888169 1.431347 8 0.377679 -0.215843 -0.633797 16 2.166005 -0.028066 -0.515698 8 2.322683 1.308562 0.047720 8 2.724287 -1.182719 0.165411	-484.6874, 18.2260, 52.9006, 73.6833, 96.9497, 157.9094, 184.7185, 237.6844, 242.4637, 268.2822, 319.2501, 401.4810, 492.4707, 513.6895, 538.3604, 550.0115, 599.3580, 656.1937, 759.4240, 827.2184, 963.3271, 1011.3589, 1097.8469, 1282.8564, 1293.6220, 1328.5142, 1574.4308
IRC	



Compound: sCI 25 + SO_2 $C_{ester}2$	**Energy (kJ mol^{-1}):** -1173.67290696018
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.575150 -0.328946 0.000001 9 2.302730 -1.047093 -1.083133 9 3.857326 -0.002343 -0.000075 9 2.302824 -1.046954 1.083252 8 1.874870 0.878202 -0.000047 6 0.524808 0.841279 0.000013 9 0.119153 2.097405 -0.000051 8 -0.191560 -0.096475 0.000103 8 -3.554650 0.056304 -1.243433 16 -3.276802 -0.639925 0.000012 8 -3.554811 0.056426 1.243351	5.3901, 13.1636, 13.2084, 35.5690, 48.4244, 83.3192, 87.0781, 108.4973, 181.3048, 378.5363, 402.3076, 427.2285, 516.3645, 552.1696, 609.9813, 670.0603, 739.8784, 777.3801, 881.6767, 1029.0054, 1139.0554, 1158.2309, 1228.1209, 1248.4840, 1284.6130, 1334.6173, 1907.1417

8.4 HFO-sCIs + HNO_3 reactions

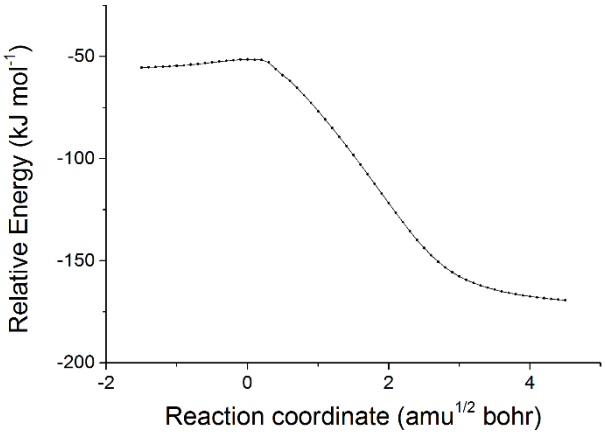
Compound: HNO_3	**Energy (kJ mol^{-1}):** -280.649387120256
Reaction Coordinates: 7 0.152578 0.031983 0.000001 8 -1.152277 -0.512972 -0.000001 1 -1.719886 0.275568 0.000002 8 0.214973 1.237996 -0.000000 8 1.018784 -0.787456 -0.000000	**Frequencies (cm^{-1}):** 479.4853, 584.8104, 646.7663, 783.1012, 896.0178, 1315.3030, 1341.5904, 1744.4127, 3711.8876

8.4.1 sCI 1 + HNO_3

Compound: sCI 1 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -470.072694506353
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.496892 -0.134866 -0.004943 8 0.667020 -1.033235 0.097948 8 2.688425 -0.260005 -0.068599 8 1.033607 1.141055 -0.058826 1 0.017702 1.095134 0.053631 6 -2.072567 -1.012782 0.120554 1 -2.498385 -1.822306 -0.459681 1 -1.658928 -1.120610 1.114625 8 -2.091056 0.101544 -0.429116 8 -1.535900 1.159208 0.283930	52.2249, 78.8218, 102.2949, 138.9453, 196.7530, 265.7980, 511.6154, 649.6811, 676.6982, 698.8865, 799.8732, 841.0081, 972.2831, 981.5672, 1060.8488, 1235.4845, 1308.1266, 1425.6956, 1481.8275, 1597.1874, 1708.0574, 2730.1492, 3121.7345, 3266.4971

Compound: sCI 1 + HNO_3 TS	**Energy (kJ mol^{-1}):** -470.068648204036
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.382578 -0.063861 -0.008349 8 0.628369 -1.058966 0.034369 8 2.580436 -0.135427 -0.065503 8 0.846896 1.149168 0.004906 1 -0.251112 1.114260 0.091169 6 -1.671765 -1.057011 0.209054 1 -1.838608 -2.006498 -0.286142 1 -1.395054 -0.967906 1.249688 8 -1.962928 -0.044666 -0.454559 8 -1.613108 1.171046 0.199461	-248.9265, 39.6720, 92.4916, 198.5650, 324.0410, 328.8518, 500.7085, 660.3195, 702.1595, 736.2226, 801.4920, 819.3851, 1019.9294, 1047.0691, 1133.6644, 1160.2011, 1235.8102, 1425.0247, 1489.9202, 1598.7784, 1614.2350, 1818.4260, 3129.3696, 3269.8948

IRC



Compound: sCI 1 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -470.123652687780
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.319520 0.088216 0.023524 8 0.339308 -0.963575 -0.181566 8 2.203213 0.022791 -0.773304 8 1.153464 0.838501 0.944072 1 -2.557702 1.413878 -0.088671 6 -0.881066 -0.827107 0.545024 1 -1.176279 -1.846124 0.792990	59.4191, 85.4098, 119.9476, 176.7737, 319.2844, 409.9451, 490.4761, 609.3846, 649.9965, 762.5552, 827.8298, 879.8808, 967.8881, 1053.3829, 1314.9395, 1324.3246, 1376.4783, 1413.3481,

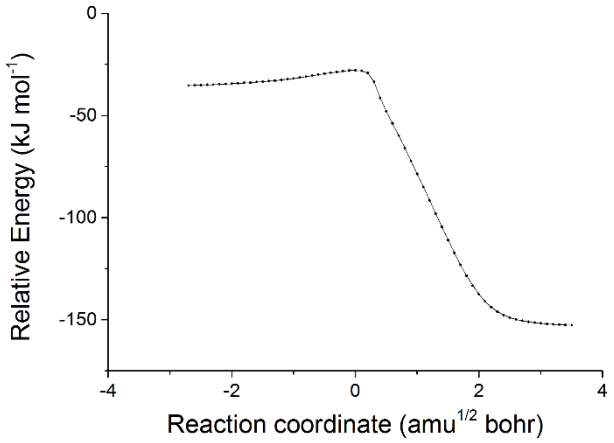
1 -0.722852 -0.212452 1.427306 8 -1.915046 -0.352282 -0.253432 8 -1.717616 1.078293 -0.431574	1450.9690, 1729.9552, 3075.3309, 3143.0899, 3755.3317

8.4.2 sCI 23 + HNO_3

Compound: sCI 23 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -806.869427684078
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.515030 -0.052204 -0.107496 6 1.389569 -0.745025 0.644316 1 1.560507 -1.689924 1.142933 8 0.227784 -0.294611 0.738235 8 -0.080258 0.887326 0.149683 9 2.227109 0.088467 -1.399867 9 3.605581 -0.830507 0.003357 9 2.793296 1.139411 0.420540 7 -3.324819 -0.165770 -0.101840 8 -2.563876 -1.114006 -0.129467 8 -4.520237 -0.167655 -0.204149 8 -2.760562 1.079774 0.072769 1 -1.771052 0.930738 0.116199	10.6140, 29.7830, 41.8008, 71.7241, 87.0513, 112.6532, 156.6378, 230.4114, 250.4582, 346.9186, 480.9087, 511.7626, 534.9130, 590.1757, 637.4624, 683.9769, 759.8603, 795.8386, 829.4514, 880.5639, 898.0185, 915.0071, 944.1144, 1161.7325, 1192.1409, 1241.8657, 1328.2504, 1371.8255, 1456.0238, 1578.6816, 1718.6016, 3124.6857, 3206.9984

Compound: sCI 23 + HNO_3 TS	**Energy (kJ mol^{-1}):** -806.865419736050
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.457042 -0.475653 -0.141690 6 0.852838 0.357702 1.001659 1 1.011599 -0.015041 2.007643 8 0.497497 1.549201 0.927013 8 0.160563 1.992571 -0.376021 9 2.631826 0.100273 -0.447165 9 0.735781 -0.596154 -1.240535 9 1.705108 -1.697626 0.349632 7 -2.096267 -0.333890 0.053274 8 -1.146941 -0.657051 0.801488 8 -3.113098 -0.960538 -0.038094 8 -1.997430 0.768090 -0.684379 1 -1.056180 1.263359 -0.537811	-203.8987, 49.4921, 52.7535, 87.1304, 156.0214, 182.5010, 225.3687, 278.4959, 313.8332, 331.5867, 435.8589, 494.9747, 533.3277, 566.1095, 672.6409, 713.0831, 749.8274, 795.0142, 821.6187, 871.5104, 928.1138, 1012.3118, 1072.1094, 1156.5460, 1157.5824, 1203.4557, 1278.5401, 1364.2600, 1517.8599, 1612.8964, 1678.5251, 1999.6916, 3181.7398

IRC

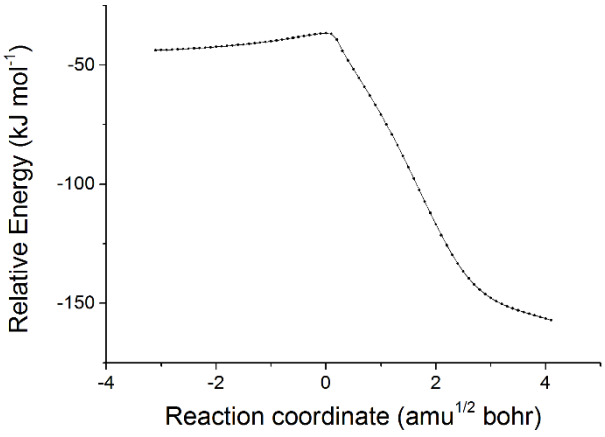


Compound: sCI 23 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -806.932710531538
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.234029 -0.565793 0.129147 6 -0.349089 0.145478 -0.926576 1 -0.712055 -0.170001 -1.906167 8 -0.403111 1.520637 -0.953015 8 -0.576378 2.097828 0.361211 1 0.337481 2.085119 0.692904 8 0.970650 -0.458847 -0.960221 7 1.946953 -0.186099 0.064084 8 2.831375 -0.979569 0.047569 8 1.800977 0.790017 0.754362 9 -2.448500 -0.017571 0.164558 9 -0.709971 -0.557213 1.359726 9 -1.368583 -1.853111 -0.240951	44.3668, 69.3809, 93.2717, 165.4610, 193.4546, 225.3272, 240.7962, 311.0701, 340.0379, 373.9625, 427.2332, 497.8110, 521.5399, 571.7072, 598.0567, 692.9346, 751.7581, 791.1962, 835.0732, 879.9702, 908.8883, 950.6032, 1108.0501, 1146.4447, 1199.1320, 1261.5324, 1325.5211, 1370.8742, 1383.7320, 1426.0054, 1726.0957, 3084.8214, 3675.8920

8.4.3 sCI 24 + HNO_3

Compound: sCI 24 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -806.873300576158
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.112628 -0.328139 0.028361 6 0.908402 0.441619 -0.483405 1 0.465875 0.214030 -1.445228 8 0.470057 1.364109 0.223449 8 -0.606103 2.078684 -0.261243 9 1.843444 -1.636496 -0.000813 9 2.452909 0.025482 1.261816 9 3.148127 -0.092228 -0.796140 7 -2.653927 -0.536448 -0.005582 8 -1.512598 -0.885133 -0.284588 8 -3.621877 -1.233995 0.095295 8 -2.859805 0.794106 0.223427 1 -1.972286 1.247236 0.060069	21.4603, 39.8574, 42.1601, 82.6932, 121.6740, 130.1110, 185.7289, 193.1965, 279.0018, 384.2481, 408.0808, 414.2012, 549.8226, 560.8570, 642.0486, 692.4597, 699.3590, 796.8093, 883.5112, 893.9237, 921.1985, 934.1911, 964.5752, 1152.1060, 1186.0423, 1272.6374, 1309.2140, 1361.4585, 1467.2626, 1597.6705, 1714.9508, 2962.3969, 3199.0004

Compound: sCI 24 + HNO_3 TS	**Energy (kJ mol^{-1}):** -806.868520205216
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.818613 -0.336853 0.015696 6 0.680377 0.567369 -0.455800 1 0.360756 0.545037 -1.488749 8 0.341153 1.489782 0.307661 8 -0.741762 2.259824 -0.211481 9 1.744065 -1.513427 -0.599055 9 1.807029 -0.513721 1.330099 9 2.975078 0.255896 -0.335374 7 -2.227662 -0.599860 -0.008985 8 -1.026866 -0.871200 -0.254858 8 -3.079524 -1.435682 0.103724 8 -2.586961 0.664416 0.137561 1 -1.744927 1.355041 -0.029616	-260.2949, 27.4937, 40.4603, 88.1780, 105.7760, 179.0839, 203.4849, 275.8988, 319.4801, 377.8967, 409.7391, 454.2256, 548.0832, 575.2912, 655.4133, 700.2323, 714.5006, 798.0752, 842.4628, 879.2374, 953.5183, 1023.6301, 1113.2491, 1146.1651, 1152.6934, 1201.8256, 1269.3687, 1355.5625, 1491.3837, 1604.5822, 1620.3004, 1807.0887, 3208.5505
IRC	



Compound: sCI 24 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -806.931663308635
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.554013 -0.423933 -0.077892 6 0.164526 0.246695 -0.151113 1 -0.026945 0.562928 -1.173348 8 0.130797 1.346934 0.710919 8 -0.158323 2.541173 -0.049835 1 -1.116845 2.619476 0.077256 8 -0.738620 -0.763913 0.274806 7 -2.123510 -0.506101 -0.059810 8 -2.841991 -1.374969 0.312222 8 -2.360662 0.517636 -0.645814 9 1.603211 -1.485321 -0.897005 9 1.854320 -0.826693 1.159300 9 2.481083 0.455219 -0.476695	49.4586, 57.3126, 79.0791, 84.2792, 143.7444, 200.6062, 254.1429, 293.8911, 327.8966, 346.1094, 396.5055, 460.3064, 534.3509, 564.3218, 632.4380, 686.2828, 735.0960, 768.6991, 831.3235, 896.1398, 956.4319, 1034.0722, 1083.2847, 1165.6245, 1186.5185, 1265.2167, 1315.8773, 1363.6233, 1367.2948, 1402.3144, 1735.4845, 3121.9660, 3715.7873

8.4.4 sCI 25 + HNO_3

Compound: sCI 25 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -906.045603878535
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.658334 0.372214 0.473504 6 1.097655 -0.333428 -0.787865 9 1.505255 0.115087 -1.928174 8 0.375536 -1.332887 -0.814800 8 -0.098135 -1.807086 0.428713 9 0.703171 0.787599 1.281294 9 2.381676 1.417913 0.071727 9 2.455978 -0.487057 1.107298 7 -2.601910 0.376304 -0.044351 8 -1.580861 0.753597 -0.602810 8 -3.656535 0.942884 0.004730 8 -2.555480 -0.829958 0.598602 1 -1.613484 -1.181122 0.491835	16.2163, 36.9939, 57.1225, 63.5689, 97.7905, 148.4175, 177.8060, 206.6922, 232.4838, 295.4329, 326.5404, 364.4840, 479.4276, 504.9650, 581.2690, 625.4322, 646.2131, 689.5643, 693.3045, 778.4011, 796.2974, 908.9884, 915.6068, 960.0898, 1154.7636, 1195.1805, 1236.8306, 1317.4677, 1410.4083, 1478.1360, 1633.9975, 1716.9084, 2949.9386

Compound: sCI 25 + HNO_3 TS	**Energy (kJ mol^{-1}):** -906.045088871693

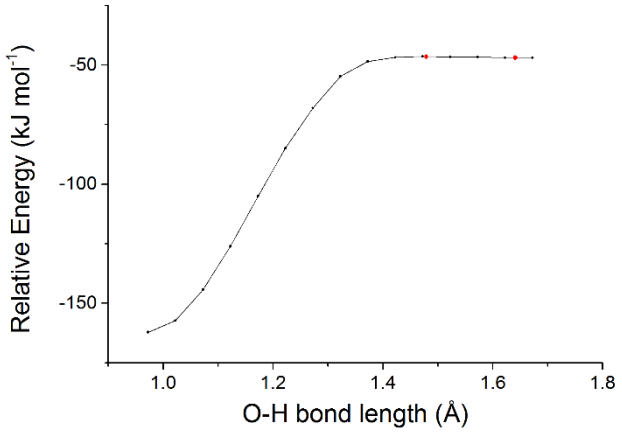
Reaction Coordinates:

```
6 1.398496 -0.436428 -0.468817
6 0.867915 0.352803 0.765201
9 1.204294 -0.149419 1.903834
8 0.443344 1.516117 0.791631
8 -0.032299 1.992907 -0.477231
9 1.702773 -1.669054 -0.072328
9 2.524212 0.191170 -0.837436
9 0.572753 -0.496022 -1.489867
7 -2.249696 -0.361885 0.046000
8 -1.207449 -0.703022 0.633327
8 -3.263342 -0.998166 0.032105
8 -2.260915 0.801357 -0.617246
1 -1.321586 1.271330 -0.538819
```

Frequencies (cm^{-1}):

```
-59.3438, 41.5877, 45.9090,
81.3198, 146.6454, 182.1514,
202.5032, 222.6189, 271.4277,
289.0449, 340.0328, 368.7527,
476.7036, 511.9915, 584.5135,
618.8684, 662.2343, 671.8021,
717.1168, 778.5606, 796.8572,
913.2326, 1001.6289, 1052.8716,
1137.9920, 1188.2205, 1246.8738,
1258.8145, 1399.1859, 1525.1097,
1626.9631, 1707.7546, 2259.7416
```

IRC



Compound: sCI 25 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -906.106548786604

Reaction Coordinates:

```
6 1.227307 -0.388855 -0.480905
6 0.286623 -0.045093 0.725794
9 0.807811 -0.639351 1.815327
8 0.136881 1.282818 1.051278
8 0.468229 2.163071 -0.038453
1 -0.399261 2.247293 -0.469648
8 -0.957084 -0.760446 0.587626
7 -2.061352 -0.183353 -0.162301
8 -3.001400 -0.904766 -0.146699
8 -1.908607 0.888922 -0.681185
9 2.401415 0.221046 -0.353700
9 0.674689 -0.061869 -1.653575
9 1.431750 -1.710595 -0.479619
```

Frequencies (cm^{-1}):

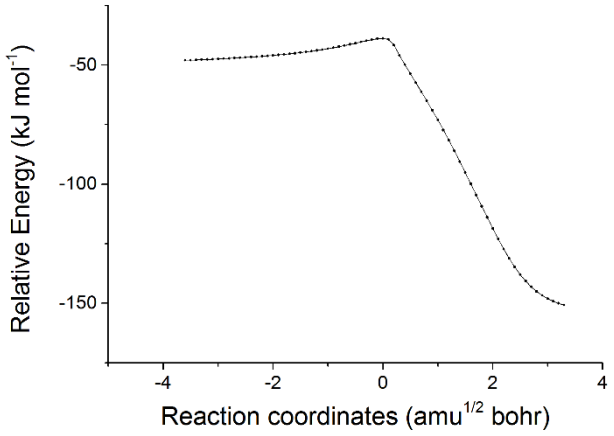
```
44.8465, 68.6884, 90.0800,
170.5517, 192.8878, 215.5921,
220.9380, 292.2829, 303.6735,
329.7248, 378.8194, 385.4820,
439.3492, 486.2138, 534.3046,
589.1877, 605.8283, 733.3051,
735.8503, 759.7463, 794.2091,
817.1514, 973.8141, 1002.2183,
1112.1058, 1174.8338, 1190.1717,
1216.3470, 1324.8542, 1344.1334,
1428.7677, 1744.5606, 3684.7511
```

8.4.5 sCI 26 + HNO_3

Compound: sCI 26 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -906.050679111630
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.024036 -0.408554 -0.156972 6 -0.898435 0.547176 0.259645 9 -0.631948 0.608199 1.510031 8 -0.341672 1.256494 -0.586459 8 0.674143 2.112512 -0.136549 9 -1.770253 -1.623626 0.317061 9 -2.134048 -0.448742 -1.475439 9 -3.171585 0.032730 0.373663 7 2.638426 -0.592217 -0.022548 8 1.462692 -0.892302 0.143819 8 3.584626 -1.326169 -0.000491 8 2.919907 0.722010 -0.265209 1 2.038779 1.216373 -0.226934	-342.4923, 28.9714, 49.3276, 82.5971, 111.5724, 174.9899, 207.6669, 232.6207, 279.7650, 309.1249, 355.8683, 366.6454, 409.2298, 501.2836, 577.5929, 604.5163, 676.6835, 720.4099, 732.5958, 797.3823, 829.3727, 869.4917, 1027.6151, 1063.0087, 1141.1869, 1163.0930, 1198.8878, 1257.3653, 1389.4405, 1472.1235, 1595.3393, 1632.8779, 1786.9313

Compound: sCI 26 + HNO_3 TS	**Energy (kJ mol^{-1}):** -906.046705839706
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.742183 -0.435894 -0.157683 6 -0.650973 0.584244 0.238844 9 -0.525944 0.808845 1.494184 8 -0.237295 1.366965 -0.637231 8 0.816568 2.232361 -0.169389 9 -1.731318 -1.463165 0.675897 9 -1.565256 -0.847937 -1.401863 9 -2.924779 0.191290 -0.062463 7 2.212431 -0.656382 0.002688 8 1.005196 -0.854236 0.295766 8 3.032763 -1.530154 0.004117 8 2.608305 0.559055 -0.321911 1 1.793287 1.311347 -0.228389	-342.4923, 28.9714, 49.3276, 82.5971, 111.5724, 174.9899, 207.6669, 232.6207, 279.7650, 309.1249, 355.8683, 366.6454, 409.2298, 501.2836, 577.5929, 604.5163, 676.6835, 720.4099, 732.5958, 797.3823, 829.3727, 869.4917, 1027.6151, 1063.0087, 1141.1869, 1163.0930, 1198.8878, 1257.3653, 1389.4405, 1472.1235, 1595.3393, 1632.8779, 1786.9313

IRC



Compound: sCI 26 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -906.107641820181
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.465714 -0.616502 -0.018853 6 -0.115197 0.174139 0.129909 9 -0.052168 0.626231 1.411907 8 0.029375 1.215056 -0.779855 8 -0.915161 2.264455 -0.484275 1 -0.365195 2.867713 0.039005 8 0.871098 -0.747902 -0.156537 7 2.324097 -0.279474 -0.042045 8 3.035235 -1.130435 -0.445880 8 2.511379 0.791426 0.427935 9 -1.437120 -1.713019 0.746717 9 -1.643942 -0.981473 -1.289204 9 -2.497153 0.135148 0.363674	35.8609, 48.3223, 97.7733, 106.6229, 136.6438, 216.4055, 218.5739, 253.9864, 277.4184, 303.7563, 362.2100, 388.0438, 420.9834, 486.3317, 532.0771, 574.0953, 591.9207, 684.5924, 740.6256, 752.6333, 787.4242, 825.9496, 976.3362, 1070.5744, 1118.2801, 1131.5996, 1199.1168, 1211.7936, 1299.2723, 1364.2598, 1411.7186, 1805.9040, 3725.8754

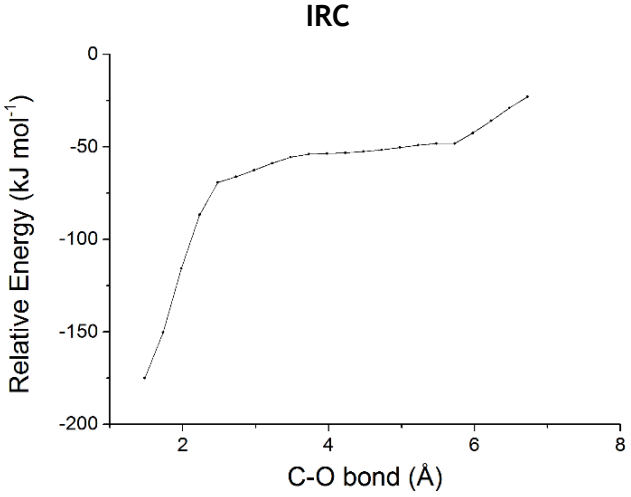
8.5 HFO-sCIs reactions with Trifluoroacetic Acid (TFA)

Compound: TFA (CF_3COOH) conformer 1	**Energy (kJ mol^{-1}):** -526.396690747069
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.600232 -0.000700 0.000001 6 -0.943150 0.162408 0.000002 8 -1.495890 1.220466 0.000000 8 -1.526983 -1.040018 0.000002 1 -2.487822 -0.910329 -0.000003 9 0.999822 -0.678016 -1.087812 9 1.192393 1.189052 0.000043 9 0.999820 -0.678091 1.087766	30.3904, 237.0884, 242.9524, 384.3951, ,420.8035, 503.5971, 582.5530, 595.2069, 666.0224, 787.6331, 791.1373, 1135.0381, 1156.4050, 1192.2434, 1246.2417, 1400.8344, 1853.8568, 3732.4833

8.5.1 sCI 1 + TFA

Compound: sCI 1 + TFA PRC	**Energy (kJ mol^{-1}):** -715.814752163838
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.117654 -0.201348 -0.000023 6 -0.740521 0.519046 0.000004 8 -0.649473 1.715143 -0.000182 8 0.232966 -0.368608 0.000253 1 1.134260 0.077798 0.000265 9 -2.248565 -0.983360 1.087847 9 -3.118080 0.678690 -0.000299 9 -2.248314 -0.983755 -1.087640 6 4.708687 -0.314834 -0.000181 1 5.296134 -1.223034 -0.000511 1 5.113259 0.690859 0.000074 8 3.472618 -0.479587 -0.000102 8 2.679877 0.637179 0.000306	15.3101, 29.2792, 36.3834, 50.1211, 77.4504, 101.5880, 169.1057, 257.8198, 279.2418, 395.5788, 433.3071, 515.8541, 550.4847, 591.1333, 681.1988, 706.1226, 780.6440, 807.7600, 880.7623, 972.0749, 1018.4284, 1141.8677, 1169.1472, 1202.8182, 1242.1331, 1335.0572, 1418.3576, 1486.5195, 1576.3894, 1824.8056, 3021.8298, 3114.8857, 3264.5288

Compound:	sCI 1 + TFA TS reaction profile



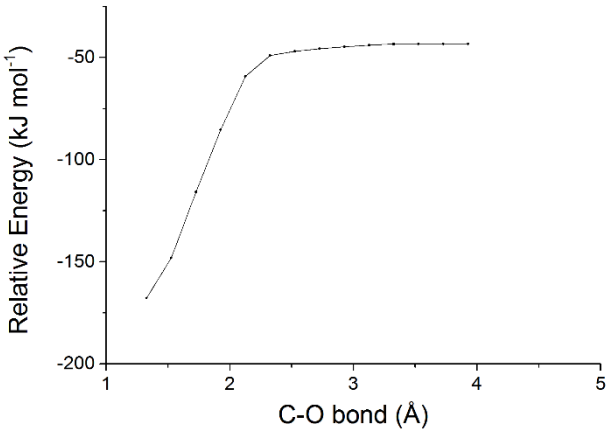
Compound: sCI 1 + TFA Pr	**Energy (kJ mol^{-1}):** -715.871685168671
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.697881 0.022687 0.042552 6 0.163468 0.215542 -0.116231 8 -0.437279 -0.958119 -0.095178 8 -0.330901 1.305557 -0.235475 1 -2.196182 1.415419 -0.011856 9 2.182883 -0.686901 -0.989582 9 2.314212 1.200094 0.072752 9 1.976930 -0.636459 1.175780 6 -1.892893 -1.058709 -0.328960 1 -2.076150 -2.112990 -0.142555 1 -2.090489 -0.767998 -1.358185 8 -2.652048 -0.337966 0.557765 8 -3.044039 0.927759 -0.027376	26.1591, 61.2351, 109.7878, 146.1666, 202.8784, 235.0052, 284.5678, 340.3942, 425.7682, 460.6063, 515.6973, 550.8166, 556.4842, 587.4142, 741.1113, 785.3393, 817.4884, 856.4786, 912.6225, 1084.6461, 1146.4313, 1157.7037, 1164.2388, 1217.5341, 1304.1561, 1338.5859, 1429.5640, 1470.8223, 1479.9155, 1804.5397, 3083.1395, 3158.9283, 3560.1146

8.5.2 sCI 23 + TFA

Compound: sCI 23 + TFA PRC	**Energy (kJ mol^{-1}):** -1052.601700422370
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.799697 -0.091409 -0.000002 6 -2.347221 0.459861 -0.000005 8 -2.108307 1.633985 -0.000084 8 -1.484502 -0.540871 0.000090 1 -0.547214 -0.201783 0.000087 9 -4.020862 -0.851857 1.087808 9 -4.685788 0.902500 -0.000097 9 -4.020806 -0.852015 -1.087714 6 2.986750 -1.120937 -0.000139 1 3.407058 -2.117903 -0.000289 6 3.892144 0.100749 0.000001 9 5.160273 -0.346119 -0.000099 9 3.707438 0.844929 1.088662 9 3.707372 0.845228 -1.088443 8 1.736864 -1.066737 -0.000094 8 1.120900 0.141888 0.000090	7.4879, 14.3532, 20.6102, 31.1970, 55.4650, 76.5639, 94.0482, 96.9370, 212.7209, 246.4799, 256.8046, 272.6323, 344.7727, 397.8334, 434.7728, 480.6449, 513.6752, 515.4363, 534.8743, 588.9227, 589.4324, 700.5560, 761.7026, 777.5234, 804.9535, 826.1389, 882.6705, 910.8651, 921.5577, 1144.3144, 1159.2873, 1167.2045, 1194.3575, 1203.5754, 1241.3283, 1319.8137, 1369.8098, 1464.7495, 1574.1753, 1831.1291, 3185.8483, 3207.3049

Compound: sCI 23 + TFA TS reaction profile

IRC



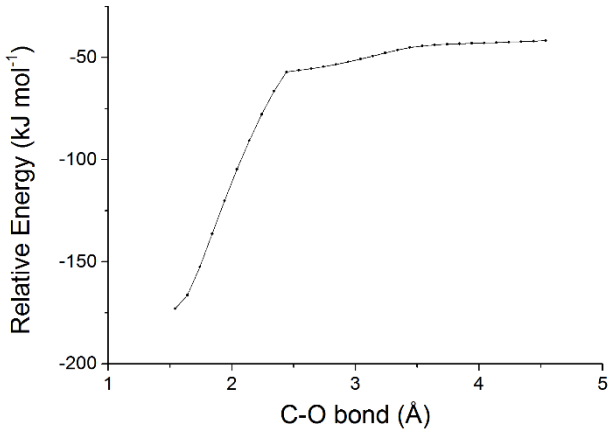
Compound: sCI 23 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.676223405220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.466755 -0.218822 -0.010253 6 1.077154 0.480250 -0.048466 8 0.223035 -0.229661 0.676838 8 0.898034 1.503630 -0.647334 1 -0.795315 2.179440 -0.631200 9 2.920504 -0.276317 1.250781 9 2.376110 -1.467759 -0.486261 9 3.341071 0.457006 -0.747324 6 -1.184517 0.121186 0.891958 1 -1.378609 -0.275710 1.886916 6 -2.012724 -0.706613 -0.124124 9 -1.906052 -2.007793 0.205177 9 -1.584011 -0.572463 -1.382367 9 -3.299166 -0.365633 -0.056782 8 -1.472670 1.453093 0.975477 8 -1.716172 2.040048 -0.324908	20.9216, 46.4107, 59.5233, 66.9627, 140.9286, 180.6824, 208.0201, 222.3190, 241.0757, 274.9078, 308.1438, 334.1048, 362.8241, 433.7150, 463.3602, 517.3656, 523.8811, 555.0554, 587.9584, 609.8561, 615.5457, 729.8126, 772.5619, 776.2809, 802.3635, 872.2091, 915.3374, 953.1669, 1107.5102, 1140.5180, 1162.3852, 1165.8355, 1202.4495, 1221.0011, 1267.8230, 1322.9942, 1382.6886, 1408.0581, 1477.9667, 1816.0211, 3111.6009, 3521.6190

8.5.3 sCI 24 + TFA

Compound: sCI 24 + TFA PRC	**Energy (kJ mol^{-1}):** -1052.615934886960
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.826946 -0.368024 -0.000004 6 -2.584060 0.564096 -0.000003 8 -2.680549 1.758804 -0.000038 8 -1.477753 -0.157249 0.000039 1 -0.672574 0.431164 0.000037 9 -3.828923 -1.159749 1.087783 9 -4.953816 0.341783 -0.000036 9 -3.828888 -1.159792 -1.087759 6 2.969286 0.773171 0.000006 1 3.182798 1.836550 0.000002 6 4.078973 -0.256742 -0.000008 9 4.845283 -0.070606 1.085930 9 4.845246 -0.070616 -1.085974 9 3.615989 -1.499861 0.000006 8 1.792081 0.363588 0.000023 8 0.792750 1.288215 0.000034	8.0185, 13.9625, 17.7010, 31.4483, 52.0818, 71.8914, 86.6937, 120.1090, 190.2986, 210.7532, 256.8293, 275.0837, 386.6084, 394.2236, 396.0285, 421.2855, 451.0603, 515.4830, 554.8464, 559.4263, 589.1000, 698.3424, 705.4141, 777.8235, 805.1851, 889.5173, 920.3806, 930.2730, 947.7599, 1144.8606, 1151.5780, 1165.9538, 1177.1230, 1203.4499, 1274.2055, 1321.6529, 1361.6588, 1469.0207, 1581.1019, 1829.5164, 3173.9935, 3180.2493

Compound: sCI 24 + TFA TS reaction profile

IRC



Compound: sCl 24 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.680470535266

Reaction Coordinates:

```
6 2.483742 -0.372757 0.043442
6 1.223571 0.514359 -0.157311
8 0.130443 -0.232202 -0.054291
8 1.287584 1.692255 -0.374094
1 -0.321270 2.775251 -0.088311
9 3.581760 0.373543 -0.007121
9 2.436718 -0.993124 1.228581
9 2.548991 -1.301029 -0.922371
6 -1.164747 0.389585 -0.277037
1 -1.228744 0.736793 -1.306612
6 -2.179111 -0.747309 -0.045264
9 -2.159505 -1.183022 1.216602
9 -1.911159 -1.779682 -0.857902
9 -3.407912 -0.300273 -0.326609
8 -1.428419 1.408876 0.610965
8 -1.293451 2.685692 -0.053664
```

Frequencies (cm^{-1}):

```
17.8491, 45.2659, 57.3567, 85.9303,
91.0158, 151.4031, 198.4283,
211.4683, 224.0042, 267.5022,
321.0179, 347.0376, 363.7984,
417.9770, 437.2892, 506.6700,
519.4156, 526.9220, 556.0132,
568.8105, 623.4046, 705.7929,
743.5205, 783.8159, 844.5009,
924.0822, 935.2929, 966.8157,
1099.5354, 1155.7595, 1167.5156,
1170.7616, 1193.8652, 1221.3136,
1272.0266, 1319.1611, 1369.9295,
1392.6546, 1461.7710, 1815.8484, ,
3107.3684, 3594.7285
```

8.5.4 sCl 25 + TFA

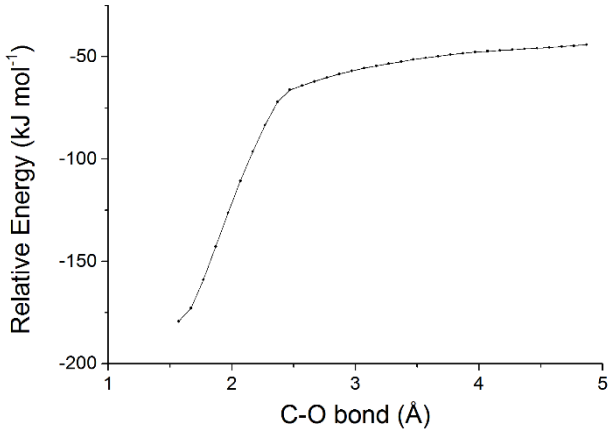
Compound: sCl 25 + TFA PRC	**Energy (kJ mol^{-1}):** -1151.785667585767

Reaction Coordinates:

```
6 -4.026188 0.115087 -0.000003
6 -2.590419 -0.478626 0.000010
8 -2.387789 -1.660124 0.000042
8 -1.698604 0.494542 -0.000019
1 -0.769777 0.125201 -0.000013
9 -4.225296 0.881788 -1.087785
9 -4.941674 -0.852194 0.000027
9 -4.225289 0.881850 1.087737
6 2.783742 0.841986 0.000010
9 3.411589 1.974591 0.000026
6 3.639321 -0.443219 -0.000005
9 4.924581 -0.087026 0.000003
9 3.385389 -1.156257 -1.088876
9 3.385383 -1.156287 1.088843
8 1.548119 0.894821 0.000007
8 0.850635 -0.318584 -0.000011
```

Frequencies (cm^{-1}):

```
7.5674, 12.4297, 19.3225, 31.2593,
50.4704, 72.6003, 74.4628, 94.2524,
216.1131, 223.6194, 256.7145,
267.3417, 268.5318, 320.3421,
365.0210, 398.2187, 434.9504,
492.4184, 502.1436, 515.5134,
583.1883, 588.9652, 634.5484,
681.7848, 703.3383, 778.2821,
779.5247, 806.1318, 916.0536,
931.0692, 1144.0082, 1159.5167,
1167.1897, 1203.5568, 1210.5858,
1215.0487, 1326.4277, 1409.5507,
1475.7611, 1612.9563, 1828.5912,
3134.7645
```

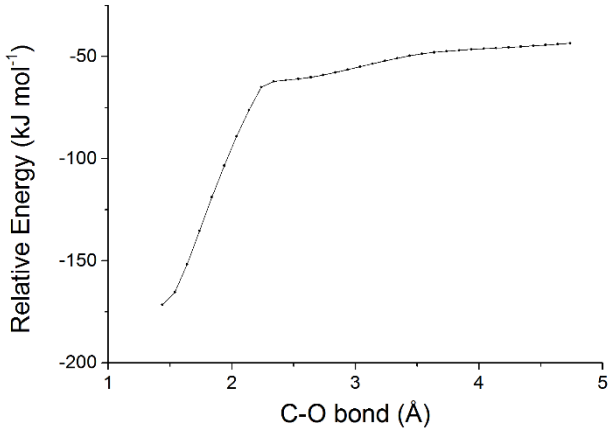
Compound: sCI 25 + TFA TS reaction profile
IRC 

Compound: sCI 25 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.676223405220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.570852 -0.220706 -0.048599 6 1.190871 0.497624 -0.075921 8 0.283900 -0.301589 0.489465 8 1.044352 1.588401 -0.545206 1 -0.664295 2.301576 -0.536636 9 3.492197 0.545148 -0.621273 9 2.937107 -0.467545 1.215532 9 2.502004 -1.383092 -0.709593 6 -1.101065 0.050357 0.709143 9 -1.402883 -0.578986 1.851964 6 -1.936484 -0.600185 -0.449206 9 -1.876419 -1.929874 -0.319117 9 -1.443070 -0.281041 -1.649312 9 -3.207065 -0.219797 -0.371946 8 -1.331892 1.376630 0.958426 8 -1.583557 2.108129 -0.257954	20.2362, 43.7482, 55.1268, 71.0110, 130.8120, 182.2072, 200.8834, 216.0355, 230.5157, 259.6638, 289.3327, 312.5332, 347.1908, 356.0338, 399.2152, 434.5129, 490.6210, 515.8851, 523.0897, 560.4187, 596.1424, 614.6958, 622.2812, 679.8581, 747.6963, 769.5610, 778.4174, 874.1228, 952.1876, 996.2569, 1112.7478, 1154.2816, 1169.0466, 1189.6280, 1209.4820, 1220.9972, 1226.1166, 1321.2883, 1351.3150, 1478.4904, 1827.5146, 3538.5897

8.5.5 sCI 26 + TFA

Compound: sCI 26 + TFA PRC	**Energy (kJ mol^{-1}):** -1151.790445383220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 4.041057 -0.371401 -0.006528 6 2.784865 0.542457 -0.033261 8 2.860138 1.727432 -0.196890 8 1.695334 -0.181267 0.147064 1 0.879129 0.394538 0.130234 9 3.966641 -1.314052 -0.963965 9 5.150320 0.337787 -0.206780 9 4.150014 -0.995914 1.180402 6 -2.746033 0.517700 0.030689 9 -3.121296 1.746140 0.046299 6 -3.846116 -0.543715 -0.034636 9 -4.564366 -0.357332 -1.144769 9 -4.648539 -0.404246 1.023560 9 -3.319784 -1.757664 -0.040486 8 -1.552125 0.186312 0.064841	10.8869, 16.0276, 18.2924, 33.1220, 39.6677, 68.5474, 72.3076, 109.6280, 158.5230, 203.3723, 257.2177, 263.1301, 323.1912, 339.7670, 376.5955, 402.9848, 407.9736, 441.1388, 515.5822, 519.6200, 576.9508, 589.1252, 690.4387, 700.7299, 732.6585, 778.2141, 805.1062, 866.9637, 878.4136, 931.1100, 1143.9517, 1159.9433, 1166.6482, 1175.0592, 1203.4005, 1242.0594, 1324.6173, 1404.8743, 1470.9930, 1632.4361, 1829.4762, 3145.9245

8 -0.603184 1.197866 0.120465	

Compound: sCI 26 + TFA TS reaction profile
IRC 

Compound: sCI 26 + TFA Pr	**Energy (kJ mol-1):** -1151.857358431300
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.478273 -0.365041 0.052667 6 -1.231413 0.534401 -0.189079 8 -0.195732 0.002265 0.469856 8 -1.274726 1.527937 -0.851783 1 0.139962 2.699595 -0.432420 9 -3.536735 0.153442 -0.559265 9 -2.258822 -1.595347 -0.428923 9 -2.738447 -0.458172 1.362722 6 1.185449 0.380691 0.339739 9 1.599361 0.605801 1.597192 6 1.928243 -0.878655 -0.221274 9 1.470194 -1.176197 -1.441770 9 1.716059 -1.919260 0.583947 9 3.236846 -0.646728 -0.291123 8 1.475822 1.397572 -0.509050 8 0.999621 2.647248 0.032861	16.5182, 35.7526, 42.6654, 58.4852, 128.4627, 176.2977, 193.2411, 204.6366, 231.9707, 261.3122, 277.9253, 325.7491, 342.7255, 366.9216, 381.0447, 427.6308, 485.9296, 514.6093, 529.4620, 555.3729, 562.0244, 587.2120, 642.9921, 722.2777, 750.2701, 769.7615, 816.3052, 860.7169, 949.7770, 1006.6998, 1096.7814, 1147.6885, 1168.4412, 1201.0525, 1210.1647, 1225.0795, 1225.6274, 1317.1342, 1334.0822, 1463.8412, 1831.1421, 3559.6296

8.6 HFO-sCI Reactions with HF

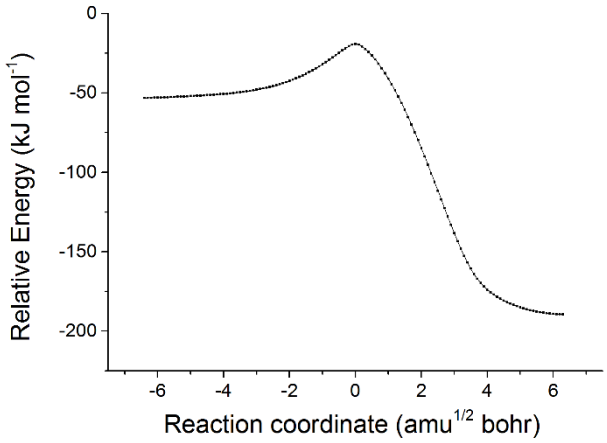
Compound: HF	**Energy (kJ mol^{-1}):** -100.388736810254
Reaction Coordinates:	**Frequencies (cm^{-1}):**
9 0.000000 0.000000 0.092410 1 0.000000 0.000000 -0.831689	4072.1142

8.6.1 sCI 1 + HF

Compound: sCI 1 + HF PRC	**Energy (kJ mol^{-1}):** -289.808532547218
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.968789 -0.977363 -0.000007 1 1.860439 -1.590782 0.000013 1 -0.050820 -1.352498 -0.000039 8 1.192344 0.252290 0.000012 8 0.149073 1.146514 -0.000009 1 -1.194974 0.358284 -0.000001 9 -1.906524 -0.304584 0.000005	79.1803, 152.0807, 307.7401, 557.6608, 691.8667, 864.2225, 887.5397, 1046.3924, 1095.0887, 1278.6763, 1433.0717, 1562.9479, 3045.8930, 3102.0931, 3246.6880

Compound: sCI 1 + HF TS	**Energy (kJ mol^{-1}):** -289.791769474177
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.304787 1.051637 0.223711 1 -0.360805 2.020957 -0.260655 1 0.124674 0.914501 1.204044 8 -0.967644 0.141252 -0.333197 8 -0.540291 -1.132555 0.180239 1 0.624123 -0.809496 0.047753 9 1.500468 -0.056152 -0.123305	-829.2644, 336.8971, 483.6272, 530.5988, 696.5045, 765.8268, 835.9935, 1117.4420, 1197.3750, 1234.8638, 1420.0552, 1580.7735, 1822.9523, 3125.6008, 3268.4885

IRC



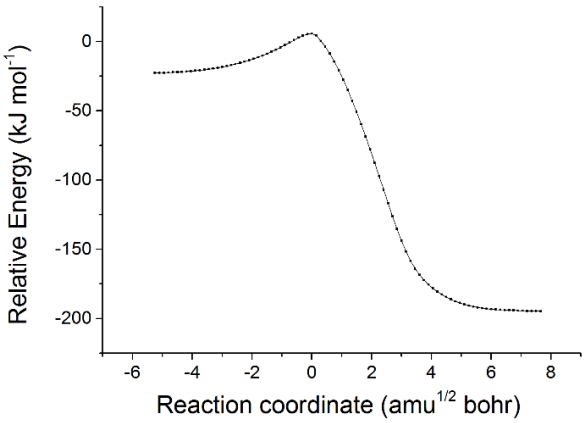
Compound: sCI 1 + HF Pr	**Energy (kJ mol^{-1}):** -289.865197002865
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.631649 0.519902 0.269119 1 1.175202 1.409728 -0.049661 1 0.499281 0.459144 1.348441 8 -0.574863 0.581176 -0.391641 8 -1.469572 -0.389753 0.211664	168.4645, 277.9778, 421.6778, 595.9358, 882.7828, 995.6691, 1077.0262, 1160.2288, 1287.4215, 1383.4539, 1415.0926, 1480.2425, 3056.8428, 3125.4267, 3737.5366

1 -1.362095 -1.142101 -0.388781 9 1.361467 -0.597507 -0.120544	

8.6.2 sCI 23 + HF

Compound: sCI 23 + HF PRC	**Energy (kJ mol^{-1}):** -626.606991675634
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.371755 0.052827 0.000001 6 -0.311811 -1.035991 -0.000000 1 -0.594705 -2.080061 0.000002 8 0.919805 -0.815171 -0.000003 8 1.370679 0.461411 -0.000005 9 -2.569662 -0.558544 0.000006 9 -1.289552 0.816787 -1.088349 9 -1.289546 0.816792 1.088347 1 3.031578 0.273012 -0.000001 9 3.964389 0.095644 0.000003	26.9508, 54.9483, 84.1009, 132.1838, 246.9818, 247.4661, 354.7131, 480.7731, 510.2538, 534.0738, 590.3146, 749.8774, 756.3514, 821.6079, 866.9841, 896.0442, 918.1111, 1161.0342, 1191.3784, 1242.0397, 1370.7088, 1572.2553, 3208.6780, 3509.336

Compound: sCI 23 + HF TS	**Energy (kJ mol^{-1}):** -626.586057924863
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.889086 -0.029145 0.056776 6 0.302863 -0.341538 -0.860655 1 0.039340 -0.360371 -1.915298 8 1.376077 -0.931380 -0.588680 8 1.887292 -0.545928 0.692138 9 -1.656484 -1.145380 -0.046981 9 -1.575119 0.987143 -0.465474 9 -0.652471 0.193255 1.329209 1 1.652604 0.682188 0.400681 9 1.186123 1.489509 -0.204506	-744.6703, 64.3780, 155.9795, 218.8689, 290.9263, 305.9879, 388.0168, 478.4261, 514.3063, 536.6919, 562.2071, 731.4878, 809.2587, 838.2783, 880.0394, 1017.9591, 1097.0831, 1182.4137, 1196.0533, 1309.7201, 1372.5351, 1594.9569, 1789.9811, 3154.0510
IRC	



Compound: sCI 23 + HF Pr	**Energy (kJ mol^{-1}):** -626.673546284392
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.834570 -0.148326 0.006261 6 0.403604 0.587437 -0.563339 1 0.154218 0.966869 -1.556157 8 1.519250 -0.186749 -0.771280 8 1.871523 -0.876548 0.454931 9 -1.921667 0.615688 -0.223556	56.8425, 135.9833, 203.5157, 232.7615, 265.9833, 305.1939, 368.6668, 433.8158, 523.9364, 580.0369, 619.4572, 762.1754, 860.2378, 911.8567, 1057.9257, 1104.4746, 1150.6938, 1188.4176,

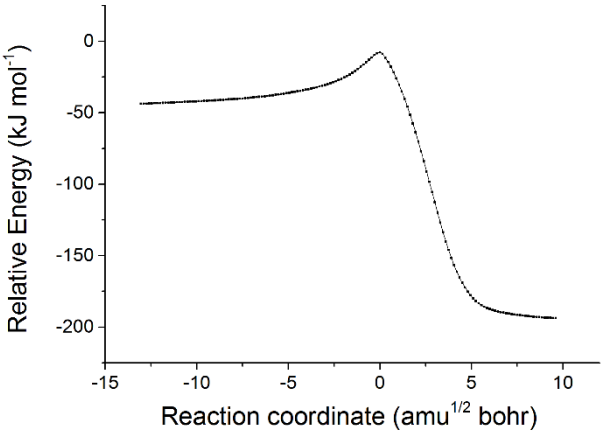
9 -0.766233 -0.375379 1.316841 9 -1.007864 -1.313996 -0.628918 1 2.545035 -0.281518 0.817457 9 0.669137 1.649949 0.270295	1283.4743, 1344.2761, 1394.2047, 1408.6765, 3084.3933, 3733.0817

8.6.3 sCl 24 + HF

Compound: sCl 24 + HF PRC	**Energy (kJ mol^{-1}):** -626.610016871772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.276051 0.122225 0.000000 6 0.238154 0.075338 0.000006 1 0.838781 0.982707 0.000012 8 0.768267 -1.055007 -0.000001 8 2.128693 -1.184191 0.000001 9 -1.691044 0.792038 -1.086257 9 -1.691051 0.792061 1.086241 9 -1.825166 -1.087203 0.000011 1 2.778804 0.267521 -0.000000 9 2.922163 1.222879 -0.000001	25.8279, 77.5369, 107.2193, 170.3821, 207.5782, 288.9583, 383.9496, 395.5151, 441.0878, 557.4098, 560.1105, 699.9805, 843.3993, 888.2642, 940.8348, 962.1647, 1046.2065, 1153.2153, 1187.3539, 1277.1579, 1388.8897, 1567.4454, 3116.9891, 3196.4029

Compound: sCl 24 + HF TS	**Energy (kJ mol^{-1}):** -626.592526379491
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.096361 -0.003094 -0.004462 6 -0.359680 -0.155275 -0.438103 1 -0.663416 0.236291 -1.398539 8 -1.066073 -0.963183 0.210641 8 -2.446944 -0.742017 -0.123188 9 1.292227 -0.377960 1.252167 9 1.472246 1.263687 -0.159861 9 1.844629 -0.776019 -0.813585 1 -2.284641 0.482190 0.001683 9 -1.649980 1.431772 0.093791	-850.5241, 34.8760, 114.4545, 182.7985, 287.3622, 336.1011, 376.2820, 453.9894, 513.0961, 549.5780, 621.8010, 675.8334, 751.4147, 869.5333, 909.5337, 990.2752, 1150.4901, 1190.6701, 1203.7874, 1284.1834, 1363.3160, 1575.9778, 1814.8849, 3212.0268

IRC



Compound: sCl 24 + HF Pr	**Energy (kJ mol^{-1}):** -626.675135107360
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.969274 -0.137135 -0.021241 6 -0.481096 0.279164 -0.340046 1 -0.659604 0.233344 -1.414282 8 -1.307314 -0.572338 0.355007 8 -2.626661 -0.476319 -0.234610 9 1.816862 0.714657 -0.615447 9 1.209603 -1.366423 -0.497401 9 1.215729 -0.131085 1.291727	65.4287, 108.2183, 184.1493, 231.2871, 271.0036, 350.3917, 357.5479, 394.4965, 522.2061, 565.1454, 617.2866, 716.1753, 879.1933, 954.1929, 1050.5288, 1128.3522, 1171.5778, 1185.5722, 1272.5277, 1359.8608, 1390.0408, 1400.2829, 3095.2578, 3732.6363

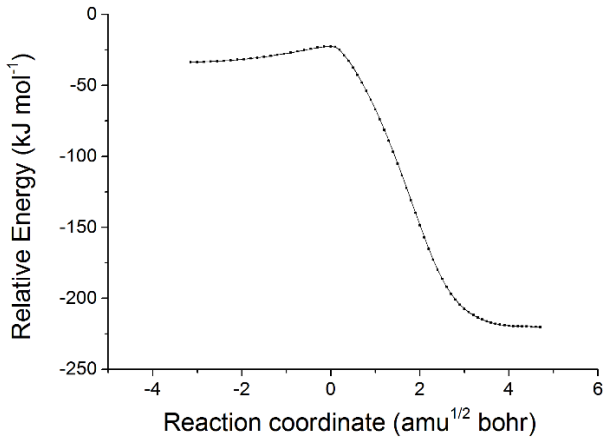
1 -3.077769 0.085638 0.413486 9 -0.655516 1.584862 0.066159	

8.6.4 sCI 25 + HF

Compound: sCI 25 + HF PRC	**Energy (kJ mol^{-1}):** -725.776277323618
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.869815 -0.421998 -0.153846 6 -0.057258 0.866122 0.122023 9 -0.705444 1.716305 0.859512 8 1.041347 1.252070 -0.287829 8 1.874968 0.393522 -1.032891 9 -1.160303 -0.995607 1.009684 9 -0.271405 -1.272555 -0.951345 9 -2.015111 -0.010512 -0.727888 1 2.114898 -0.665378 0.158952 9 1.943042 -1.122532 0.987564	39.0244, 59.7387, 76.7172, 200.0033, 227.3232, 252.6997, 259.1565, 334.3436, 367.7980, 483.1061, 505.5070, 571.4816, 615.5282, 690.0793, 772.8026, 790.5163, 904.4336, 1008.4787, 1127.7364, 1176.1445, 1275.3385, 1391.3018, 1613.3843, 3263.4439

Compound: sCI 25 + HF TS	**Energy (kJ mol^{-1}):** -725.769990619824
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.911285 -0.279396 -0.087736 6 0.299622 0.697087 -0.086988 9 -0.032873 1.863438 0.356311 8 1.359429 0.666224 -0.746314 8 1.914009 -0.673218 -0.801520 9 -1.555553 -0.185057 1.066053 9 -0.621937 -1.530199 -0.352728 9 -1.709117 0.200215 -1.066745 1 1.697315 -0.807733 0.510584 9 1.228942 -0.530892 1.432714	-380.2160, 57.5077, 139.3986, 207.0471, 239.1676, 263.7697, 320.3367, 363.6198, 390.7479, 486.7055, 527.9314, 592.5551, 610.0036, 681.7931, 781.8620, 904.2735, 1094.1675, 1117.9363, 1172.3312, 1246.5506, 1283.4670, 1385.0778, 1607.1290, 1837.8803

IRC



Compound: sCI 25 + HF Pr	**Energy (kJ mol^{-1}):** -725.857806332430
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.889167 -0.292627 -0.009267 6 0.415104 0.571256 0.005386 9 0.164758 1.722671 -0.629602 8 1.490616 0.038298 -0.679680 8 1.861000 -1.213187 -0.064101 9 -1.914062 0.459599 0.411129	39.7363, 126.2403, 202.0897, 225.5792, 249.4652, 288.7103, 343.6012, 376.3539, 399.9664, 489.8662, 531.6127, 590.5430, 653.5497, 687.2684, 782.6821, 980.2959, 1090.2120, 1155.7713,

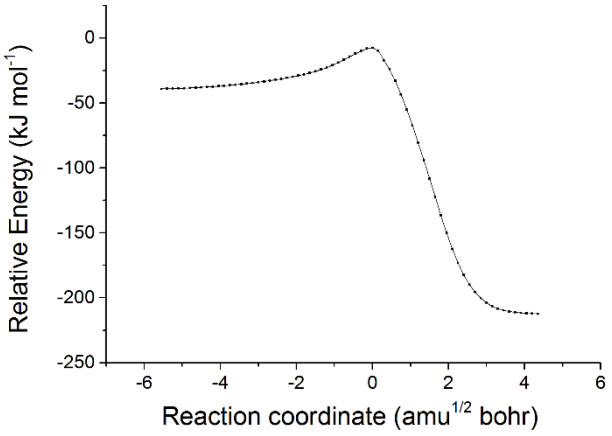
9 -0.792497 -1.353455 0.790426 9 -1.142632 -0.705041 -1.253049 1 2.609374 -0.935161 0.485985 9 0.731328 0.838726 1.290825	1192.3813, 1201.6568, 1214.8916, 1350.7749, 1413.8516, 3727.6606

8.6.5 sCI 26 + HF

Compound: sCI 26 + HF PRC	**Energy (kJ mol^{-1}):** -725.783185514069
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.346110 0.061678 -0.133186 6 0.098792 -0.185894 0.312407 9 0.521788 0.510871 1.301754 8 0.788018 -1.043836 -0.255240 8 2.103466 -1.228631 0.181675 9 -1.485883 1.341631 -0.475855 9 -2.163912 -0.201940 0.891456 9 -1.655856 -0.715041 -1.159465 1 2.712299 0.234128 -0.283211 9 2.743833 1.141245 -0.580512	30.4167, 43.0085, 72.9994, 156.8884, 180.1979, 258.9762, 302.7274, 353.6017, 371.6271, 405.6737, 519.5743, 576.0599, 697.7263, 726.7195, 729.3323, 852.1026, 862.2567, 943.3627, 1160.6948, 1179.4724, 1241.3002, 1404.9745, 1636.1444, 3393.8484

Compound: sCI 26 + HF TS	**Energy (kJ mol^{-1}):** -725.770085507023
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.160862 -0.032260 -0.105695 6 0.320445 -0.209963 0.292269 9 0.608204 0.190085 1.479794 8 1.027540 -1.005634 -0.363899 8 2.432868 -0.685533 -0.155085 9 -1.328521 -0.276154 -1.394517 9 -1.554072 1.199715 0.183001 9 -1.888106 -0.903457 0.609456 1 2.131169 0.574495 -0.392815 9 1.410058 1.390720 -0.497152	-665.3587, 34.4507, 114.8127, 178.8817, 256.6845, 300.9149, 309.4190, 360.2051, 402.1590, 431.0590, 525.5625, 578.3785, 668.3228, 719.8528, 823.8600, 842.9141, 1036.0573, 1142.1647, 1151.2266, 1195.4510, 1254.3528, 1400.3879, 1606.9244, 1817.2889

IRC



Compound: sCI 26 + HF Pr	**Energy (kJ mol^{-1}):** -725.860158374757
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.071132 -0.164947 -0.001594 6 -0.426713 0.274719 -0.004529 9 -0.640177 1.108402 -1.036237 8 -1.174458 -0.867810 -0.087232 8 -2.571414 -0.496277 -0.117625 9 1.845035 0.918898 0.084820 9 1.369026 -0.819623 -1.124342 9 1.322689 -0.957224 1.043687	60.1460, 121.4786, 168.5796, 220.2847, 255.1560, 295.0352, 336.5640, 374.0731, 376.8953, 523.2280, 529.6868, 594.5260, 606.2032, 738.2555, 833.3664, 943.2474, 1094.1752, 1144.8046, 1184.4607, 1206.5191, 1211.8461, 1345.0714, 1411.1882, 3726.8452

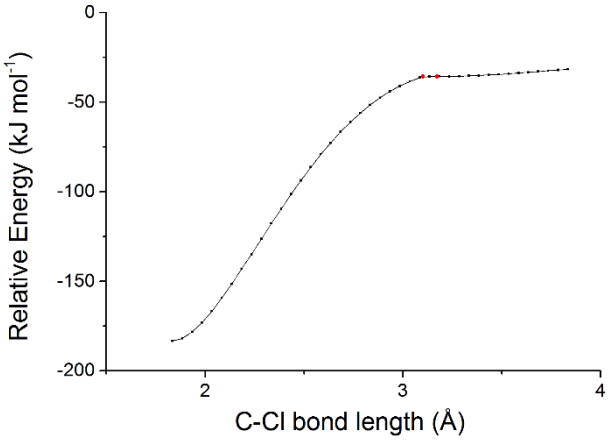
1 -2.829982 -0.688425 0.797048 9 -0.682080 0.965379 1.129688	

8.7 HFO-sCI reactions with HCl

Compound: HCl	**Energy (kJ mol^{-1}):** -460.373228449128
Reaction Coordinates: 17 0.000000 0.000000 0.071311 1 0.000000 0.000000 -1.212290	**Frequencies (cm^{-1}):** 2935.7855

8.7.1 sCI 1 + HCl

Compound: sCI 1 + HCL PRC	**Energy (kJ mol^{-1}):** -649.786096409260
Reaction Coordinates: 6 -1.336144 1.008146 0.177187 1 -1.868220 1.826217 -0.292080 1 -0.680692 1.112214 1.032231 8 -1.535125 -0.111981 -0.335374 8 -0.828331 -1.180579 0.194099 1 0.554522 -0.654641 0.096022 17 1.701112 0.118107 -0.045241	**Frequencies (cm^{-1}):** 60.4557, 176.4811, 230.4019, 509.8882, 663.3721, 754.8100, 850.5504, 1022.5705, 1035.4059, 1244.4996, 1423.1906, 1578.1814, 11.5544:13, 1619.2991, 1528.6350, 3120.4571, 3265.3577

Compound: sCI 1 + HCL TS	**Energy (kJ mol^{-1}):** -649.785673633254
Reaction Coordinates: 6 -1.290274 1.012234 0.181602 1 -1.794768 1.846515 -0.290202 1 -0.647019 1.095745 1.047673 8 -1.515281 -0.099860 -0.338189 8 -0.822644 -1.182523 0.193323 1 0.504896 -0.678863 0.099185 17 1.669526 0.113074 -0.046314	**Frequencies (cm^{-1}):** -93.7733, 179.6707, 237.6760, 498.5803, 659.3270, 803.9659, 842.1572, 1033.4816, 1060.7591, 1247.6658, 1385.9919, 1428.7903, 1579.5775, 3122.0712, 3266.8750
IRC	
	

Compound: sCI 1 + HCL Pr	**Energy (kJ mol^{-1}):** -649.851301605594
Reaction Coordinates: 6 0.003850 0.838496 0.263509 1 0.297621 1.812033 -0.116982 1 -0.155121 0.828835 1.337016	**Frequencies (cm^{-1}):** 143.1167, 260.0739, 365.5883, 494.0492, 664.4717, 877.6148, 996.3526, 1078.6954, 1267.3400,

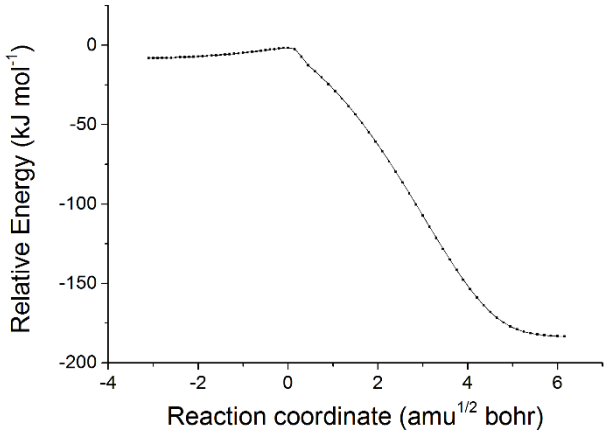
8 -1.125194 0.483448 -0.438558 8 -1.737316 -0.651057 0.217450 1 -1.350257 -1.388632 -0.279390 17 1.416749 -0.290726 -0.044285	1322.2118, 1390.8227, 1456.2616, 3091.0927, 3169.7044, 3717.0894

8.7.2 sCl 23 + HCl

Compound: sCl 23 + HCl PRC	**Energy (kJ mol^{-1}):** -986.587116795699
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.914503 -0.050458 0.000001 6 -0.847721 1.030051 -0.000000 1 -1.123123 2.075925 0.000001 8 0.383224 0.799262 -0.000004 8 0.828024 -0.476783 -0.000006 9 -3.108809 0.568984 0.000006 9 -1.839190 -0.816240 1.088202 9 -1.839196 -0.816235 -1.088204 1 2.617586 -0.277000 -0.000004 17 3.910215 -0.040288 0.000002	18.7102, 37.3389, 83.0612, 92.6607, 213.5202, 246.5783, 337.0294, 479.6058, 504.7996, 533.0463, 534.5479, 590.3170, 642.5689, 762.8747, 814.3955, 883.6309, 920.2579, 1159.4939, 1188.9489, 1241.8058, 1369.4349, 1565.8153, 2527.4977, 3209.9424

Compound: sCl 23 + HCL TS	**Energy (kJ mol^{-1}):** -986.576964395944
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.137573 -0.246816 -0.047542 6 -0.290786 0.621775 0.888296 1 -0.577372 0.576857 1.933905 8 0.466574 1.578942 0.609843 8 1.039573 1.594156 -0.656418 9 -1.287606 -1.449642 0.511022 9 -0.741805 -0.374196 -1.292953 9 -2.349561 0.364692 -0.044438 1 1.696166 0.354117 -0.489858 17 2.047819 -0.907835 0.077726	-358.2410, 48.0071, 105.4872, 151.4765, 218.8015, 291.2973, 302.2909, 431.4392, 491.8270, 528.5665, 560.3076, 734.0336, 813.2396, 820.9045, 858.0104, 896.8840, 1023.7636, 1096.4000, 1188.0244, 1307.9946, 1370.7250, 1398.7693, 1581.5061, 3174.8648

IRC



Compound: sCl 23 + HCL Pr	**Energy (kJ mol^{-1}):** -986.659667626854
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.016093 -0.086265 0.021645 6 -0.362052 -0.043383 -0.679606 1 -0.215083 -0.351869 -1.712506 8 -0.930566 1.207428 -0.779110 8 -1.082098 1.795492 0.533299 9 1.623303 -1.247388 -0.288003 9 0.963234 0.009638 1.348314 9 1.778337 0.913227 -0.447178 1 -1.999280 1.557641 0.741066	59.1331, 127.2325, 176.6045, 208.4503, 234.4071, 305.8910, 328.7563, 382.3320, 505.5717, 524.4360, 577.9461, 715.5376, 806.8403, 845.2028, 905.7538, 1083.8250, 1135.3758, 1167.9676, 1262.5845, 1268.2043, 1380.2082, 1398.1375, 3116.5427, 3717.2765

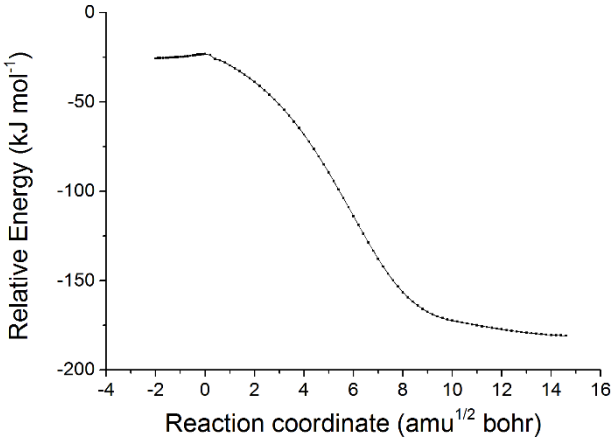
17 -1.464261 -1.266502 0.080441	

8.7.3 sCl 24 + HCl

Compound: sCl 24 + HCL PRC	**Energy (kJ mol^{-1}):** -986.588821076460
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.582120 -0.230508 0.004148 6 0.216761 0.291935 0.403795 1 -0.350700 -0.175656 1.199747 8 -0.219477 1.289563 -0.205145 8 -1.454922 1.771203 0.136133 9 1.479664 -1.523676 -0.327477 9 2.406751 -0.134788 1.061239 9 2.105067 0.442975 -1.013836 1 -2.403940 0.424704 0.044861 17 -2.856870 -0.833197 -0.036442	21.7466, 41.5599, 106.4836, 157.8438, 195.5869, 236.1469, 381.4594, 399.6774, 414.5187, 550.3914, 559.1233, 605.1213, 699.8698, 797.7048, 886.7464, 909.3514, 939.2583, 1151.0214, 1182.2896, 1273.7220, 1365.0410, 1572.7375, 2192.8173, 3188.7321

Compound: sCl 24 + HCL TS	**Energy (kJ mol^{-1}):** -986.585206698211
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.475079 0.187092 -0.003645 6 0.113282 -0.345669 -0.423827 1 -0.380015 0.037238 -1.307222 8 -0.350271 -1.303630 0.229611 8 -1.634527 -1.704090 -0.136852 9 1.424826 1.518227 0.057538 9 2.368854 -0.162839 -0.945122 9 1.869014 -0.298242 1.166832 1 -2.230512 -0.494197 -0.058986 17 -2.470912 0.938580 0.039749	-400.1643, 26.3909, 67.7722, 177.8239, 199.7647, 266.5886, 373.9922, 399.3114, 423.0809, 539.4095, 564.3907, 685.5681, 723.5873, 842.5092, 873.5717, 899.9578, 1006.9712, 1152.7589, 1193.0976, 1275.6814, 1348.0393, 1369.7483, 1576.1347, 3208.3909

IRC



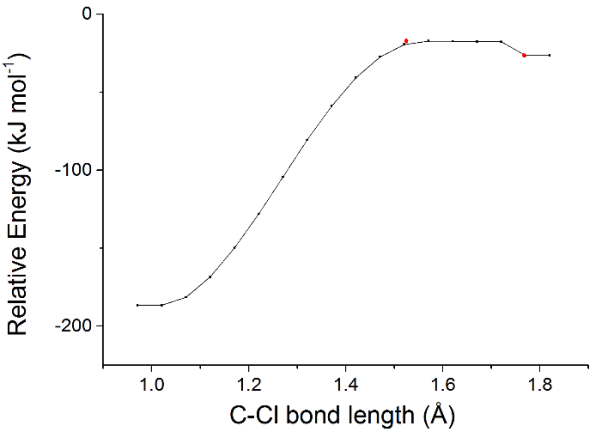
Compound: sCl 24 + HCL Pr	**Energy (kJ mol^{-1}):** -986.660655427993
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.117713 -0.163739 -0.020203 6 -0.382956 -0.078604 -0.356523 1 -0.522871 -0.220769 -1.424751 8 -1.013282 -1.059037 0.380371 8 -2.293145 -1.322743 -0.231825 9 1.796699 0.773587 -0.693662 9 1.589405 -1.363303 -0.395803 9 1.356619 -0.008933 1.284400 1 -2.885091 -0.816900 0.346833	62.6223, 105.0812, 183.4353, 187.3409, 251.3766, 322.8491, 339.7521, 364.9799, 461.5709, 534.4284, 562.4427, 700.6468, 762.1871, 878.4267, 954.3954, 1100.9976, 1141.3416, 1180.7016, 1259.3337, 1285.8863, 1358.3179, 1399.9080, 3119.8932, 3717.5641

17 -1.013745 1.584342 0.023264	

8.7.4 sCl 25 + HCl

Compound: sCl 25 + HCL PRC	**Energy (kJ mol^{-1}):** -1085.756886776330
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.788499 -0.376521 -0.000005 6 0.756492 0.768406 0.000006 9 1.213983 1.981969 -0.000002 8 -0.473795 0.640091 0.000021 8 -0.994569 -0.653408 0.000031 9 3.009876 0.160989 -0.000023 9 1.643236 -1.121713 -1.088590 9 1.643265 -1.121708 1.088587 1 -2.736778 -0.349696 0.000010 17 -4.022323 -0.058289 -0.000011	14.4742, 35.2968, 60.1189, 94.2784, 219.7336, 222.6743, 266.1698, 304.8624, 364.6273, 483.8170, 500.3309, 549.8405, 578.5807, 631.2857, 675.8252, 683.1820, 780.3017, 920.0740, 1160.6457, 1207.0769, 1210.1306, 1406.4075, 1607.6839, 2477.0829

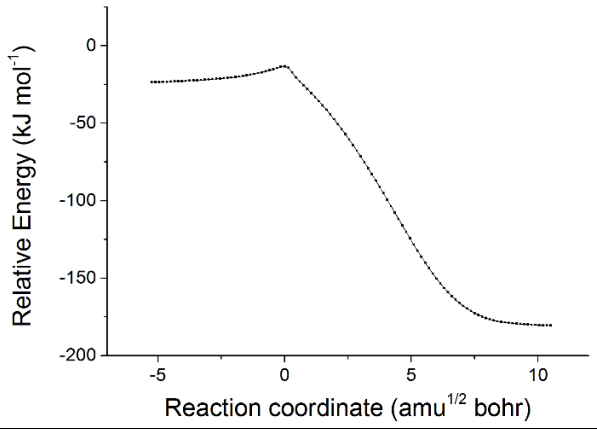
Compound: sCl 25 + HCL TS	**Energy (kJ mol^{-1}):** -1085.755515324460
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.061675 -0.485134 0.206104 6 0.379040 0.780930 -0.373687 9 0.884630 1.135589 -1.513276 8 -0.374195 1.615144 0.150847 8 -1.098287 1.227245 1.298940 9 1.142806 -1.405621 -0.747312 9 0.490864 -0.980490 1.275721 9 2.309365 -0.081099 0.520230 1 -1.903232 0.158409 0.567437 17 -2.259423 -0.746336 -0.410500	-80.0949, .7463, 83.4905, 155.8752, 212.6513, 252.4910, 265.0050, 288.4477, 368.3748, 478.8249, 506.8511, 578.2229, 615.7454, 668.1614, 732.7236, 777.3729, 902.0691, 1007.4100, 1112.4128, 1181.8976, 1278.3178, 1385.3241, 1592.9476, 1757.0919
IRC	



Compound: sCl 25 + HCL Pr	**Energy (kJ mol^{-1}):** -1085.834620970350
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.060856 -0.008297 -0.189123 6 0.355338 -0.108230 0.475200 9 0.197689 -0.699204 1.669813 8 0.927380 1.111898 0.791717 8 1.101114 1.895565 -0.401700 9 -1.647677 -1.209971 -0.157015 9 -1.008596 0.402535 -1.453358 9 -1.808957 0.848469 0.512907 1 2.027791 1.705099 -0.618622 17 1.434426 -1.126006 -0.551124	50.2033, 121.4143, 171.8280, 217.7511, 223.4230, 278.6540, 312.2242, 345.4722, 366.0803, 405.1581, 506.9394, 538.8667, 590.2412, 624.2460, 743.7466, 909.3164, 980.1865, 1102.6952, 1157.4600, 1191.4081, 1211.5291, 1295.0756, 1416.7299, 3710.0443

8.7.5 sCl 26 + HCl

Compound: sCl 26 + HCL PRC	**Energy (kJ mol^{-1}):** -1085.762584407700
Reaction Coordinates: 6 1.652214 -0.266535 -0.132727 6 0.351559 0.434522 0.266554 9 -0.039641 0.277222 1.479483 8 -0.252232 1.146365 -0.549289 8 -1.429760 1.763605 -0.136867 9 1.529614 -1.576698 0.079388 9 2.646860 0.200300 0.630556 9 1.929256 -0.041822 -1.407761 1 -2.492164 0.382844 -0.129858 17 -2.980549 -0.847149 -0.130520	**Frequencies (cm^{-1}):** 26.6352, 29.6193, 55.4301, 131.9833, 181.2789, 204.0811, 294.9425, 344.6381, 364.5925, 405.7232, 517.2215, 526.6510, 576.2596, 686.3177, 706.9846, 728.9803, 860.5920, 873.3529, 1157.9005, 1176.9629, 1240.1319, 1399.6990, 1626.7741, 2402.4687

Compound: sCl 26 + HCL TS	**Energy (kJ mol^{-1}):** -1085.758646350020
Reaction Coordinates: 6 1.444993 -0.202352 -0.117201 6 0.113833 0.485166 0.242495 9 -0.193524 0.488128 1.486587 8 -0.439482 1.208925 -0.609714 8 -1.744542 1.629281 -0.252622 9 1.461858 -1.426052 0.392147 9 2.440338 0.511295 0.427362 9 1.603459 -0.248916 -1.429169 1 -2.214678 0.368181 -0.166095 17 -2.204428 -1.099459 -0.092902	**Frequencies (cm^{-1}):** -581.3091, 32.0565, 70.2436, 158.4864, 182.2178, 211.7313, 297.6019, 335.8299, 359.1080, 405.1791, 496.9126, 577.5197, 610.7858, 727.0141, 760.3198, 856.8177, 858.9326, 929.6950, 1145.8207, 1192.6900, 1252.5531, 1387.6973, 1411.2767, 1610.8001
IRC  	

Compound: sCl 26 + HCL Pr	**Energy (kJ mol^{-1}):** -1085.837345614150
Reaction Coordinates: 6 -1.194899 -0.120815 -0.111015 6 0.331124 -0.083210 0.229355 9 0.474675 -0.305365 1.551533 8 0.899285 -1.074209 -0.524802 8 2.303812 -1.172668 -0.216102 9 -1.841384 0.800655 0.603411 9 -1.693257 -1.321710 0.195276 9 -1.401636 0.111274 -1.408265 1 2.690449 -0.706358 -0.974330 17 1.001285 1.549519 -0.134476	**Frequencies (cm^{-1}):** 64.4258, 128.1095, 167.6467, 186.4425, 223.1601, 270.7713, 308.4509, 349.4830, 369.6766, 425.8388, 452.6172, 546.5202, 575.5520, 706.3830, 742.8602, 932.2223, 962.3080, 1078.0033, 1146.1876, 1198.7855, 1211.6191, 1288.9764, 1413.0046, 3714.6669

8.8 Reactions with H_2S

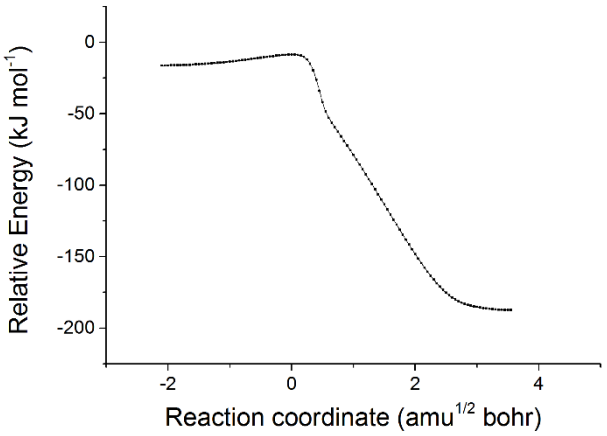
Compound: H_2S	**Energy (kJ mol^{-1}):** -398.964896610182
Reaction Coordinates:	**Frequencies (cm^{-1}):**
16 0.000000 -0.000000 0.103242 1 -0.000000 0.971861 -0.825934 1 -0.000000 -0.971861 -0.825934	1206.0101, 2682.8315, 2695.9979

8.8.1 sCl 1 + H_2S

Compound: sCl 1 + H_2S PRC1	**Energy (kJ mol^{-1}):** -588.373411489393
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.383147 1.052216 -0.190803 1 0.857402 1.062232 -1.135927 1 1.750328 1.932456 0.319036 8 1.620589 -0.035140 0.381047 8 1.154027 -1.183091 -0.196698 16 -1.894674 0.073705 -0.044649 1 -0.816788 -0.757434 -0.095069 1 -1.971973 0.016017 1.296363	63.4000, 131.8291, 149.4863, 162.3626, 233.3899, 476.4641, 530.3435, 672.4471, 883.9619, 975.7551, 1211.1926, 1238.8171, 1410.6771, 1558.3845, 2475.3799, 2689.0854, 3126.9057, 3271.963

Compound: sCl 1 + H_2S TS1	**Energy (kJ mol^{-1}):** -588.366724078241
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.850344 1.071250 -0.227889 1 0.603134 0.952593 -1.271614 1 0.880621 2.037578 0.259668 8 1.403926 0.127025 0.404241 8 1.163723 -1.125721 -0.183869 16 -1.571014 -0.031723 -0.035438 1 -0.410264 -0.882903 -0.126424 1 -1.580531 -0.037629 1.309724	-287.4348, 192.8922, 266.6416, 346.5469, 470.9489, 503.0721, 727.6948, 853.5293, 903.8597, 1013.4027, 1212.6890, 1229.2910, 1385.7411, 1535.5675, 1640.5057, 2683.0310, 3132.3039, 3269.0933

IRC



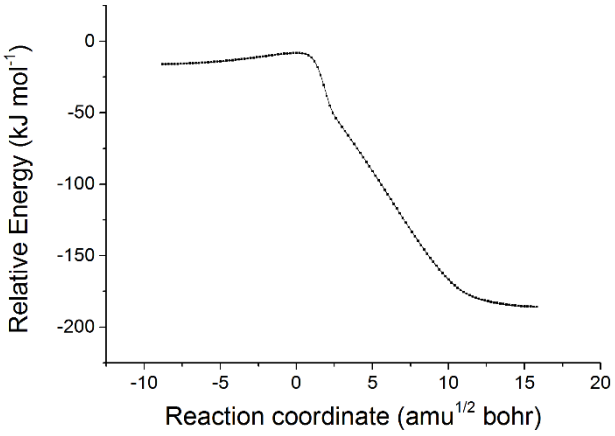
Compound: sCl 1 + H_2S Pr1	**Energy (kJ mol^{-1}):** -588.446035792738
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.001168 0.835726 0.290620 1 -0.181880 0.839497 1.364179 1 0.259165 1.833670 -0.056535 8 -1.165429 0.503394 -0.417719 8 -1.733621 -0.684680 0.175653	141.7941, 250.1772, 306.7244, 361.7041, 504.1382, 667.7742, 797.3210, 884.0190, 1004.4493, 1070.2357, 1270.4039, 1327.6749,

16 1.415014 -0.309297 0.024241 1 -1.234849 -1.384014 -0.276466 1 1.702732 0.095537 -1.226224	1388.0540, 1442.1300, 2670.1919, 3063.0127, 3131.2502, 3694.8508

Compound: sCl 1 + H_2S PRC2	**Energy (kJ mol^{-1}):** -588.373317449885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.374106 1.051493 0.211173 1 0.855371 1.043508 1.160152 1 1.727983 1.941423 -0.291192 8 1.615258 -0.026559 -0.376434 8 1.163584 -1.185240 0.192467 16 -1.875235 0.076608 -0.116169 1 -0.812930 -0.764087 0.024453 1 -2.242037 -0.061138 1.169987	63.0680, 130.1110, 145.4168, 162.6574, 245.2900, 464.0536, 527.5536, 671.0392, 883.0327, 974.9178, 1215.9064, 1239.3125, 1410.1846, 1558.0192, 2476.9496, 2688.8034, 3126.9908, 3272.3093

Compound: sCl 1 + H_2S TS2	**Energy (kJ mol^{-1}):** -588.366581083392
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.849619 1.069515 0.237062 1 0.578535 0.941856 1.273377 1 0.890091 2.038022 -0.245086 8 1.413656 0.127668 -0.389692 8 1.159069 -1.127293 0.188155 16 -1.550820 -0.025704 -0.128931 1 -0.404959 -0.883882 0.065341 1 -1.930063 -0.104826 1.159185	-295.7329, 192.3838, 268.3680, 346.2326, 491.6914, 513.1666, 715.6320, 853.2832, 888.9700, 1003.2864, 1205.4724, 1243.2746, 1385.4237, 1534.7258, 1629.1815, 2683.1069, 3135.1386, 3273.1921

IRC



Compound: sCl 1 + H_2S Pr2	**Energy (kJ mol^{-1}):** -588.445571445584
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.012289 0.836673 0.292041 1 0.137899 0.843930 1.369473 1 -0.261437 1.835409 -0.062595 8 1.182629 0.525484 -0.380415 8 1.707413 -0.699298 0.182137 16 -1.445103 -0.237773 -0.114264 1 1.423595 -1.344209 -0.482939 1 -1.225017 -1.160284 0.838262	138.0723, 205.9238, 297.5899, 356.7590, 494.4525, 686.5323, 780.5804, 886.2457, 1009.5045, 1062.2832, 1278.9894, 1319.8557, 1377.8454, 1439.6650, 2680.0174, 3066.0637, 3129.7951, 3725.2061

8.8.2 sCI 23 + H_2S

Compound: sCI 23 + H_2S PRC1	**Energy (kJ mol^{-1}):** -925.175112004368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.484229 -0.344913 -0.006771 6 -0.855916 0.661362 0.935858 8 0.009345 1.502272 0.588972 8 0.449903 1.536780 -0.681884 1 -1.150956 0.698319 1.974948 9 -2.154044 0.255184 -0.994064 9 -0.584013 -1.177125 -0.531100 9 -2.361052 -1.072857 0.711674 16 3.190953 -0.600746 0.031241 1 4.010342 0.349054 0.514893 1 2.344237 0.306641 -0.499502	9.9024, 23.7127, 61.6911, 106.0087, 107.9417, 135.5994, 181.9940, 245.6847, 314.0242, 327.5125, 477.9915, 506.4081, 535.5159, 589.4703, 757.9055, 792.8041, 883.2286, 931.3426, 1155.0768, 1180.1698, 1209.2232, 1242.6978, 1366.4837, 1550.9099, , 2626.7917, 2690.7441, 3215.4330

Compound: sCI 23 + H_2S TS1	**Energy (kJ mol^{-1}):** -925.168836880090
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.079377 -0.272562 0.017459 6 0.062519 0.407790 -0.903023 8 -0.458449 1.540497 -0.680542 8 -0.719497 1.804417 0.660310 1 0.145936 0.148250 -1.951564 9 2.137961 0.548220 0.135183 9 0.674673 -0.606080 1.237017 9 1.493402 -1.393073 -0.605044 16 -1.985813 -0.912407 0.044771 1 -2.799656 -0.366896 -0.878246 1 -1.755408 0.304882 0.684309	-186.5290, 50.4707, 126.9609, 154.6013, 210.6029, 314.1125, 322.1871, 331.7323, 435.1666, 465.2846, 510.9986, 542.6879, 571.0339, 731.1105, 763.7064, 845.8696, 865.8312, 913.6169, 1145.9236, 1154.6731, 1216.9637, 1258.5030, 1344.6574, 1524.9039, 2125.4049, 2679.8543, 3182.1468

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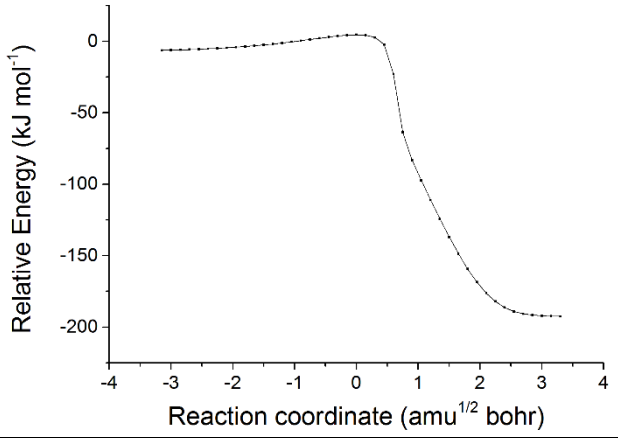

Compound: sCI 23 + H_2S Pr1	**Energy (kJ mol^{-1}):** -925.256025297439
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.023936 -0.130202 0.007316 6 -0.359856 -0.030549 -0.670201 8 -0.837859 1.281713 -0.779296 8 -1.004095 1.851805 0.537383 1 -0.222963 -0.334569 -1.706347 9 1.801492 0.896816 -0.354922 9 0.959825 -0.154651 1.346215	60.8407, 124.4968, 176.2385, 192.0415, 221.4286, 285.4577, 327.4123, 332.3845, 379.4655, 502.9899, 524.0442, 568.9290, 712.1710, 780.1388, 832.6499, 895.8157, 966.2179, 1039.8374, 1122.2301, 1175.2785, 1249.6693,

9 1.632480 -1.266220 -0.389625 16 -1.524866 -1.200782 0.148899 1 -2.278442 -1.380984 -0.949920 1 -1.893773 1.540930 0.771481	1260.7064, 1364.3021, 1394.9375, 2680.3929, 3106.7373, 3692.8576
Compound: sCI 23 + H_2S PRC2	**Energy (kJ mol^{-1}):** -925.174429805702
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.021718 -0.038630 0.002520 6 -0.932518 1.013408 0.041877 8 0.295322 0.750975 0.020220 8 0.714242 -0.524723 -0.042152 1 -1.182713 2.063680 0.091864 9 -1.978894 -0.759165 -1.119635 9 -1.960687 -0.858685 1.053557 9 -3.203548 0.606804 0.042095 16 4.235132 0.005906 -0.070083 1 4.435857 -0.406631 1.193404 1 2.921818 -0.310813 -0.039009	9.7858, 20.5426, 55.3474, 63.8132, 84.8668, 177.3682, 191.4593, 247.0686, 328.2667, 354.2698, 479.2267, 508.8930, 536.1159, 591.1425, 758.8193, 791.7027, 884.2323, 934.7058, 1155.4684, 1181.4413, 1216.3689, 1242.5905, 1366.8974, 1550.6684, 2608.8873, 2691.3503, 3215.2254

Compound: sCI 23 + H_2S TS2	**Energy (kJ mol^{-1}):** -925.167972073153
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.084640 -0.267962 0.020490 6 0.061333 0.409724 -0.893056 8 -0.466565 1.540319 -0.671974 8 -0.744439 1.796104 0.668712 1 0.150330 0.153688 -1.942151 9 2.171907 0.524589 0.062317 9 0.721390 -0.535782 1.268061 9 1.442690 -1.426479 -0.567284 16 -2.059113 -0.840429 -0.076063 1 -1.625042 -1.640531 0.913255 1 -1.791177 0.330804 0.639548	-200.4295, 46.0578, 134.0311, 158.5604, 213.1732, 290.9336, 312.7965, 319.5703, 408.7537, 472.4336, 517.6245, 550.6113, 573.3513, 731.3071, 761.6964, 844.7599, 865.9906, 916.4786, 1140.3623, 1152.3552, 1224.1910, 1264.0710, 1345.3041, 1524.3551, 2085.2288, 2694.0451, 3181.0752

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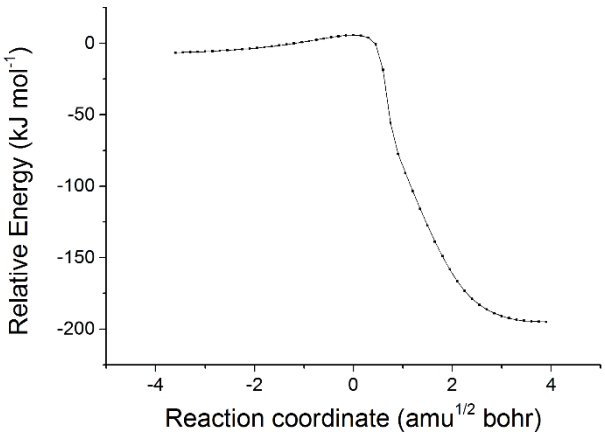

Compound: sCI 23 + H_2S Pr2	**Energy (kJ mol^{-1}):** -925.257286575136
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.038101 -0.073681 0.017437 6 -0.345508 -0.051413 -0.667474 8 -0.874309 1.246164 -0.774009 8 -1.218307 1.740515 0.541365 1 -0.172466 -0.327747 -1.708250	57.7190, 119.0022, 183.5200, 191.0234, 220.5122, 285.8439, 322.5651, 331.8899, 379.7520, 507.0559, 523.3513, 575.9561, 710.5756, 730.3250, 850.4188,

9 1.795556 0.938754 -0.429649 9 0.976078 0.020668 1.354219 9 1.674062 -1.222024 -0.282036 16 -1.485535 -1.318144 -0.007489 1 -1.301491 -1.020792 1.290740 1 -2.183383 1.659403 0.515897	893.4750, 976.3478, 1031.4681, 1131.8965, 1166.8457, 1247.6794, 1285.3044, 1356.0743, 1388.4082, 2684.6621, 3088.2825, 3730.1768

8.8.3 sCl 24 + H_2S

Compound: sCl 24 + H_2S PRC1	**Energy (kJ mol^{-1}):** -925.175112004368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.505791 -0.283359 -0.011193 6 0.260325 0.445841 -0.455155 1 -0.241765 0.189576 -1.378153 8 -0.136738 1.398076 0.254026 8 -1.246501 2.074357 -0.133452 9 2.508066 -0.023426 -0.873639 9 1.895522 0.071654 1.210826 9 1.286545 -1.606577 -0.032310 16 -2.822560 -0.892838 -0.052930 1 -2.655982 0.447927 0.043415 1 -2.683283 -1.081307 1.271215	16.7560, 35.6648, 94.9104, 129.5199, 144.0315, 187.5120, 195.2086, 226.6565, 356.3090, 388.4219, 406.5327, 422.0334, 552.0897, 561.1364, 699.6543, 868.5870, 888.1502, 960.6589, 1135.9140, 1176.5214, 1209.5645, 1267.4663, 1356.5936, 1553.5525, 2574.0746, 2688.7827, 3207.5983

Compound: sCl 24 + H2S TS1	**Energy (kJ mol^{-1}):** -925.172857190441
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.310051 -0.131310 -0.019387 6 0.013684 0.470188 -0.452503 8 0.483121 1.387908 0.280974 8 1.747748 1.813111 -0.134919 1 0.324899 0.372530 -1.482418 9 -1.370451 -0.327937 1.299070 9 -1.499155 -1.299640 -0.643653 9 -2.318385 0.691074 -0.367375 16 2.010557 -1.162230 -0.043231 1 2.319981 0.217673 -0.042042 1 1.809374 -1.207415 1.286670	-211.4560, 36.1197, 92.0602, 175.9207, 196.7871, 283.0048, 313.1884, 378.3885, 411.0245, 418.9613, 486.3471, 552.6049, 586.6452, 698.7495, 805.2558, 876.8659, 919.3305, 933.5828, 1139.9428, 1182.4716, 1216.9751, 1254.8214, 1338.8958, 1515.4506, 1912.7856, 2681.5459, 3207.0263

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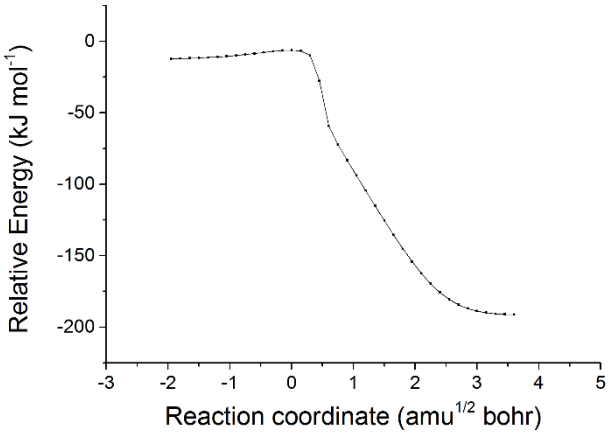

Compound: sCl 24 + H_2S Pr1	**Energy (kJ mol^{-1}):** -925.257735936140

Reaction Coordinates:	Frequencies (cm^{-1}):
6 1.126290 -0.140551 -0.031638 6 -0.374715 -0.078433 -0.357479 8 -0.970615 -1.118009 0.379968 8 -2.255017 -1.394028 -0.209024 1 -0.488446 -0.255832 -1.427000 9 1.372263 0.107002 1.266689 9 1.623239 -1.352756 -0.318668 9 1.801010 0.759696 -0.761611 16 -1.116036 1.571429 -0.048806 1 -0.702156 1.668348 1.228465 1 -2.825833 -0.770645 0.268896	63.8128, 102.0609, 186.4836, 187.1548, 245.7465, 301.4951, 321.9712, 351.3219, 365.2552, 454.8641, 534.7094, 561.6093, 685.2206, 715.5061, 873.8865, 932.6839, 970.9561, 1059.7406, 1138.6731, 1177.0163, 1243.1934, 1311.3835, 1339.9383, 1399.0168, 2671.5249, 3082.4983, 3694.2213

Compound: sCI 24 + H_2S PRC2	Energy (kJ mol^{-1}): -925.174429805702
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.503567 -0.284485 -0.011828 6 0.262393 0.449685 -0.460027 1 -0.232363 0.202682 -1.389467 8 -0.140290 1.396906 0.252344 8 -1.244397 2.078583 -0.143226 9 2.521171 0.007486 -0.846631 9 1.866725 0.037533 1.226876 9 1.293556 -1.607184 -0.077163 16 -2.780476 -0.902092 0.105562 1 -2.645184 0.445483 0.070505 1 -3.286178 -0.950318 -1.139579	16.8693, 36.2707, 93.7280, 127.5679, 142.8341, 192.0942, 193.9604, 235.7731, 350.9350, 388.0237, 405.4637, 420.8305, 552.1704, 560.7231, 699.7189, 868.7005, 887.7995, 959.2261, 1134.4405, 1177.7167, 1212.8077, 1267.9318, 1356.3589, 1554.0258, 2572.1811, 2688.1979, 3207.6933

Compound: sCI 24 + H_2S TS2	Energy (kJ mol^{-1}): -925.172354744837
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.313290 -0.136608 -0.016959 6 0.012714 0.461428 -0.447671 8 0.472921 1.396341 0.269616 8 1.739945 1.815318 -0.146902 1 0.338165 0.341324 -1.470376 9 -1.399575 -0.286104 1.303791 9 -1.479678 -1.327746 -0.605359 9 -2.320475 0.664428 -0.417352 16 1.993002 -1.140977 0.118183 1 2.311340 0.234651 0.001975 1 2.360541 -1.417753 -1.146189	-217.3443, 37.4007, 92.6508, 175.1327, 197.5688, 276.0734, 313.8069, 377.8487, 409.8519, 428.7319, 504.0821, 553.3237, 586.0863, 698.2452, 797.9012, 875.7437, 913.3066, 924.9756, 1137.9528, 1181.1166, 1221.2218, 1260.3439, 1339.4354, 1516.3591, 1892.3908, 2682.5789, 3211.9961

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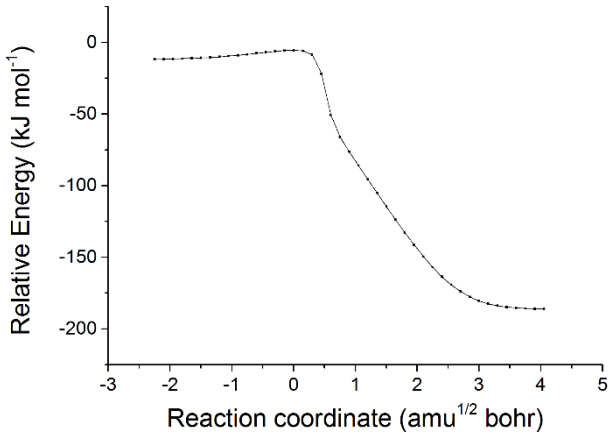

Compound: sCI 24 + H_2S Pr2	**Energy (kJ mol^{-1}):** -925.255754732320
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.134988 -0.125424 -0.029628 6 -0.364644 -0.085999 -0.364057 8 -0.934831 -1.167480 0.329847 8 -2.255123 -1.380183 -0.204046 1 -0.472188 -0.217740 -1.438933 9 1.367666 0.136530 1.266332 9 1.653715 -1.330722 -0.307283 9 1.796972 0.781311 -0.764700 16 -1.089668 1.545198 0.104755 1 -1.766818 1.718580 -1.042276 1 -2.793900 -0.858226 0.411706	60.8375, 103.4306, 134.5855, 184.9709, 193.2162, 286.4429, 316.1939, 345.9497, 365.6998, 459.7549, 532.6234, 561.6597, 689.6998, 743.5890, 858.3025, 935.5761, 969.8389, 1060.0747, 1133.8875, 1176.0136, 1248.1780, 1284.2039, 1341.6047, 1396.1450, 2689.6046, 3097.4785, 3703.1385

8.8.4 sCI 25 + H_2S

Compound: sCI 25 + H_2S PRC1	**Energy (kJ mol^{-1}):** -1024.345549005980
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.255536 -0.535628 0.094499 6 0.626941 0.785770 -0.380958 8 -0.126808 1.515607 0.276098 8 -0.522536 1.094310 1.539803 9 0.962643 1.208923 -1.564048 9 2.026957 -0.306980 1.155540 9 0.326616 -1.431341 0.398410 9 2.015402 -1.018278 -0.892853 16 -3.000013 -0.564130 -0.301112 1 -3.719085 0.534199 -0.591370 1 -2.365378 0.040780 0.727263	13.8664, 36.9070, 53.5079, 92.9337, 136.2438, 162.2992, 185.3213, 221.2522, 268.6021, 293.8398, 361.4009, 365.2395, 483.2266, 495.6568, 581.6967, 629.1721, 660.3300, 779.6001, 920.3828, 1158.5904, 1193.0932, 1207.0404, 1213.5979, 1399.6569, 1594.5146, 2610.1312, 2690.0168

Compound: sCI 25 + H_2S TS1	**Energy (kJ mol^{-1}):** -1024.344013062570
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.068099 -0.371050 -0.242756 6 -0.149806 0.520690 0.627818 8 0.372002 1.604912 0.291859 8 0.697364 1.725914 -1.073496 9 -0.348033 0.376851 1.912128 9 -2.176887 0.344798 -0.489359 9 -0.545925 -0.760632 -1.390633 9 -1.409574 -1.449026 0.466501 16 2.142449 -0.885776 -0.036405 1 2.851505 -0.192450 0.873466 1 1.945591 0.212507 -0.835992	-91.8475, 37.6949, 103.0268, 109.1560, 196.2418, 251.7585, 272.1509, 290.8062, 306.5540, 368.1350, 388.3813, 476.4108, 503.3478, 581.3188, 599.5715, 622.8849, 636.5919, 779.7094, 918.7570, 1129.6648, 1176.7367, 1214.0730, 1236.0744, 1354.9605, 1549.5736, 2369.6784, 2681.9410
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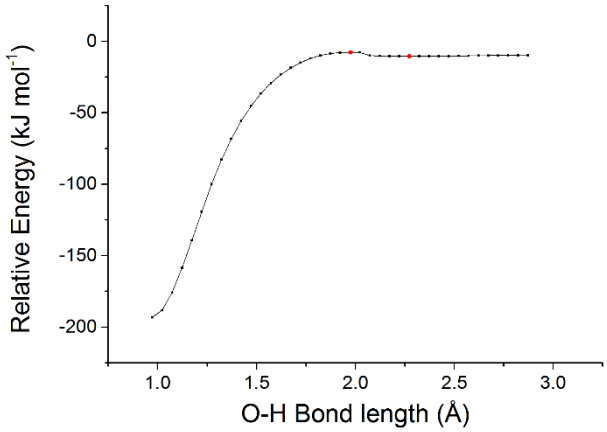

Compound: sCI 25 + H_2S Pr1	**Energy (kJ mol^{-1}):** -1024.429431015390
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.063006 -0.096610 -0.176165 6 0.364858 -0.080465 0.466586 8 0.807099 1.210387 0.789287 8 0.864917 2.002775 -0.408568 9 0.265422 -0.664548 1.686821 9 -1.843260 0.815874 0.402587 9 -1.015127 0.146435 -1.491994 9 -1.618803 -1.302127 -0.000355 16 1.534813 -1.013646 -0.610945 1 2.431715 -1.133411 0.385610 1 1.729943 1.748193 -0.772298	54.3934, 121.0861, 167.5154, 207.0012, 213.8160, 266.5950, 294.2510, 326.0987, 341.1989, 365.7182, 402.0517, 504.0054, 533.5151, 570.6240, 619.2433, 741.0527, 848.8025, 965.6506, 986.2968, 1073.9629, 1140.1976, 1183.4904, 1203.7794, 1296.0267, 1415.5088, 2674.3831, 3673.9102

Compound: sCI 25 + H_2S PRC2	**Energy (kJ mol^{-1}):** -1024.345353229650
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.290490 -0.529706 0.062238 6 0.625134 0.799092 -0.334777 8 -0.151494 1.465079 0.362419 8 -0.534378 0.958574 1.598056 9 0.948948 1.301501 -1.489789 9 2.048350 -0.347356 1.141503 9 0.386033 -1.469738 0.301393 9 2.070049 -0.927379 -0.947657 16 -3.108159 -0.396842 -0.360503 1 -2.936307 -1.694105 -0.052990 1 -2.420334 0.024770 0.723423	12.1242, 35.9569, 52.7329, 92.3689, 131.0919, 163.6602, 185.7154, 220.6224, 268.9694, 293.8148, 352.6309, 364.3246, 483.3067, 495.7094, 581.7737, 629.2548, 660.4071, 779.5938, 920.6439, 1159.0171, 1193.5348, 1206.2207, 1213.6770, 1399.8534, 1594.0341, 2612.4339, 2691.7932

Compound: sCI 25 + H_2S TS2	**Energy (kJ mol^{-1}):** -1024.343079346060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.071211 -0.363698 -0.245937 6 -0.143560 0.530370 0.609849 8 0.395490 1.605527 0.265975 8 0.765781 1.693599 -1.091961 9 -0.369535 0.414344 1.892212 9 -2.212221 0.326010 -0.415284 9 -0.596972 -0.699277 -1.430353 9 -1.348295 -1.474452 0.441689	-106.4507, 34.4170, 112.2563, 116.6783, 198.6133, 249.1393, 270.2184, 276.6378, 290.3873, 369.0565, 394.2326, 476.6437, 508.8478, 581.8044, 606.0935, 631.4851, 641.8063, 780.1505, 918.8704, 1125.8058, 1174.7524,

16 2.182199 -0.810150 0.100843 1 1.863614 -1.755094 -0.800983 1 1.962861 0.224832 -0.782456	1218.2103, 1239.2021, 1353.1718, 1543.8164, 2316.0817, 2695.1504

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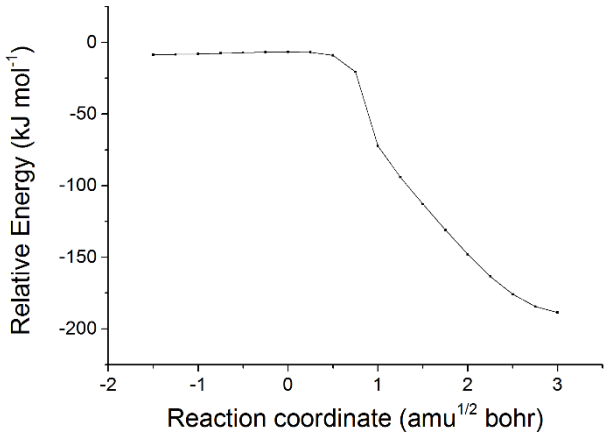

Compound: sCI 25 + H_2S Pr2	**Energy (kJ mol^{-1}):** -1024.428919132390
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.106304 0.072990 -0.218224 6 0.285982 -0.089087 0.463772 8 0.862223 1.170956 0.686912 8 1.642238 1.563219 -0.463465 1 2.518795 1.636667 -0.056694 9 0.033549 -0.561191 1.715421 16 1.413265 -1.206650 -0.455943 1 0.747460 -2.301924 -0.046329 9 -1.901340 0.848771 0.527851 9 -0.982485 0.632823 -1.423831 9 -1.704417 -1.120976 -0.359747	57.2635, 70.9939, 175.7844, 201.2701, 214.0455, 240.9941, 300.2199, 308.2382, 339.6347, 369.4160, 400.5555, 502.7278, 530.9276, 585.2028, 602.8116, 736.3936, 886.0484, 946.5138, 983.6877, 1100.7233, 1134.3376, 1177.3711, 1198.8231, 1281.0401, 1405.6513, 2679.1684, 3732.9729

8.8.5 sCI 26 + H_2S

Compound: sCI 26 + H_2S PRC1	**Energy (kJ mol^{-1}):** -1024.352019623190
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.497901 -0.354035 0.113257 6 0.326787 0.557329 -0.235223 9 -0.019078 0.609081 -1.476740 8 -0.193080 1.273361 0.636115 8 -1.239250 2.096406 0.275803 9 2.611061 0.116300 -0.469978 9 1.680445 -0.398850 1.426610 9 1.270769 -1.583402 -0.350508 16 -2.739843 -0.999585 -0.011305 1 -2.696080 0.342916 0.141142 1 -2.844680 -1.215609 1.311733	24.1450, 33.1121, 65.0647, 98.5150, 140.2987, 166.9719, 185.3141, 197.8389, 294.3611, 326.7809, 360.0382, 382.8149, 406.7516, 511.8452, 576.5956, 655.5405, 728.7778, 856.9027, 892.9799, 1146.7193, 1172.6328, 1209.1424, 1230.9405, 1399.6934, 1611.3284, 2609.0297, 2689.4607

Compound: sCI 26 + H_2S TS1	**Energy (kJ mol^{-1}):** -1024.345922619310
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.336779 -0.162720 -0.101569 6 -0.019006 0.479715 0.216224	-212.8655, 41.9183, 92.7584, 169.9711, 177.8020, 214.1780,

8 -0.515172 1.245306 -0.649683 8 -1.802057 1.722392 -0.318134 9 -0.263186 0.631311 1.489973 9 1.395870 -0.518762 -1.382031 9 1.531605 -1.232089 0.666795 9 2.316371 0.720581 0.146452 16 -1.882243 -1.286634 0.014244 1 -2.329438 0.029629 -0.155333 1 -1.749424 -1.496399 -1.308676	286.9091, 319.6417, 355.8809, 364.4907, 404.7532, 463.5875, 507.2484, 576.2040, 629.5656, 721.3812, 762.2249, 829.4224, 881.0242, 1129.7304, 1178.1249, 1207.3719, 1225.3137, 1358.6645, 1530.2690, 2071.9114, 2682.1682

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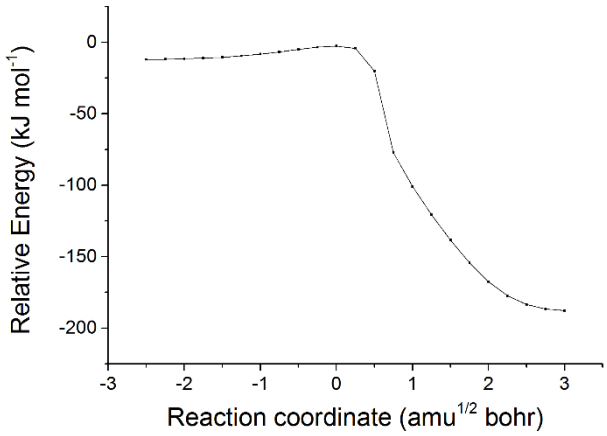

Compound: sCl 26 + H_2S Pr1	**Energy (kJ mol^{-1}):** -1024.433159728430
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.200903 -0.095266 -0.099958 6 0.326675 -0.089049 0.223901 8 0.843690 -1.117581 -0.540345 8 2.245704 -1.284167 -0.257708 9 0.464397 -0.342426 1.555653 9 -1.413293 0.221313 -1.387446 9 -1.725040 -1.300860 0.129524 9 -1.837661 0.792828 0.664830 16 1.114990 1.556337 -0.055220 1 0.651037 1.684950 -1.311783 1 2.643713 -0.604157 -0.826976	66.2156, 137.0343, 156.8050, 176.9816, 200.0302, 245.6916, 278.2893, 295.7701, 347.7871, 367.4199, 411.0122, 439.2158, 545.3320, 571.0266, 694.6552, 738.6398, 887.3473, 938.7696, 993.2027, 1069.6573, 1123.6025, 1182.6165, 1203.6161, 1282.2079, 1414.9629, 2679.6380, 3680.8781
Compound: sCl 24 + H_2S PRC2	**Energy (kJ mol^{-1}):** -1024.352020666000
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.489163 -0.357160 -0.112118 6 -0.325648 0.564108 0.235950 9 0.005099 0.635842 1.480987 8 0.200272 1.270865 -0.639145 8 1.238752 2.103600 -0.278495 9 -2.612149 0.122593 0.444942 9 -1.651870 -0.429464 -1.426202 9 -1.266596 -1.575910 0.381370 16 2.710350 -1.019175 -0.143759 1 2.696623 0.331667 -0.190098 1 3.044108 -1.039826 1.158502	24.7913, 33.7033, 65.0276, 97.7672, 141.4668, 166.3063, 186.3025, 196.5192, 293.6860, 323.5083, 358.0252, 379.9072, 406.7070, 511.7565, 576.6243, 655.0017, 728.6802, 856.4586, 892.6362, 1145.3146, 1172.1473, 1210.5034, 1232.6576, 1399.1867, 1611.2523, 2611.1316, 2690.4468
Compound: sCl 26 + H_2S TS2	**Energy (kJ mol^{-1}):** -1024.345712139260
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 1.337645 -0.163068 -0.103782 6 -0.018713 0.475773 0.220019 8 -0.507990 1.263483 -0.629415 8 -1.797439 1.732071 -0.294004 9 -0.268582 0.597141 1.496683 9 1.413666 -0.473263 -1.392902 9 1.515718 -1.259729 0.631286 9 2.317632 0.705926 0.191884 16 -1.859989 -1.285882 -0.160405 1 -2.322831 0.034760 -0.220607 1 -2.193410 -1.431987 1.134461	-214.3248, 43.9396, 94.7246, 172.0993, 177.1296, 218.7101, 287.8239, 316.2546, 346.1578, 363.8654, 405.7866, 461.7908, 513.6250, 576.1385, 630.2736, 720.9692, 758.5877, 828.0010, 879.3764, 1128.0337, 1176.9447, 1213.5395, 1228.9550, 1357.9335, 1531.4213, 2070.7635, 2687.8493

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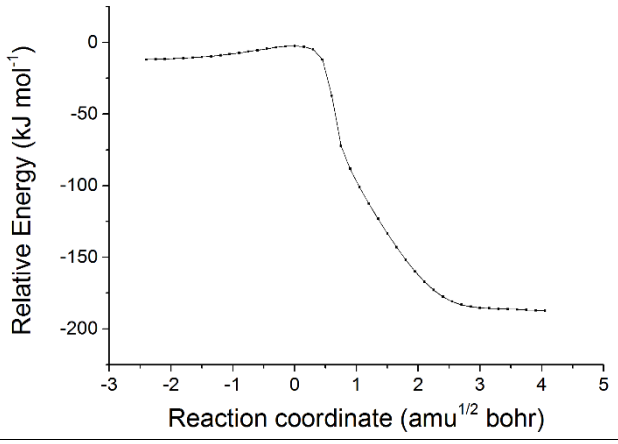

Compound: sCl 26 + H_2S Pr2	**Energy (kJ mol^{-1}):** -1024.433112228060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.202362 -0.089113 -0.109268 6 0.318048 -0.089101 0.243524 8 0.827351 -1.177761 -0.442171 8 2.255224 -1.241345 -0.260519 9 0.431335 -0.281065 1.592046 9 -1.379704 0.255548 -1.393450 9 -1.735591 -1.297017 0.084936 9 -1.853762 0.786093 0.658312 16 1.058272 1.538292 -0.208423 1 1.989300 1.468211 0.758434 1 2.563125 -0.830796 -1.084279	60.9853, 112.5120, 142.6837, 171.9181, 186.3778, 257.8669, 279.9189, 301.2905, 349.5684, 369.4286, 417.1116, 449.7881, 543.9532, 571.0201, 686.0786, 737.2994, 855.3090, 942.0929, 999.5997, 1067.2588, 1100.2573, 1187.4977, 1204.3373, 1292.5349, 1408.4410, 2689.6565, 3708.1167

8.9 Reactions with H_2O

Compound:	H_2O	**Energy (kJ mol^{-1}):**	-76.372669648641
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
8 -0.000000 -0.000000 0.116992 1 -0.000000 0.763520 -0.467967 1 -0.000000 -0.763520 -0.467967		1626.9293, 3796.3639, 3899.0961	

8.9.1 sCI 1 + H_2O

Compound:	sCI 1 + H_2O PRC	**Energy (kJ mol^{-1}):**	-265.786257491251
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
8 0.357047 -1.171861 -0.000014 8 1.289920 -0.173564 0.000019 6 0.924903 1.024191 -0.000004 1 -0.129754 1.281859 -0.000044 1 1.739280 1.736480 0.000025 8 -2.012469 0.273086 -0.000021 1 -1.353128 -0.449947 -0.000007 1 -2.881795 -0.134832 0.000186		21.8780, 75.7289, 148.6369, 209.9306, 493.6039, 549.1761, 629.7151, 691.8102, 881.1881, 1017.5999, 1272.0176, 1429.7599, 1558.0952, 1645.6134, 3091.7849, 3248.5013, 3499.8200, 3871.1216	

Compound:	sCI 1 + H_2O TS1	**Energy (kJ mol^{-1}):**	-265.772122072372
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
8 -0.950605 -0.946963 0.167769 8 -0.886084 0.399108 -0.376202 6 0.046206 0.999114 0.246331 1 0.186984 0.820730 1.304039 1 0.394195 1.921099 -0.209200 8 1.446354 -0.374579 -0.005867 1 0.557419 -0.948603 0.076115 1 1.706835 -0.408441 -0.934541		-433.3116, 326.5769, 426.8495, 531.9388, 597.5414, 656.1524, 809.2086, 899.0486, 1157.5178, 1211.4121, 1251.2657, 1392.4448, 1546.5882, 1605.7472, 2196.2030, 3103.8784, 3225.5749, 3798.4004	

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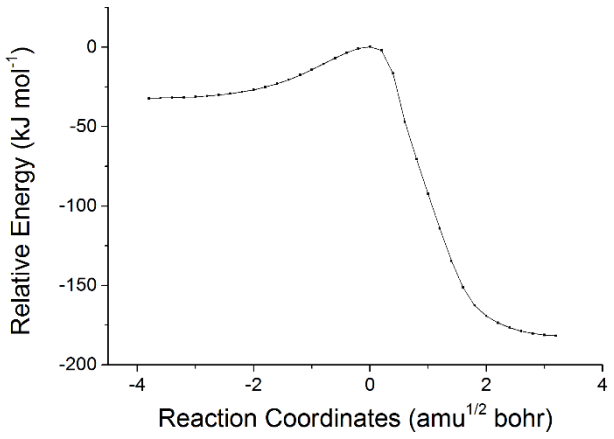

Compound:	sCl 1 + H_2O Pr1	**Energy (kJ mol^{-1}):**	-265.849083661745

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.613216 0.542122 0.285606 8 1.381072 -0.594495 -0.014848 8 -0.614068 0.578422 -0.401400 8 -1.485958 -0.421022 0.182400 1 0.443979 0.526639 1.360537 1 1.100746 1.469391 -0.028131 1 -1.183095 -1.228893 -0.258159 1 1.710703 -0.523108 -0.917100	159.0267, 283.2184, 374.4906, 424.9952, 616.1269, 877.8835, 1010.2947, 1032.0533, 1068.5203, 1276.8372, 1369.8581, 1382.2124, 1414.7043, 1484.3437, 3030.0864, 3111.6326, 3728.0279, 3798.4265

Compound:	sCl 1 + H_2O TS2	**Energy (kJ mol^{-1}):**	-265.770736044301

Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 0.934736 -0.958068 0.182645 8 0.902650 0.394968 -0.348596 6 -0.043467 0.997720 0.247728 1 -0.205224 0.815507 1.302611 1 -0.372999 1.921901 -0.214833 8 -1.412711 -0.344459 -0.213952 1 -0.543987 -0.941192 -0.052972 1 -2.014398 -0.522066 0.518046	-455.6181, 348.7363, 410.1920, 526.9050, 613.2280, 689.4603, 815.0326, 880.2699, 1126.8327, 1206.7266, 1219.8467, 1386.7034, 1527.2808, 1634.3676, 2149.3718, 3103.4468, 3222.4555, 3813.0408

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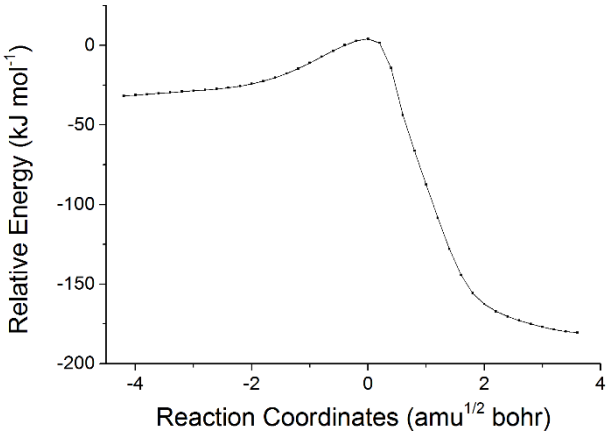

Compound:	sCl 1 + H_2O Pr2	**Energy (kJ mol^{-1}):**	-265.848846609638

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.647196 0.538648 0.261567 8 0.625293 0.629426 -0.338740 8 1.425464 -0.454794 0.213290 1 1.601714 -0.966752 -0.587818 1 -0.529616 0.517625 1.347966 1 -1.138554 1.456034 -0.061035 8 -1.414034 -0.537971 -0.192946 1 -1.144148 -1.332081 0.278647	167.4320, 205.9488, 363.0291, 433.1822, 606.0638, 871.9321, 998.8296, 1044.5819, 1074.2590, 1272.8836, 1372.2326, 1384.1981, 1412.5021, 1484.6978, 3025.6587, 3107.6286, 3758.6628, 3815.8683

8.9.2 sCI 23 + H_2O

Compound: sCI 23 + H_2O PRC	**Energy (kJ mol^{-1}):** -602.585302654489
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.418122 -0.035776 -0.000003 6 0.319563 1.008948 -0.000001 8 -0.904792 0.737430 0.000011 8 -1.312365 -0.546032 0.000023 1 0.561195 2.062640 -0.000010 9 1.370649 -0.806322 1.087881 9 1.370633 -0.806333 -1.087879 9 2.594145 0.620050 -0.000015 8 -4.162630 0.061529 -0.000005 1 -4.718098 -0.722268 -0.000085 1 -3.249743 -0.269386 0.000006	12.9685, 28.0322, 34.6398, 84.0523, 109.5999, 211.6467, 247.2163, 334.3561, 375.5031, 479.5982, 510.8715, 534.4531, 536.6024, 591.4602, 759.7032, 800.6129, 884.1656, 931.3447, 1157.2991, 1183.4831, 1242.5624, 1368.6752, 1557.3767, 1658.4346, 3213.8618, 3648.1189, 3869.8220

Compound: sCI 23 + H_2O TS1	**Energy (kJ mol^{-1}):** -602.571519549324
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.880942 -0.040291 0.035680 6 0.374737 -0.063934 -0.855948 8 1.370730 -0.828340 -0.705354 8 1.782336 -0.820106 0.676516 1 0.161124 0.207677 -1.886552 9 -1.469403 -1.243069 -0.117446 9 -0.724983 0.193086 1.324767 9 -1.712041 0.890310 -0.469775 8 1.168700 1.545355 0.045488 1 1.846465 1.896020 -0.545448 1 1.613361 0.783438 0.582497	-335.6905, 48.6609, 176.1151, 213.7137, 280.4627, 322.3603, 348.6340, 448.8651, 514.6696, 537.3357, 550.1125, 572.5144, 667.5975, 744.2436, 808.1946, 872.6150, 993.2852, 1139.3767, 1148.0772, 1195.9793, 1292.0680, 1346.8227, 1554.7138, 1616.4176, 2586.7975, 3144.4219, 3801.2117

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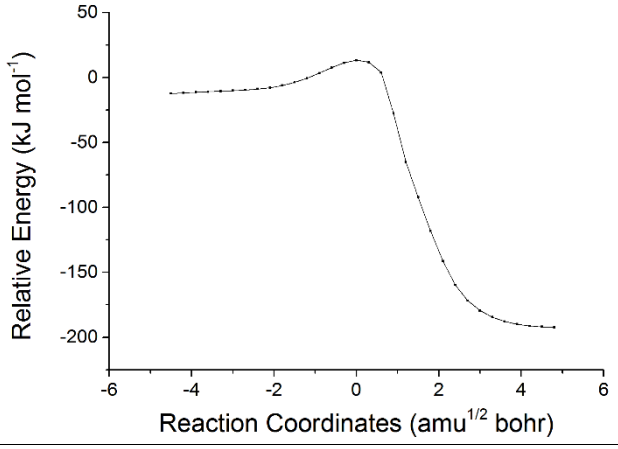
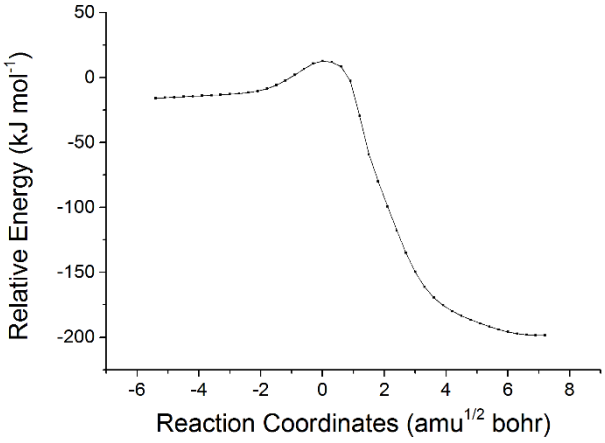


Compound: sCI 23 + H_2O Pr1	**Energy (kJ mol^{-1}):** -602.660056059595
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.840616 -0.134696 0.006007 6 0.411407 0.581582 -0.551944 8 1.505490 -0.266093 -0.775674 8 1.864918 -0.931170 0.458894 1 0.162315 0.911744 -1.564471 9 -1.020367 -1.310094 -0.610249 9 -0.798843 -0.344692 1.322507	64.6652, 135.2115, 205.5945, 222.1310, 272.2757, 294.3622, 343.4660, 378.4008, 436.4043, 525.6920, 583.1678, 617.3587, 763.2320, 842.4769, 902.3706, 1043.7056, 1097.6907, 1131.6755, 1170.8830, 1236.4595, 1291.7286,

9 -1.922869 0.632033 -0.251339 8 0.694373 1.640349 0.310457 1 1.185863 2.316989 -0.166310 1 2.387533 -0.249960 0.908728	1366.8442, 1389.1393, 1442.1396, 3049.9342, 3723.7563, 3812.8925

Compound: sCI 23 + H_2O TS2	**Energy (kJ mol^{-1}):** -602.571987979725
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.872000 -0.055866 0.026501 6 0.388125 -0.059725 -0.862867 8 1.376054 -0.829330 -0.693386 8 1.752043 -0.797944 0.701867 1 0.188509 0.212024 -1.895001 9 -1.361524 -1.300237 0.049360 9 -0.744726 0.376239 1.278093 9 -1.777175 0.740324 -0.583722 8 1.278925 1.534698 -0.102153 1 0.727023 2.081282 0.470334 1 1.682365 0.793917 0.498653	-353.5599, 32.7498, 178.7265, 213.7614, 289.5076, 323.6146, 366.4348, 447.5482, 507.7217, 533.8073, 567.4192, 588.3382, 709.5027, 739.4606, 811.9352, 864.6585, 1000.0724, 1111.6344, 1160.0164, 1190.1058, 1257.9738, 1345.9494, 1542.6598, 1655.3576, 2544.8281, 3157.6649, 3805.1193
IRC  	

Compound: sCI 23 + H_2O Pr2	**Energy (kJ mol^{-1}):** -602.658023397310
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.841050 -0.157441 0.010445 6 0.405739 0.532657 -0.593230 8 1.494897 -0.309691 -0.777127 8 1.946041 -0.824612 0.499873 1 0.139028 0.801180 -1.622219 9 -1.170039 -1.245554 -0.691500 9 -0.722055 -0.493929 1.295152 9 -1.878208 0.721576 -0.076130 8 0.792725 1.643641 0.164788 1 0.020802 2.136425 0.465070 1 2.515462 -0.102443 0.805901	45.8073, 137.2188, 149.7556, 211.4607, 231.3373, 267.9918, 313.5215, 368.2515, 437.2812, 520.0905, 583.4169, 618.8499, 755.5434, 854.2256, 905.1872, 1039.2504, 1097.6375, 1127.1441, 1192.6499, 1236.5467, 1296.0157, 1351.6378, 1398.2769, 1425.9067, 3020.2585, 3727.7188, 3803.4861

8.9.3 sCI 24 + H_2O

Compound: sCI 24 + H_2O PRC	**Energy (kJ mol^{-1}):** -602.589934294451
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.265134 0.155609 -0.000000 6 -0.238467 0.008675 0.000003 8 -0.691074 -1.158101 -0.000001 8 -2.031785 -1.370658 0.000001 1 -0.897012 0.874551 0.000007 9 1.644005 0.852596 1.085581 9 1.897770 -1.014649 -0.000008 9 1.644000 0.852607 -1.085576 8 -2.920854 1.280203 0.000006 1 -3.823997 1.606901 -0.000046 1 -2.961273 0.306298 -0.000000	18.9310, 29.3495, 78.1991, 106.2923, 155.7969, 203.6063, 225.9814, 381.2152, 394.8102, 416.6995, 467.3076, 556.2957, 557.9028, 579.8286, 700.0094, 892.9234, 942.1189, 959.7400, 1141.7667, 1183.2773, 1280.4930, 1388.8948, 1556.7441, 1626.8972, 3124.7371, 3577.8101, 3872.5923

Compound: sCI 24 + H_2O TS1	**Energy (kJ mol^{-1}):** -602.577917489654
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.039070 -0.051694 -0.022089 6 -0.419427 -0.182932 -0.448222 8 -1.146757 -0.949377 0.249124 8 -2.521237 -0.668508 -0.120692 1 -0.665573 0.023250 -1.482782 9 1.617879 0.945434 -0.698388 9 1.153163 0.194419 1.287084 9 1.694390 -1.188659 -0.300101 8 -1.326421 1.520273 -0.024545 1 -1.163554 1.758943 0.897664 1 -2.122302 0.845713 -0.021481	-344.2658, 39.3846, 140.2218, 175.5019, 268.4806, 340.7036, 381.7182, 433.9197, 491.8150, 551.9982, 564.2127, 603.5697, 674.9171, 717.4654, 848.3778, 884.9556, 1079.4615, 1171.3551, 1184.0130, 1221.8795, 1258.0253, 1343.7326, 1536.7055, 1608.3451, 2435.5100, 3172.2175, 3783.6617

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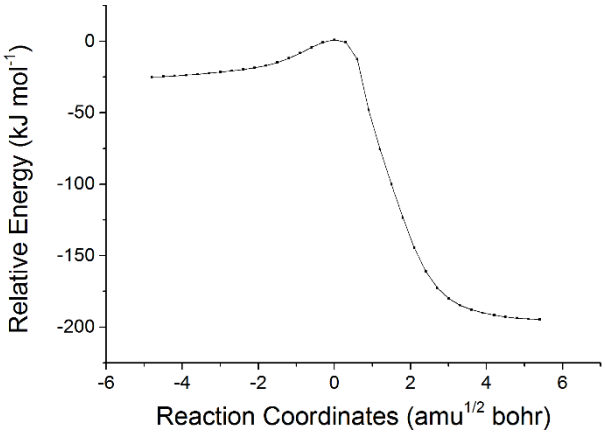

Compound: sCI 24 + H_2O Pr1	**Energy (kJ mol^{-1}):** -602.662813970698
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.963295 -0.146555 -0.034177 6 0.480869 0.288837 -0.359532 8 1.306945 -0.586625 0.368263 8 2.626042 -0.522137 -0.216993 1 0.654164 0.172304 -1.428349 9 -1.168282 -1.440472 -0.294445	66.6299, 105.1886, 185.4932, 233.3104, 264.2291, 352.9867, 355.6744, 385.5909, 428.9955, 519.5011, 563.7230, 626.6447, 712.4712, 857.8522, 949.6848, 1040.3403, 1088.3219, 1151.0923,

9 -1.249598 0.074900 1.266542 9 -1.829589 0.568705 -0.767756 8 0.691587 1.629400 -0.052602 1 0.435506 1.791110 0.864764 1 3.035510 0.189595 0.297415	1194.1080, 1250.6670, 1293.5017, 1361.2445, 1390.1415, 1437.9011, 3102.6609, 3728.9304, 3764.5581

Compound: sCI 24 + H_2O TS2	**Energy (kJ mol^{-1}):** -602.576912007240
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.039856 -0.049677 -0.010843 6 0.419539 -0.170430 -0.434149 8 1.150764 -0.956828 0.233990 8 2.523335 -0.666412 -0.143361 1 0.657816 0.049055 -1.468419 9 -1.552721 1.085282 -0.508187 9 -1.729827 -1.080080 -0.533333 9 -1.194383 -0.057248 1.306915 8 1.306977 1.471994 0.180893 1 1.388018 2.132416 -0.517541 1 2.119841 0.817564 0.095175	-364.8804, 52.2464, 143.0267, 175.9772, 274.1325, 343.0331, 381.2444, 435.7241, 478.2902, 553.8646, 583.4874, 590.5433, 694.4015, 732.1931, 850.8644, 881.0498, 1063.1370, 1153.9872, 1161.0462, 1190.5992, 1280.3717, 1337.8593, 1529.0559, 1631.0497, 2387.3409, 3161.7624, 3808.2251

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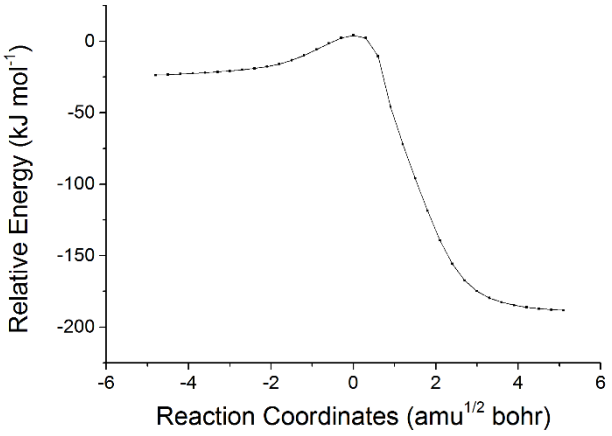

Compound: sCI 24 + H_2O Pr2	**Energy (kJ mol^{-1}):** -602.660922289812
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.977653 -0.122020 -0.020540 6 0.472388 0.292316 -0.339887 8 1.280676 -0.678073 0.280541 8 2.623938 -0.461809 -0.218113 1 0.609833 0.242347 -1.422859 9 -1.229129 -1.358117 -0.477948 9 -1.232482 -0.098538 1.291950 9 -1.828074 0.720918 -0.628725 8 0.676183 1.576208 0.153493 1 1.316213 2.032740 -0.399749 1 3.066331 -0.165837 0.590302	67.1172, 105.0116, 130.0950, 184.4267, 243.6539, 324.8792, 345.4993, 359.5577, 404.8713, 522.4187, 565.5794, 632.5000, 706.2299, 854.7571, 950.9452, 1050.2587, 1103.0362, 1142.7893, 1177.1310, 1242.9134, 1283.6311, 1354.4268, 1388.8170, 1458.0452, 3049.1963, 3747.1703, 3833.6975

8.9.4 sCI 25 + H_2O

Compound: sCI 25 + H_2O PRC1	**Energy (kJ mol^{-1}):** -701.757032802282
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.967467 -0.448045 -0.009361 6 0.154124 0.861668 -0.039692 8 -0.853476 1.115458 0.628635 8 -1.371797 0.108216 1.448886 9 0.598175 1.811820 -0.805522 9 1.460108 -0.630382 1.215244 9 0.228312 -1.484773 -0.360912 9 1.985779 -0.325431 -0.866525 8 -2.659392 -0.685120 -0.979841 1 -3.601914 -0.543870 -1.101342 1 -2.501686 -0.587409 -0.026351	8.9142, 50.9829, 56.8709, 125.1006, 160.5746, 181.1844, 225.8585, 279.1395, 292.2263, 336.4398, 363.7598, 481.9951, 500.3346, 573.4040, 583.7145, 626.9831, 674.6696, 778.6339, 914.2553, 1156.3613, 1190.7739, 1224.5363, 1401.3945, 1608.7930, 1641.3966, 3642.7446, 3869.6071

Compound: sCI 25 + H_2O TS1	**Energy (kJ mol^{-1}):** -701.754722973199
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.922876 -0.252529 0.014628 6 0.362255 0.565884 -0.294872 8 1.349650 0.211899 -0.976788 8 1.789010 -1.121052 -0.588485 9 0.114206 1.848404 -0.318084 9 -1.590196 -0.321598 -1.153003 9 -0.722079 -1.470293 0.466790 9 -1.669098 0.426961 0.885625 8 1.193811 0.106194 1.564075 1 1.851343 0.781472 1.770174 1 1.657121 -0.589197 0.988920	-182.9477, 43.9809, 165.4231, 198.8283, 243.5936, 262.9655, 302.4476, 351.3823, 371.3221, 477.0843, 499.7850, 525.3643, 565.6404, 605.5389, 625.5149, 679.1056, 780.3852, 887.6970, 1089.4681, 1123.5063, 1179.4890, 1256.3551, 1357.2587, 1570.7234, 1615.7012, 2887.0314, 3807.7211

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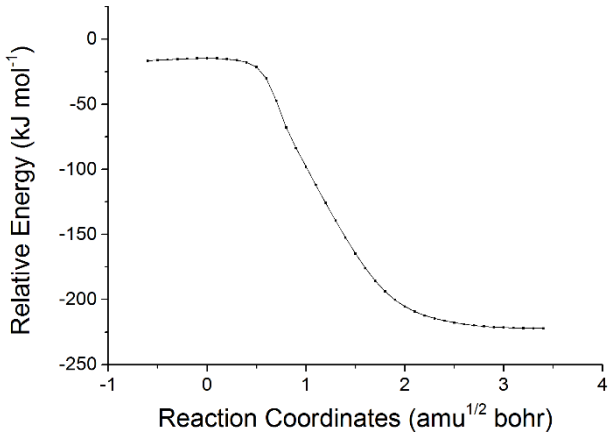


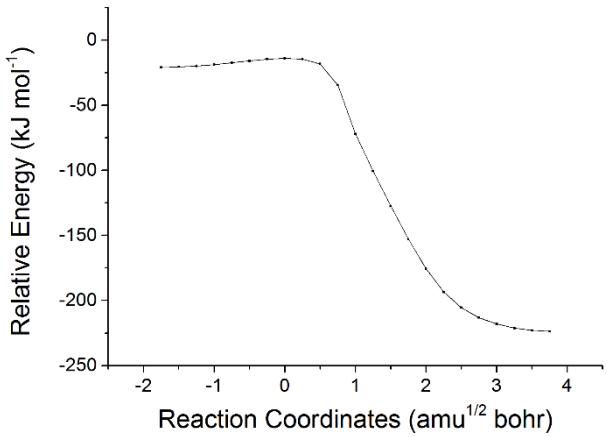
Compound: sCI 25 + H_2O Pr1	**Energy (kJ mol^{-1}):** -701.845677031827
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.889789 -0.270159 -0.010129 6 -0.431897 0.565724 -0.011041 8 -1.498264 -0.049484 0.670262 8 -1.771437 -1.321015 0.048761 9 -0.220327 1.671207 0.757854 9 1.087753 -0.810191 1.194456 9 0.872008 -1.241878 -0.923082 9 1.921381 0.540493 -0.285449	51.9068, 129.7086, 196.6813, 208.7458, 233.2065, 285.1346, 323.0522, 346.4562, 381.7148, 419.7601, 492.7066, 538.4071, 588.2672, 653.1779, 672.0489, 781.1123, 972.7409, 1033.4888, 1094.4151, 1182.9092, 1202.5091,

8 -0.714328 0.904974 -1.300334 1 -1.390579 1.595805 -1.297851 1 -2.431879 -1.081688 -0.618650	1207.0919, 1232.2767, 1402.9368, 1432.4007, 3728.7382, 3765.6990

Compound: sCI 25 + H_2O PRC2	**Energy (kJ mol^{-1}):** -701.757770997730
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.977575 -0.375535 -0.047959 6 0.014302 0.825274 0.048720 8 -0.967734 0.922922 0.791449 8 -1.354925 -0.209247 1.516763 9 0.320286 1.874211 -0.652500 9 1.562304 -0.551250 1.138425 9 0.366719 -1.487941 -0.415148 9 1.920185 -0.080620 -0.948960 8 -2.458473 -0.520975 -1.109929 1 -2.795570 -1.317291 -1.528523 1 -2.432075 -0.712349 -0.158653	22.4289, 55.7258, 71.6779, 148.8436, 161.0054, 182.5709, 232.8751, 282.2735, 294.0666, 364.2100, 373.9421, 478.9771, 500.5261, 510.9374, 581.3517, 626.6840, , 671.8741, 778.5441, 913.6810, 1155.7015, 1186.0906, 1223.3890, 1399.8811, 1611.1781, 1643.5507, 3661.4245, 3872.2454

Compound: sCI 25 + H_2O TS2	**Energy (kJ mol^{-1}):** -701.754639690128
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.917298 -0.252424 -0.015764 6 0.371649 0.577981 -0.264789 8 1.364908 0.247768 -0.952222 8 1.799098 -1.098137 -0.590989 9 0.113971 1.855245 -0.249161 9 -1.583242 -0.275303 -1.178912 9 -0.722470 -1.491868 0.394882 9 -1.667441 0.384204 0.892193 8 1.278018 0.176684 1.517952 1 0.761571 -0.259947 2.205324 1 1.708783 -0.554405 0.949053	-224.4680, 28.2180, 165.0634, 199.2546, 254.2594, 262.0571, 307.3955, 357.3279, 373.8725, 477.9454, 515.0983, 551.0126, 567.1130, 602.8137, 611.6785, 727.2799, 786.6461, 895.3756, 1061.2898, 1139.5150, 1176.2030, 1240.2368, 1354.8576, 1556.1705, 1650.3191, 2770.0033, 3814.6039

IRC



Compound: sCI 25 + H_2O Pr2	**Energy (kJ mol^{-1}):** -701.845674474457
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.888438 -0.308532 -0.010458 6 0.410990 0.559492 0.002560 8 1.463801 0.006090 -0.725260 8 1.980769 -1.149354 -0.036166	46.9670, 131.6299, 205.9108, 226.8588, 245.4856, 290.8668, 306.3950, 347.6743, 377.9855, 414.5608, 484.6199, 529.2277,

9 0.109977 1.683447 -0.712380 9 -1.317669 -0.516289 -1.252096 9 -0.715606 -1.485877 0.590294 9 -1.851494 0.359527 0.669975 8 0.819587 0.863153 1.266749 1 0.065762 1.113776 1.815604 1 2.658803 -0.745908 0.527062	590.4181, 642.2163, 692.5148, 784.1847, 968.1183, 1044.0527, 1092.7799, 1158.1546, 1195.9693, 1221.8558, 1289.7655, 1378.5484, 1419.4410, 3725.9129, 3782.9088

8.9.5 sCI 26 + H_2O

Compound: sCI 26 + H_2O PRC1	**Energy (kJ mol^{-1}):** -701.764103446066
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.253199 0.089592 0.115211 6 -0.153286 -0.368008 -0.261044 8 -0.872970 -0.931109 0.575069 8 -2.156873 -1.298958 0.195285 9 -0.507050 -0.188673 -1.485279 9 1.402006 1.379556 -0.186073 9 1.477454 -0.097338 1.407847 9 2.147090 -0.615696 -0.594844 8 -2.203577 1.547561 0.297113 1 -2.753188 2.142143 -0.220012 1 -2.654432 0.687754 0.280419	32.7360, 46.8598, 92.4712, 157.7812, 179.9572, 181.7624, 189.5062, 294.9945, 332.2552, 361.8550, 371.8605, 406.9222, 515.8260, 532.4507, 576.6471, 676.3573, 728.5135, 858.4915, 876.1783, 1149.8613, 1173.9584, 1235.9757, 1403.0899, 1628.8278, 1641.2467, 3658.9141, 3871.8932

Compound: sCI 26 + H_2O TS1	**Energy (kJ mol^{-1}):** -701.756908629529
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.126733 -0.047615 -0.093143 6 0.367795 -0.221556 0.235940 8 1.063441 -0.897170 -0.559318 8 2.478562 -0.642997 -0.295352 9 0.643596 -0.130985 1.504069 9 -1.657265 0.907431 0.663875 9 -1.279619 0.274686 -1.378264 9 -1.769314 -1.197000 0.143966 8 1.217696 1.555346 -0.143389 1 1.005306 1.861075 -1.034714 1 2.034135 0.945334 -0.240420	-292.2117, 38.7233, 137.0646, 175.9347, 252.9241, 290.7045, 310.8719, 365.5904, 388.1022, 418.6521, 507.5719, 527.4436, 574.7313, 656.1128, 696.2299, 726.4874, 809.6219, 845.9113, 1123.2579, 1160.3658, 1191.9307, 1222.6289, 1369.5290, 1563.9859, 1622.8314, 2744.9152, 3792.4031

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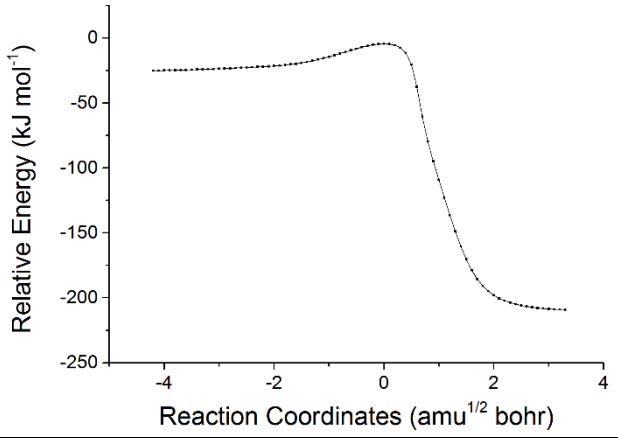

Compound: sCI 26 + H_2O Pr1	**Energy (kJ mol^{-1}):** -701.845741873404
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.062154 -0.164450 0.008092 6 0.430105 0.300164 -0.048891 8 1.168471 -0.873619 0.086297 8 2.569482 -0.553850 -0.039440 9 0.649193 0.876050 -1.249055 9 -1.314131 -1.157639 -0.839044 9 -1.351761 -0.581518 1.259980	62.5858, 126.1553, 156.3520, 187.5452, 228.7942, 295.2365, 316.7880, 342.0580, 377.0116, 393.9381, 521.8175, 530.1352, 587.2667, 609.4954, 733.9792, 831.8169, 943.4958, 1051.7784, 1091.0788, 1157.7878, 1177.4707,

9 -1.864993 0.861751 -0.279192 8 0.705758 1.255653 0.899749 1 0.356738 0.972335 1.754092 1 2.821091 -0.399880 0.883653	1219.1982, 1284.5333, 1384.6587, 1403.4261, 3729.2527, 3786.2786

Compound: sCI 26 + H_2O TS2	**Energy (kJ mol^{-1}):** -701.757550624596
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.127586 -0.061446 -0.098574 6 -0.368149 -0.185799 0.245111 8 -1.066102 -0.970698 -0.432758 8 -2.481840 -0.695167 -0.198366 9 -0.636159 0.097016 1.495767 9 1.600071 1.101582 0.352276 9 1.794427 -1.054918 0.506831 9 1.320420 -0.142869 -1.406306 8 -1.193324 1.473055 -0.506932 1 -1.313450 2.140834 0.178902 1 -2.021883 0.877816 -0.490794	-294.5242, 49.7277, 138.2138, 175.5823, 256.1652, 276.7056, 308.7521, 363.4740, 390.8796, 419.0342, 512.6498, 542.4217, 576.1978, 644.9694, 692.3609, 722.8270, 805.8408, 845.4312, 1078.8819, 1142.1180.9943, 1236.9997, 1357.9910, A, 1561.3891, 1646.0271, 2797.5934, 3809.6964

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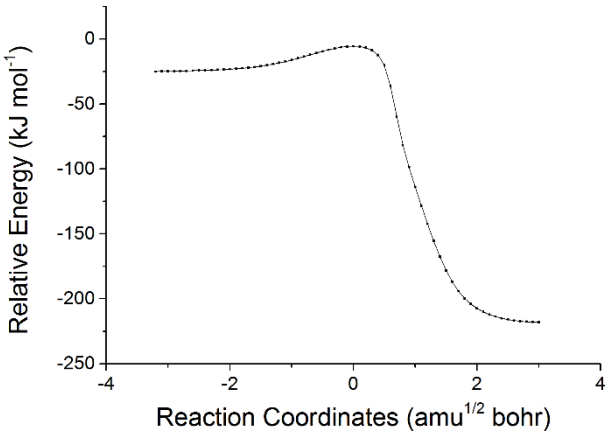

Compound: sCI 26 + H_2O Pr2	**Energy (kJ mol^{-1}):** -701.848967983056
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.061640 -0.178518 0.026237 6 0.433844 0.274899 -0.021704 8 1.170177 -0.885298 -0.006673 8 2.574014 -0.556023 -0.067483 9 0.594253 0.968979 -1.194790 9 -1.393384 -0.902540 -1.041940 9 -1.309837 -0.892268 1.126667 9 -1.837660 0.920355 0.053817 8 0.763942 1.076495 1.038769 1 0.429834 1.968970 0.887611 1 2.791526 -0.479383 0.874497	67.4708, 125.8551, 166.0025, 224.1819, 237.1201, 253.3577, 306.5786, 340.7011, 375.3352, 389.2286, 520.6247, 526.0073, 586.7124, 605.7663, 733.6858, 829.3280, 939.0000, 1044.0602, 1068.6489, 1176.7477, 1183.4267, 1211.4081, 1330.7134, 1346.9850, 1414.6427, 3722.6833, 3796.5626

7.10 sCI Reactions with $(H_2O)_2$

Compound: $(H_2O)_2$	**Energy (kJ mol^{-1}):** -152.753039538317
Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 -1.516947 0.000002 -0.121143 1 -1.926876 -0.000012 0.747807 1 -0.561489 -0.000002 0.044554 8 1.391185 -0.000002 0.109911 1 1.747231 -0.766159 -0.351264 1 1.747228 0.766171 -0.351242	136.9386, 159.6379, 161.0494, 190.5114, 364.4335, 626.4275, 1628.1114, ,1647.2164, 3675.9138, 3791.8236, 3871.0307, 3890.8064

8.10.1 sCI 1 + $(H_2O)_2$

Compound: sCI 1 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -342.172906791257
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.941512 -1.103855 0.343798 8 -1.411547 -0.220247 -0.397069 8 -1.297519 1.104921 0.041057 1 -0.528363 -0.842561 1.308425 1 -1.044879 -2.119710 -0.010485 8 1.374142 1.413463 0.128117 1 0.383318 1.436018 0.084927 1 1.688347 2.087966 -0.479194 8 1.534375 -1.298054 -0.030337 1 1.664081 -0.321597 -0.036516 1 1.890960 -1.617648 -0.864079	34.7620, 92.3912, 128.1685, 229.3716, 245.7725, 251.4917, 264.5672, 292.4871, 435.7695, 509.2517, 527.9532, 708.4598, 757.5050, 820.9549, 928.0187, 1050.4965, 1233.0677, 1420.8772, 1585.0220, 1657.2334, 1667.4210, 3135.5422, 3229.4431, 3276.7943, 3402.4775, 3852.3723, 3864.9663

Compound: sCI 1 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -342.168010859089
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.192422 0.529632 0.316311 8 1.160920 -0.499868 -0.434508 8 0.318766 -1.553240 0.115411 1 0.932868 0.410061 1.360688 1 1.931337 1.267746 0.027052 8 -1.845919 -0.326514 0.101626 1 -0.993520 -0.964941 0.078703 1 -2.433201 -0.575827 -0.616514 8 -0.296944 1.611904 -0.010087 1 -1.070723 0.887825 -0.013058 1 -0.215877 1.939076 -0.914276	-331.9075, 71.9222, 194.6061, 351.7547, 414.3802, 422.4307, 475.2839, 500.9594, 542.9366, 635.6221, 785.6676, 811.7532, 997.0156, 1174.5653, 1210.7296, 1231.3393, 1340.8124, 1379.1202, 1510.8264, 1574.8904, 1701.3286, 1933.9475, 2324.7193, 3111.8165, 3225.2142, 3799.8888, 3856.3891
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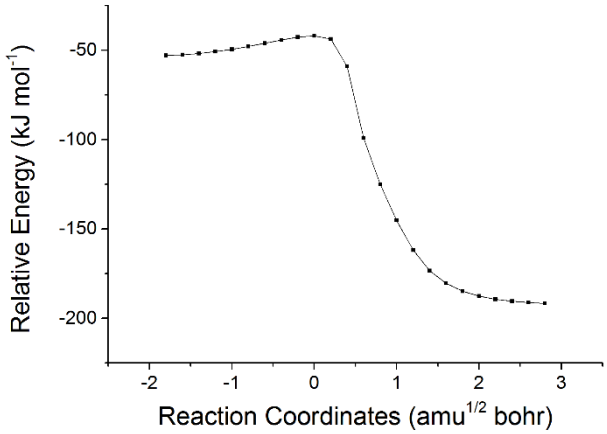


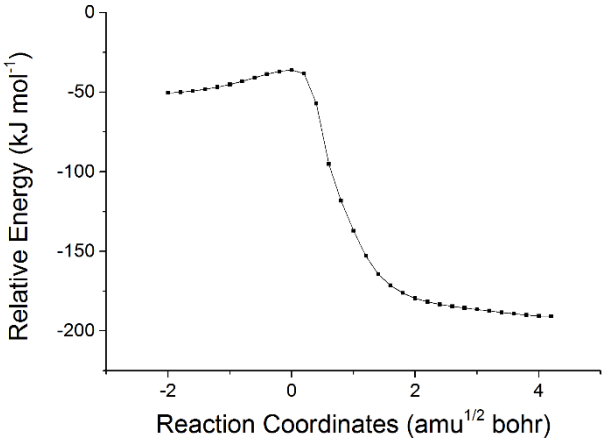
Compound: sCl 1 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -342.233729892064
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.310155 -0.387971 0.211196 8 -0.951903 0.746125 -0.518256 8 -0.007548 1.526793 0.257320 1 0.849294 1.100333 0.040465 1 -1.377092 -0.153293 1.270671 1 -2.278477 -0.684059 -0.197767 8 -0.375966 -1.458639 0.095441 1 -0.493571 -1.871459 -0.766643 8 2.199355 -0.167618 0.041687 1 2.736653 -0.384393 -0.725326 1 1.512619 -0.852597 0.101887	80.2143, 135.1051, 177.1882, 218.1612, , 245.4740, 311.2889, 418.3506, 430.3680, , 548.4011, 606.7308, 762.0375, 878.9051, 985.8147, 1044.7150, 1057.6103, 1281.4671, 1376.6100, 1409.4124, 1477.9090, 1487.4796, 1643.2095, 3043.3769, 3125.9909, 3485.3233, 3647.4380, 3800.8669, 3864.6927

Compound: sCl 1 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -342.172820831981
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.183018 1.034344 0.165699 8 1.329699 -0.039021 -0.445103 8 1.120434 -1.214004 0.287038 1 0.963648 1.023652 1.224482 1 1.336764 1.932257 -0.416177 8 -1.553924 -1.256559 -0.144544 1 -0.591428 -1.418379 0.018269 1 -2.032764 -1.857041 0.431979 8 -1.306680 1.470287 -0.041135 1 -1.570090 0.522258 -0.059751 1 -1.920468 1.905555 0.556951	44.7709, 92.2913, 121.6969, 190.2055, 221.7461, 229.2992, 252.4455, 269.8093, 454.4412, 508.4079, 558.2405, 679.0943, 700.7851, 820.4844, 849.8782, 1042.4600, 1234.4812, 1421.5825, 1590.4005, 1666.4577, 1681.3650, 3134.9513, 3276.2042, 3280.1314, 3422.0270, 3856.0097, 3867.7459

Compound: sCl 1 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -342.166034138439
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.320571 0.408091 0.121837 8 0.985248 -0.661014 -0.484936 8 0.151751 -1.508354 0.360187 1 1.343904 0.381680 1.205155 1 2.027564 1.018985 -0.425759 8 -1.846984 -0.152850 -0.195992 1 -1.096225 -0.874018 0.055889 1 -2.570960 -0.233348 0.430105	-390.4521, 77.4610, 199.6630, 350.7358, 398.6994, 428.1677, 472.3849, 496.8026, 547.9891, 695.6734, 814.1253, 819.6207, 974.9830, 1065.5883, 1190.1939, 1237.5317, 1311.3755, 1373.6134, 1500.2665, 1605.5800, 1703.6058,

8 -0.101441 1.596433 -0.018511 1 -0.949800 0.944191 -0.069664 1 -0.186498 2.120247 0.787262	1871.0365, 2225.0288, 3105.5587, 3220.4414, 3799.7280, 3857.9859

IRC



Compound: sCl 1 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -342.234765929815
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.379368 -0.331531 -0.143936 8 -0.679769 0.790306 -0.597330 8 -0.021638 1.388099 0.551088 1 0.893352 1.074027 0.403685 1 -2.043645 -0.057252 0.678174 1 -1.943257 -0.656645 -1.017525 8 -0.533159 -1.399710 0.242642 1 -0.346092 -1.309180 1.182284 8 2.153792 -0.217292 -0.222703 1 2.906674 -0.673391 0.162826 1 1.455373 -0.879593 -0.335403	109.1770, 119.5232, 156.5756, 175.0228, 220.1963, 279.2470, 378.5575, 410.0549, 490.8357, 612.7953, 691.0145, 881.9182, 1015.8576, 1037.4611, 1059.6915, 1284.5684, 1380.9111, 1410.5284, 1482.8420, 1487.0272, 1630.3323, 3034.4784, 3109.8974, 3543.4798, 3698.6881, 3813.3170, 3873.2790

Compound: sCl 1 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -342.173701402131
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.112307 1.068481 0.203569 8 1.344169 0.032511 -0.444929 8 1.171224 -1.184469 0.230492 1 0.857189 0.999313 1.252239 1 1.242551 1.998643 -0.331254 8 -1.514347 -1.304856 0.053226 1 -0.531564 -1.416493 0.119399 1 -1.799220 -1.866540 -0.672457 8 -1.363138 1.408770 -0.093024 1 -1.572574 0.445034 -0.085667 1 -1.973493 1.813512 0.530199	53.1327, 101.9900, 132.7817, 216.3090, 243.7112, 262.3092, 281.8423, 301.6424, 438.3076, 477.5225, 510.9797, , 696.7678, 816.7400, 821.8222, 950.4880, 1046.3538, 1235.4963, 1422.2397, 1589.6123, 1640.0256, 1668.4226, , 3134.9327, 3239.5935, 3277.1102, 3384.2768, 3849.1270, 3859.6874

Compound: sCl 1 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -342.168160410100
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.307862 0.444852 0.124825 8 1.010389 -0.627475 -0.492431 8 0.206552 -1.515403 0.339739	-357.3390, 83.2044, 206.4492, 353.9082, 392.4595, 425.2889, 475.5641, 507.1320, 550.1419,

1 1.306652 0.417002 1.208064 1 1.999163 1.084525 -0.409325 8 -1.868295 -0.197275 -0.001163 1 -1.074048 -0.895604 0.133812 1 -2.336835 -0.426090 -0.808385 8 -0.159866 1.602317 -0.040412 1 -0.977060 0.917827 -0.074545 1 -0.275279 2.135912 0.755561	625.3160, 800.6382, 818.4120, 964.7382, 1192.1193, 1215.3899, 1240.6843, 1362.3744, 1421.4184, 1509.2727, 1574.1521, 1652.4906, 1867.5595, 2284.4761, 3108.9557, 3225.1613, 3795.7823, 3851.9574

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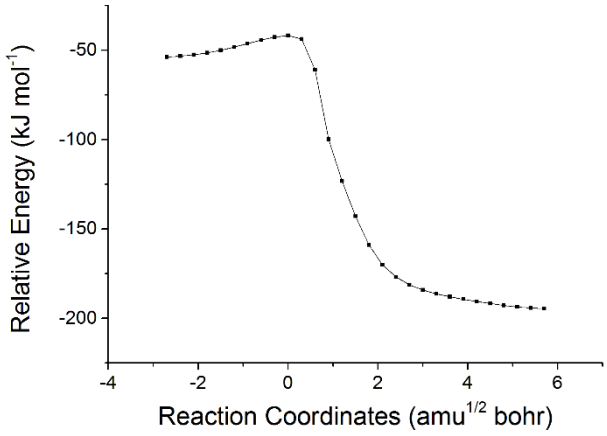

Compound: sCl 1 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -342.236055056007
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.379185 -0.321230 0.130494 8 0.687283 0.800439 0.597518 8 -0.001863 1.393427 -0.534429 1 -0.902001 1.029461 -0.396438 1 2.012555 -0.049944 -0.716190 1 1.974993 -0.634252 0.987427 8 0.525348 -1.397117 -0.215878 1 0.333934 -1.347236 -1.157888 8 -2.159058 -0.297409 0.068324 1 -2.681414 -0.178741 0.866979 1 -1.426865 -0.886630 0.308862	102.8232, 138.8594, 161.2587, 217.9648, 234.9476, 270.5088, 401.6741, 440.9790, 540.4841, 624.9479, 753.4956, 882.5366, 1015.2832, 1038.1739, 1058.5376, 1284.3506, 1377.0341, 1410.5592, 1482.3422, 1486.2977, 1632.4035, 3037.2242, 3108.2353, 3498.1506, 3681.9869, 3811.6239, 3862.6764

Compound: sCl 1 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -342.173268681123
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.035941 1.088804 0.263467 8 1.393543 0.111275 -0.419126 8 1.227174 -1.156101 0.155147 1 0.679362 0.944771 1.273830 1 1.175061 2.058545 -0.193582 8 -1.453888 -1.351848 -0.097799 1 -0.469779 -1.435667 -0.012495 1 -1.834915 -1.938947 0.560283 8 -1.452168 1.361236 0.051517 1 -1.617832 0.390095 0.007285 1 -1.864840 1.731884 -0.734030	50.1715, 95.4727, 125.9329, 230.6779, 244.3856, 258.3228, 278.3355, 306.0719, 455.3526, 497.6357, 520.4366, 705.8264, 768.2027, 821.0998, 923.8951, 1049.5097, 1230.3444, 1419.6329, 1586.9402, 1653.3753, 1680.2783, 3136.0331, 3239.6046, 3277.0653, 3385.2974, 3850.4666, 3861.9778

Compound: sCl 1 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -342.168384007199

Reaction Coordinates:	Frequencies (cm^{-1}):
6 1.218398 0.517405 0.297770 8 1.143425 -0.519292 -0.438134 8 0.301105 -1.548507 0.154723 1 1.002418 0.412531 1.353308 1 1.951131 1.244668 -0.032246 8 -1.851952 -0.311351 -0.103947 1 -1.017154 -0.960857 -0.003975 1 -2.470054 -0.505205 0.605649 8 -0.279622 1.609468 0.030322 1 -1.055363 0.888764 0.009180 1 -0.225014 1.973128 -0.862245	-323.4815, 80.5480, 190.8851, 346.9591, 381.6466, 419.4027, 479.1782, 508.9306, 558.1013, 663.7923, 772.5704, 815.4304, 1002.2355, 1105.5810, 1208.6211, 1227.3572, 1350.2545, 1391.6604, 1512.9992, 1651.4838, 1666.7662, 1957.8254, 2347.4213, 3111.9292, 3225.4165, 3795.6111, 3855.2238

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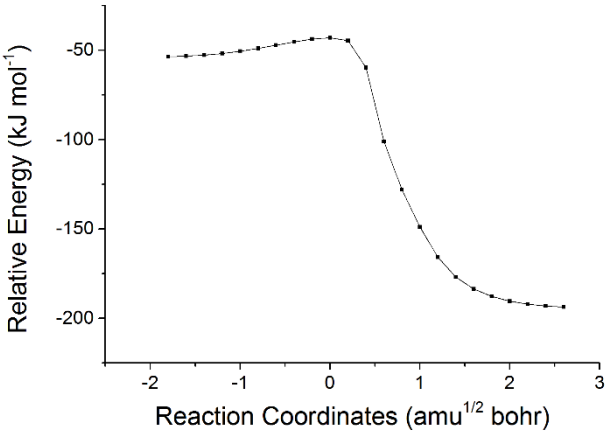


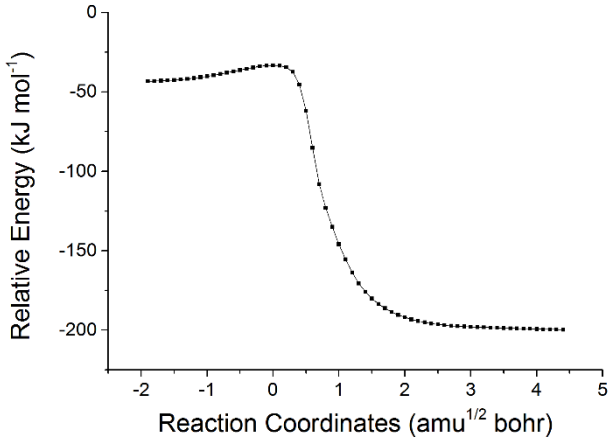
Compound: sCl 1 + $(H_2O)_2$ Pr4	Energy (kJ mol^{-1}): -342.234605099278
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.304886 -0.428786 0.217856 8 -1.000200 0.731096 -0.495025 8 -0.047719 1.514145 0.267961 1 0.809870 1.123777 -0.003827 1 -1.389838 -0.214913 1.280822 1 -2.256525 -0.761623 -0.202357 8 -0.320406 -1.449584 0.094944 1 -0.369645 -1.814832 -0.795559 8 2.196659 -0.145098 -0.146881 1 2.878349 -0.161457 0.530961 1 1.530433 -0.802702 0.114842	90.9279, 136.5893, 170.6335, 225.5069, 258.9680, 329.8411, 426.2758, 439.7446, 528.9552, 608.3053, 766.9180, 880.2249, 992.4407, 1045.1451, 1060.6803, 1281.0766, 1375.5973, 1412.5202, 1479.2496, 1496.9437, 1626.5333, 3042.1788, 3121.4472, 3499.4066, 3641.3869, 3792.6196, 3861.7379

8.10.2 sCl 23 + $(H_2O)_2$

Compound: sCl 23 + $(H_2O)_2$ PRC1	Energy (kJ mol^{-1}): -678.974835113330
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.226886 0.069658 -0.173860 6 -0.327629 -0.153120 1.036917 8 0.548333 -1.036039 1.112313 8 0.877813 -1.749719 -0.030010 1 -0.543624 0.376619 1.953269 9 -2.014559 1.127672 0.099043 9 -0.591222 0.307883 -1.313380	37.4045, 57.1535, 91.4813, 107.9226, 134.2558, 193.0122, 218.4290, 225.2269, 231.9446, 276.5813, 295.5504, 320.5879, 430.4866, 480.3114, 500.0589, 526.4522, 539.5277, 591.2657, 652.9329, 753.0271, 816.7426,

9 -2.019818 -1.000758 -0.332959 8 2.879487 0.074156 -0.588399 1 2.302773 -0.717172 -0.511804 1 3.224136 0.073448 -1.485108 8 1.106164 1.829012 0.588222 1 1.819692 1.348332 0.111352 1 0.860129 2.567097 0.022605	846.1514, 855.7267, 885.9751, 1150.1725, 1170.1522, 1262.1541, 1371.4928, 1593.0624, 1662.6313, 1668.8617, 3222.1025, 3389.2633, 3463.1346, 3847.8267, 3865.5964

Compound: sCI 23 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -678.970889225415
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.173357 -0.023374 0.164242 6 -0.151008 0.080429 -0.982054 8 0.689286 1.025230 -1.064898 8 1.119634 1.538355 0.223773 1 -0.541650 -0.236571 -1.942191 9 -2.015736 -1.041562 -0.149138 9 -0.676530 -0.288170 1.368967 9 -1.889874 1.098391 0.215695 8 2.710861 -0.401175 0.533202 1 2.185805 0.495286 0.505416 1 2.922854 -0.588301 1.451650 8 0.810773 -1.490775 -0.664878 1 1.644758 -1.159895 -0.104261 1 0.329264 -2.143876 -0.141050	-290.0059, 46.3837, 64.5511, 168.5922, 182.7072, 230.3468, 301.4527, 314.3332, 372.6685, 395.7978, 408.1420, 473.8506, 507.6275, 518.0961, 554.1721, 598.6566, 675.9497, 744.7321, 805.4973, 824.7409, 879.3618, 1008.2971, 1075.2479, 1122.4730, 1206.1978, 1262.7319, 1277.8725, 1351.6705, 1530.8641, 1673.7946, 1713.3045, 2078.5849, 2543.4807, 3168.9662, 3787.2140, 3854.6140
IRC	



Compound: sCI 23 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -679.043932127222
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.319171 -0.025832 0.129707 6 -0.099793 -0.222029 -0.803922 8 0.688475 0.894559 -0.978112 8 1.172711 1.381058 0.299920 1 2.046883 0.932451 0.348848 1 -0.505125 -0.398751 -1.805744 8 0.677895 -1.319844 -0.364164 1 0.115687 -2.093579 -0.242853 9 -2.120810 -1.120416 -0.019587 9 -1.024117 0.063500 1.425112 9 -2.028327 1.047038 -0.229328 8 3.336058 -0.357324 0.286854 1 3.755770 -0.629253 1.108307 1 2.658744 -1.022384 0.094960	36.4715, 56.0671, 125.3481, 135.0123, 185.8482, 211.5810, 235.6883, 243.2222, 254.3634, 298.8896, 330.1348, 376.5204, 437.9258, 469.2699, 520.0383, 582.8195, 611.9422, 744.2850, 754.9017, 852.2004, 908.7220, 1033.2727, 1092.9097, 1112.6719, 1195.4946, 1247.0912, 1300.8185, 1359.0143, 1425.1312, 1528.9667, 1632.6548, 3033.4111, 3443.2887, 3715.3179, 3798.3722, 3865.9905

Compound: sCI 23 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -678.975412531634
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.214882 0.071350 -0.175366 6 -0.325793 -0.161017 1.042058 8 0.545657 -1.048070 1.121063 8 0.887838 -1.752056 -0.026755 1 -0.554234 0.358827 1.961138 9 -2.001088 1.130774 0.097863 9 -0.570514 0.311513 -1.307792 9 -2.010442 -0.996175 -0.342068 8 2.774490 0.122967 -0.749245 1 2.224618 -0.679219 -0.605514 1 3.666755 -0.111412 -0.480022 8 1.103865 1.811852 0.619107 1 1.806175 1.330267 0.123785 1 0.844351 2.546984 0.055074	41.8023, 58.0072, 98.6309, 113.1135, 134.6924, 193.3712, 224.3711, 238.4057, 254.7038, 282.1835, 319.6521, 335.3226, 404.7950, 467.5258, 481.0277, 507.0066, 536.9264, 591.7953, 747.8361, 759.8966, 829.6064, 858.2697, 886.5529, 908.8787, 1149.1735, 1170.7208, 1265.3439, 1371.2946, 1593.6215, 1637.7621, 1663.6177, 3221.0408, 3359.0331, 3445.1478, 3842.8330, 3860.0165

Compound: sCI 23 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -678.972203381997
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.178354 0.022029 0.158851 6 0.147978 -0.071725 -0.980800 8 -0.697411 -1.010264 -1.065886 8 -1.114160 -1.543374 0.218888 1 0.525561 0.262066 -1.940232 9 2.018163 1.042347 -0.152675 9 0.690659 0.271855 1.367738 9 1.895185 -1.101577 0.189445 8 -2.649322 0.416120 0.673704 1 -2.152135 -0.487113 0.573358 1 -3.524230 0.315367 0.288595 8 -0.818695 1.511442 -0.634519 1 -1.653999 1.160100 -0.097130 1 -0.352551 2.142745 -0.070962	-269.7946, 50.1764, 63.9495, 173.4678, 183.5984, 229.1705, 302.2534, 313.6691, 372.7622, 379.2671, 408.0386, 477.1009, 511.5748, 517.6791, 549.2021, 595.0579, 610.6639, 742.1387, 800.8068, 814.9207, 879.3384, 1064.6348, 1124.1278, 1139.8038, 1205.8730, 1270.9158, 1347.7219, 1368.6629, 1535.3773, 1606.6560, 1661.9980, 2136.0068, 2593.0390, 3171.4988, 3783.4700, 3851.0261

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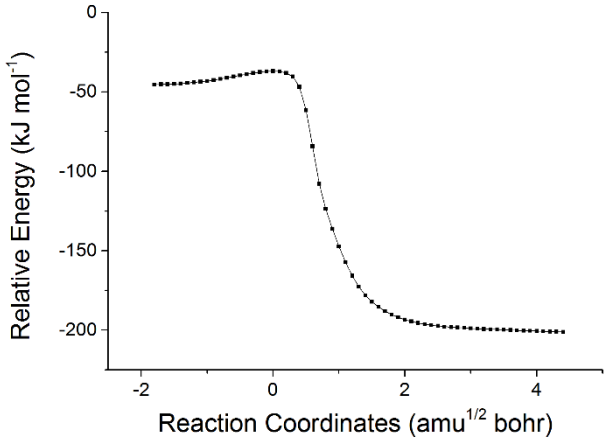

Compound: sCI 23 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -679.044522555901
Reaction Coordinates:	**Frequencies (cm^{-1}):**

6 -1.322906 -0.020520 0.112406 6 -0.084043 -0.241045 -0.789019 8 0.716228 0.869099 -0.963624 8 1.167558 1.378038 0.317840 1 2.031053 0.914065 0.408348 1 -0.467995 -0.429444 -1.797286 8 0.679699 -1.335631 -0.321104 1 0.102371 -2.044888 -0.015769 9 -2.130590 -1.110357 -0.037283 9 -1.055727 0.085110 1.412809 9 -2.012187 1.052759 -0.279522 8 3.301497 -0.378920 0.431258 1 3.995376 -0.356724 -0.234385 1 2.647576 -1.021918 0.119768	38.5690, 54.0929, 129.2809, 136.0169, 157.2516, 214.1037, 237.6501, 255.5837, 260.4528, 282.1900, 301.5859, 369.7651, 436.3490, 518.4205, 527.5382, 584.3273, 621.5032, 752.7175, 793.5276, 854.1331, 908.7737, 1041.4784, 1090.5830, 1113.8186, 1199.1434, 1244.6945, 1302.0778, 1353.1822, 1431.0382, 1512.5730, 1626.9675, 3031.5325, 3431.1048, 3713.0756, 3796.4734, 3864.3227

Compound: sCI 23 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -678.973863351660
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.190559 0.094535 -0.196108 6 -0.369816 -0.172653 1.062611 8 0.480011 -1.077431 1.176344 8 0.862903 -1.784611 0.048000 1 -0.634506 0.341912 1.974995 9 -1.984786 1.148371 0.055349 9 -0.480784 0.343171 -1.283526 9 -1.981592 -0.969140 -0.421792 8 2.702079 0.091542 -0.818995 1 2.159514 -0.701130 -0.614895 1 3.616997 -0.164226 -0.676270 8 1.073424 1.846982 0.551227 1 1.771615 1.367837 0.052656 1 1.525750 2.310843 1.261611	43.5999, 60.5434, 98.9220, 102.2304, 122.5014, 186.2915, 219.4830, 223.4351, 231.6112, 247.9051, 277.4087, 319.6655, 395.1912, 476.6845, 496.7676, 505.7365, 536.0064, 588.8097, 688.7703, 754.5842, 820.2495, 852.0429, 862.4511, 887.8182, 1150.9682, 1170.0254, 1268.7329, 1368.4085, 1591.2971, 1644.9660, 1665.7561, 3219.0326, 3402.1416, 3471.6488, 3853.1968, 3865.0665

Compound: sCI 23 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -678.970261942381
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.151495 -0.045174 -0.184872 6 0.170938 0.072243 0.998151 8 -0.653792 1.026446 1.122183 8 -1.115610 1.577872 -0.136639 1 0.591290 -0.262956 1.940555 9 2.030092 -1.024962 0.114831 9 0.607304 -0.324768 -1.358357 9 1.837879 1.100638 -0.273055 8 -2.529554 -0.422462 -0.791602 1 -2.072740 0.486607 -0.603370 1 -3.451191 -0.349556 -0.529791 8 -0.772075 -1.527413 0.614835 1 -1.582115 -1.188548 0.037894 1 -1.129066 -1.841687 1.454050	-255.0687, 55.2659, 77.0544, 168.0979, 178.5946, 222.8289, 303.1951, 315.0054, 370.2693, 390.8977, 403.1160, 468.3366, 482.4316, 519.7345, 552.4007, 603.8288, 621.6264, 742.8942, 784.0733, 809.4791, 898.8488, 1058.3895, 1108.0793, 1143.1440, 1188.6024, 1271.7654, 1305.2514, 1345.2191, 1534.5795, 1613.5212, 1707.5809, 2181.4832, 2610.1198, 3155.3420, 3805.6386, 3855.2006
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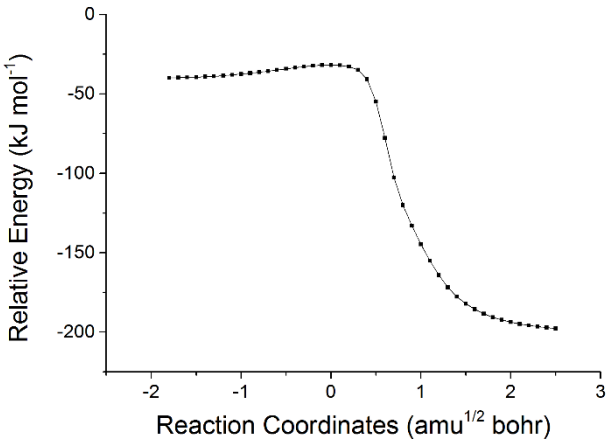
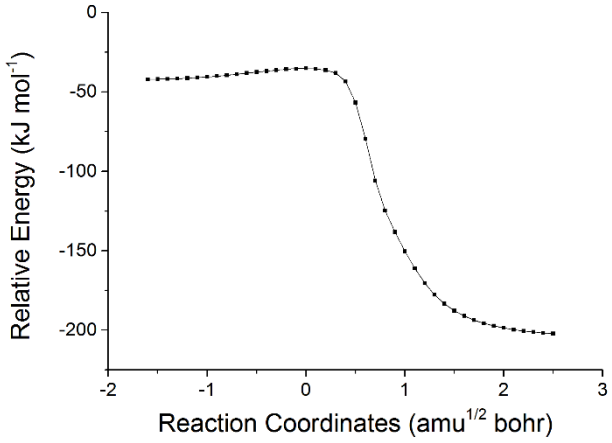


Compound: sCl 23 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -679.044046393108
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.235036 -0.074225 -0.201158 6 0.180498 -0.131186 0.928825 8 -0.576023 1.025870 1.082329 8 -1.115760 1.449222 -0.193629 1 -1.945106 0.927595 -0.260668 1 0.729962 -0.193591 1.871195 8 -0.585846 -1.296230 0.707444 1 -0.893072 -1.622913 1.558947 9 2.181647 -1.006601 0.055252 9 0.739031 -0.332562 -1.412406 9 1.839106 1.118160 -0.225203 8 -3.084291 -0.441560 -0.675776 1 -3.903200 -0.686352 -0.235492 1 -2.424486 -1.101660 -0.421706	38.0835, 64.6328, 96.1394, 135.5457, 197.8564, 201.4051, 234.9116, 243.3833, 261.0024, 303.1512, 331.9013, 371.1792, 436.1274, 449.1955, 525.3000, 582.6400, 609.0144, 750.8165, 767.7665, 844.1162, 907.7243, 1051.8707, 1076.2109, 1126.7896, 1177.7901, 1246.2906, 1291.8476, 1373.1354, 1437.7390, 1483.7264, 1632.1168, 3059.6863, 3479.9112, 3732.3887, 3815.2581, 3872.7493

Compound: sCl 23 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -678.974423926339
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.195272 0.096888 -0.192917 6 -0.363456 -0.174980 1.057263 8 0.485322 -1.082150 1.161247 8 0.865860 -1.777624 0.024545 1 -0.627595 0.330073 1.975107 9 -1.987364 1.149471 0.068122 9 -0.497726 0.350479 -1.289404 9 -1.987331 -0.966137 -0.416690 8 2.796504 0.076841 -0.680249 1 2.233024 -0.714988 -0.535574 1 2.968365 0.113539 -1.625230 8 1.069922 1.825415 0.546226 1 1.765743 1.329712 0.056432 1 1.523766 2.266039 1.270788	44.5943, 61.0444, 104.8336, 125.3744, 189.9980, 221.1578, 232.1002, 241.0143, 280.2124, 303.1346, 320.0261, 427.4818, 469.8666, 496.1996, 500.6470, 536.0040, 590.0928, 694.7367, 754.2804, 834.5125, 857.8793, 885.0821, 896.8702, 1151.3690, 1169.9219, 1265.2790, 1368.1246, 1590.6157, 1649.7949, 1669.9483, 3218.8672, 3367.2346, 3453.9721, 3847.7674, 3858.5145

Compound: sCI 23 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -678.971433697789
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.148516 -0.052598 -0.185936 6 0.180719 0.099865 1.002687 8 -0.638403 1.059164 1.109814 8 -1.110604 1.582452 -0.154346 1 0.603794 -0.220212 1.948898 9 2.026834 -1.026730 0.127879 9 0.590992 -0.363862 -1.349187 9 1.836346 1.087250 -0.317239 8 -2.611693 -0.414783 -0.662662 1 -2.124068 0.486864 -0.549865 1 -2.687895 -0.585007 -1.605794 8 -0.778960 -1.510779 0.657020 1 -1.572380 -1.177308 0.057052 1 -1.165135 -1.786280 1.497513	-242.4381, 56.9560, 77.5768, 163.9943, 178.3123, 224.0854, 302.7484, 314.3336, 362.0054, 378.2726, 389.8786, 472.0494, 518.6113, 520.7586, 551.5244, 606.7181, 632.0949, 734.4464, 779.3153, 813.3456, 899.3494, 1014.0479, 1074.2958, 1146.1441, 1188.0078, 1269.7607, 1330.6011, 1355.1327, 1539.8493, 1652.5416, 1695.9196, 2208.5205, 2657.1975, 3158.3164, 3799.5431, 3850.0937
IRC	



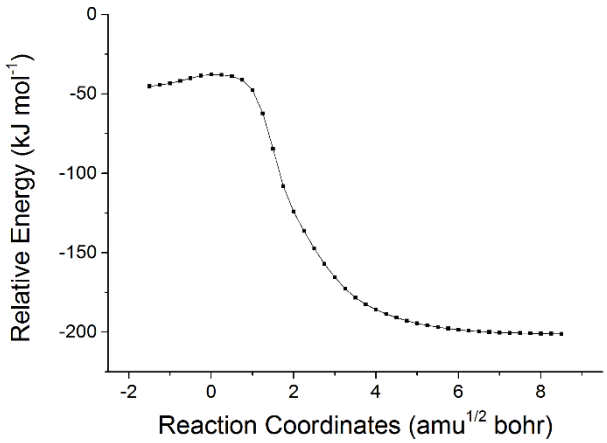
Compound: sCI 23 + $(H_2O)_2$ Pr4	**Energy (kJ mol^{-1}):** -679.045781275488
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.229414 -0.104076 -0.197877 6 0.186925 -0.032536 0.942221 8 -0.541302 1.152571 0.996142 8 -1.125871 1.444229 -0.296751 1 -1.949458 0.909925 -0.286233 1 0.744590 -0.018329 1.882382 8 -0.605649 -1.191117 0.830119 1 -1.027534 -1.354289 1.680771 9 2.160525 -1.027778 0.129379 9 0.710813 -0.462019 -1.376728 9 1.854483 1.068510 -0.341170 8 -3.100430 -0.541605 -0.489931 1 -3.472311 -0.705733 -1.361849 1 -2.339708 -1.132937 -0.401095	42.2630, 62.8676, 110.5466, 138.7273, 184.2194, 196.6160, 232.1943, 261.7272, 299.5725, 324.8941, 355.9719, 403.2916, 436.8545, 455.0373, 525.8731, 582.1368, 611.4955, 738.4935, 765.3435, 848.2237, 906.3519, 1060.1520, 1075.5174, 1128.1962, 1175.7514, 1244.6938, 1288.3378, 1370.2384, 1443.8454, 1497.8364, 1615.5190, 3054.8039, 3485.5656, 3726.2780, 3802.1332, 3865.2728

8.10.3 sCI 24 + $(H_2O)_2$

Compound: sCI 24 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -678.976463310368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.499637 0.034189 0.029921 9 -2.421756 -0.917529 -0.234744 9 -1.481601 0.246835 1.339166 9 -1.879268 1.149648 -0.601056 6 -0.161123 -0.437563 -0.509120 8 0.528005 -1.160758 0.229694 8 1.703726 -1.674615 -0.315970 1 0.107263 -0.285593 -1.545557 8 3.323108 0.443097 0.301092 1 2.903426 -0.428271 0.114598 1 4.143665 0.463451 -0.197932 8 0.947209 1.699816 -0.129811 1 1.885003 1.425164 -0.007395 1 0.952445 2.474579 -0.698853	30.2311, 48.3526, 78.3380, 121.2136, 129.1577, 183.8853, 210.7690, 233.2283, 237.6079, 250.3556, 291.0299, 378.0381, 406.7864, 419.5053, 447.6724, 548.6580, 556.0472, 567.2963, 661.5093, 697.1129, 828.2620, 881.3964, 901.0656, 932.5150, 1129.1888, 1190.4575, 1271.2460, 1360.2601, , 1593.5489, 1654.6893, 1672.7892, 3208.8953, 3342.6622, 3427.3235, 3855.6257, 3865.3133

Compound: sCI 24 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -678.974181399714
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.433893 -0.010821 0.025018 6 0.000721 0.275629 -0.421110 8 -0.642633 1.080587 0.312812 8 -1.879165 1.511302 -0.325547 1 -0.181859 0.294659 -1.490112 9 1.919606 -1.067259 -0.651454 9 2.194354 1.053299 -0.281898 9 1.536228 -0.247488 1.326860 8 -3.054122 -0.636397 0.296387 1 -2.742309 0.326894 0.061902 1 -3.810052 -0.849239 -0.256998 8 -0.720537 -1.425674 -0.112831 1 -1.747372 -1.231075 0.021585 1 -0.606141 -2.015594 -0.867951	-263.1970, 41.2328, 75.5833, 147.1956, 171.5294, 195.8320, 313.2451, 347.0769, 363.3666, 390.1600, 411.0510, 428.8565, 468.8022, 522.5049, 557.4381, 588.2506, 669.5502, 698.9099, 812.9743, 859.6684, 893.5243, 996.8146, 1104.8172, 1159.1604, 1187.8663, 1254.9663, 1279.0990, 1335.4104, 1518.4628, 1670.5092, 1710.7505, 2130.1417, 2552.0395, 3156.0023, 3798.9059, 3858.0062

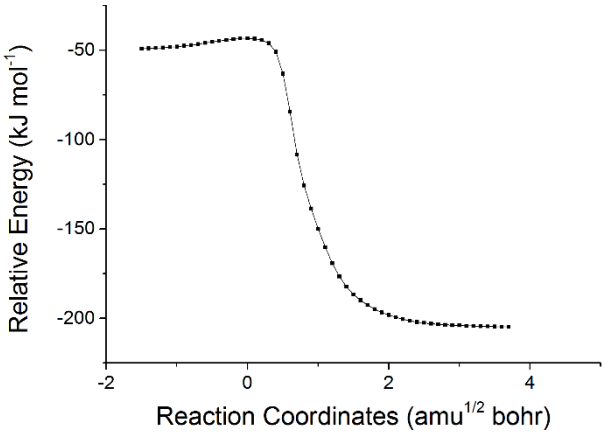
IRC



Compound: sCl 24 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -679.046695526630
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.449107 -0.036898 0.087914 6 0.037661 0.090957 -0.522040 8 -0.658996 0.963041 0.289197 8 -1.798886 1.451237 -0.458160 1 -2.502768 0.852493 -0.119323 1 0.137230 0.491542 -1.534270 8 -0.601361 -1.173366 -0.536544 1 -0.323123 -1.670114 -1.313281 9 2.147732 -0.948405 -0.627237 9 2.110176 1.125660 0.018976 9 1.428296 -0.441198 1.359734 8 -3.294813 -0.659336 0.509863 1 -4.052965 -1.078680 0.093172 1 -2.522371 -1.196702 0.280354	39.4378, 67.9434, 112.9031, 127.4279, 182.7777, 199.1615, 225.0892, 240.7713, 252.2604, 330.8000, 355.9574, 366.0785, 403.1514, 467.2147, 520.1325, 565.5773, 620.0285, 711.2871, 732.5789, 872.7445, 951.3378, 1036.5657, 1089.3071, 1145.6563, 1177.6616, 1276.8225, 1278.9342, 1379.7424, 1401.6927, 1531.8141, 1634.1229, 3045.2327, 3438.3881, 3713.2347, 3811.0091, 3869.9623

Compound: sCl 24 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -678.977263064497
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.489581 0.032561 0.017263 6 -0.130363 -0.424195 -0.483405 8 0.528723 -1.168690 0.262489 8 1.721301 -1.679972 -0.259762 1 0.165924 -0.264696 -1.511268 9 -1.863219 1.146325 -0.620301 9 -2.392537 -0.928016 -0.277285 9 -1.512613 0.240448 1.327654 8 3.328823 0.482446 0.065681 1 2.893099 -0.399289 -0.020606 1 3.863618 0.443308 0.863291 8 0.915829 1.691448 -0.041072 1 1.859539 1.407848 0.030886 1 0.895401 2.431960 -0.654738	30.6497, 52.9885, 88.3887, 126.1346, 131.7672, 188.4279, ,227.6577, 257.3088, 270.5375, 298.3777, 326.5543, 377.5462, 406.6573, 419.9501, 426.6031, 504.1159, 551.6708, 565.5651, 696.6782, 801.3020, 868.7779, 896.7671, 932.7880, 956.1836, 1130.7885, 1190.6128, 1270.0021, 1360.0737, 1591.7576, 1632.3812, 1658.9014, 3206.3576, 3280.1552, 3382.2637, 3846.1059, 3857.7617

Compound: sCl 24 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -678.976125632750
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.435077 -0.010533 0.024264 6 0.002922 0.283163 -0.418283 8 -0.638892 1.083167 0.318663 8 -1.874687 1.523888 -0.310848 1 -0.193354 0.288870 -1.484716 9 1.916127 -1.067784 -0.651339 9 2.198962 1.051509 -0.282868 9 1.537638 -0.246161 1.327155 8 -3.093194 -0.653611 0.111027 1 -2.754194 0.314963 -0.024240 1 -3.541326 -0.693970 0.960482 8 -0.723810 -1.442665 -0.094417 1 -1.744088 -1.234536 0.030523 1 -0.624922 -2.035418 -0.849864	-237.6757, 42.6112, 75.8600, 147.3213, 171.3151, 201.4235, 313.1240, 346.9833, 365.9511, 381.3066, 410.6057, 432.7579, 477.7047, 524.5486, 553.7698, 575.2125, 603.5414, 699.2346, 790.1670, 857.8705, 890.3554, 1092.8087, 1134.3888, 1160.1992, 1186.3775, 1275.9931, 1337.7155, 1346.5485, 1525.6492, 1604.5939, 1661.5278, 2196.6905, ,2613.5636, 3161.3782, 3795.8025, 3850.4897
IRC	

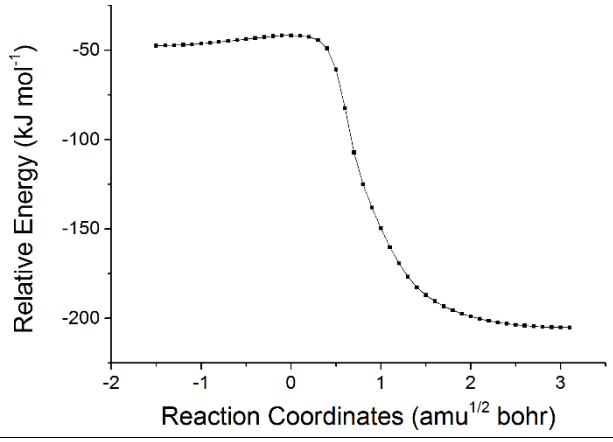


Compound: sCl 24 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -679.048259309215
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.439730 -0.040130 0.094282 6 0.041573 0.113367 -0.539534 8 -0.664860 0.966737 0.289088 8 -1.811918 1.448383 -0.451212 1 -2.503211 0.821351 -0.135658 1 0.160701 0.545794 -1.535594 8 -0.589337 -1.151117 -0.607078 1 -0.516255 -1.508389 -1.497434 9 2.166630 -0.898248 -0.650811 9 2.089350 1.131291 0.116479 9 1.385711 -0.519510 1.341232 8 -3.287949 -0.726004 0.392427 1 -3.520615 -0.824360 1.320614 1 -2.451151 -1.199605 0.271668	29.1021, 68.3708, 114.9367, 133.5549, 142.3315, 197.9780, 232.6122, 258.8916, 279.9146, 298.2524, 352.5085, 360.8069, 402.4199, 511.5738, 552.9532, 565.9581, 640.1037, 711.7799, 793.0365, 869.3275, 951.3602, 1042.2727, 1083.7799, 1149.1644, 1176.6648, 1269.7387, 1286.4346, 1366.9773, 1414.0520, 1516.4983, 1627.6177, 3054.0939, 3419.5323, 3703.4480, 3823.5165, 3861.4461

Compound: sCI 24 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -678.976758543801
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.485381 0.029360 0.008310 6 -0.118211 -0.417021 -0.481879 8 0.508388 -1.199324 0.254757 8 1.716295 -1.697852 -0.234009 1 0.213743 -0.202963 -1.488591 9 -1.903593 1.082738 -0.695441 9 -2.367865 -0.971427 -0.177248 9 -1.480214 0.342995 1.305648 8 3.317663 0.478742 0.072711 1 2.881421 -0.402415 -0.003996 1 3.910307 0.425006 0.826937 8 0.936741 1.748319 -0.204451 1 1.862031 1.456501 -0.027708 1 0.686411 2.322011 0.526067	22.7981, 33.1705, 84.6555, 116.8194, 135.7398, 183.9906, 226.2528, 250.2507, 260.1566, 277.5607, 297.0635, 378.3309, 404.9927, 413.8918, 425.4943, 540.8087, 552.1992, 568.2039, 696.2535, 731.1253, 865.8081, 891.1302, 921.7357, 942.0771, 1143.3441, 1195.7403, 1250.2764, 1360.4244, 1586.1495, 1639.6708, 1665.4309, 3208.9233, 3314.2435, 3405.6402, 3846.2551, 3863.2852

Compound: sCI 24 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -678.975252603565
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.431618 -0.011054 -0.034022 6 -0.034263 0.263996 -0.375191 8 -0.606445 1.103863 0.379333 8 -1.881019 1.551034 -0.156779 1 -0.317238 0.214681 -1.420450 9 1.934015 -0.944984 -0.846552 9 2.143596 1.110552 -0.191312 9 1.577245 -0.428714 1.234683 8 -3.089048 -0.671805 -0.096550 1 -2.739105 0.303517 -0.088996 1 -3.714809 -0.772452 0.625598 8 -0.713585 -1.470124 -0.036222 1 -1.741506 -1.277314 -0.007735 1 -0.444395 -1.721504 0.857244	-234.0953, 40.5246, 63.1378, 148.1200, 169.9852, 188.6379, 317.5559, 337.1536, 365.4847, 395.3353, 407.4014, 434.1385, 485.7447, 516.9718, 555.8605, 592.6492, 628.4843, 696.8288, 787.2052, 853.9549, 900.9870, 1084.2440, 1123.9700, 1185.4779, 1191.7999, 1247.1847, 1307.6331, 1338.5639, 1518.0518, 1617.4855, 1696.5678, 2227.8831, 2604.6378, 3168.8170, 3781.6508, 3855.6553

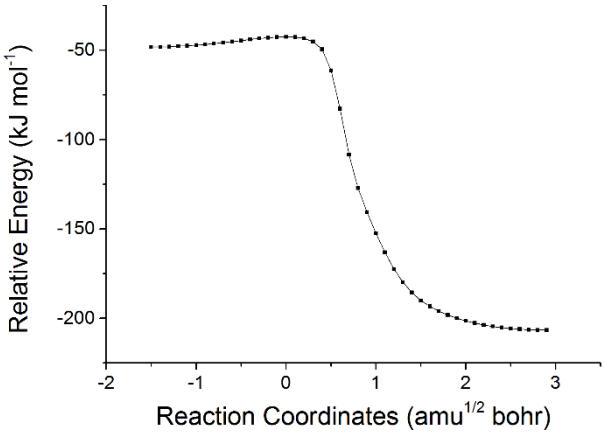
IRC



Compound: sCI 24 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -679.047730845463
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.471334 -0.037790 -0.013291 6 -0.025816 -0.002631 -0.378566 8 -0.609598 0.972687 0.429755 8 -1.751106 1.522386 -0.268795 1 -2.465622 0.891842 -0.025845 1 -0.131809 0.259331 -1.429368 8 -0.595147 -1.281875 -0.211757 1 -0.359250 -1.609005 0.666398 9 2.123837 -0.889429 -0.820830 9 2.040916 1.162355 -0.128133 9 1.642956 -0.470542 1.256125 8 -3.462714 -0.631195 0.014372 1 -3.945142 -0.971691 0.773244 1 -2.692139 -1.205440 -0.106349	42.3450, 68.1372, 93.4777, 108.7143, 196.3265, 225.6205, 232.9114, 251.4983, 300.4113, 355.5126, 363.0538, 395.7893, 417.7649, 498.8204, 529.5849, 566.0577, 617.7195, 712.3798, 766.2066, 860.6738, 952.0996, 1039.1784, 1072.2515, 1145.9665, 1198.6877, 1249.1969, 1289.4075, 1358.5433, 1439.6431, 1502.5135, 1634.4066, 3112.1802, 3454.4926, 3707.6218, 3759.0631, 3867.6327

Compound: sCI 24 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -678.977086514110
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.488498 0.031281 0.024393 6 -0.139236 -0.422659 -0.505341 8 0.517339 -1.188274 0.222487 8 1.710186 -1.685984 -0.301775 1 0.155884 -0.226073 -1.526722 9 -1.911345 1.099923 -0.654924 9 -2.386673 -0.956767 -0.156662 9 -1.449487 0.325814 1.324340 8 3.279493 0.457583 0.323859 1 2.878271 -0.422784 0.134575 1 4.085206 0.508678 -0.197337 8 0.967077 1.729600 -0.302147 1 1.874419 1.418739 -0.068966 1 0.707409 2.345586 0.389960	29.7774, 35.1066, ,82.1077, 119.2790, 134.9192, 186.3092, 224.0826, 246.1701, 255.0849, 291.8496, 316.9709, 378.1117, 405.2150, 423.9155, 457.8222, 503.7150, 551.7795, 567.5064, 697.2139, 721.0081, 871.9403, 897.5611, 925.5407, 938.4995, 1142.2460, 1193.3356, 1253.5596, 1359.8805, 1587.0451, 1645.5366, 1672.1439, 3211.2763, 3307.8078, 3403.5872, 3843.0633, 3860.4701

Compound: sCl 24 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -678.975564636070
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.434044 -0.011313 -0.024390 6 -0.022466 0.274629 -0.394792 8 -0.611372 1.101933 0.359427 8 -1.877562 1.547582 -0.196765 1 -0.280451 0.243820 -1.446862 9 1.949462 -0.936385 -0.840424 9 2.154234 1.109008 -0.151706 9 1.551251 -0.447853 1.239679 8 -3.086228 -0.660807 0.136398 1 -2.750726 0.310568 0.018441 1 -3.759521 -0.826499 -0.528976 8 -0.722771 -1.464038 -0.109070 1 -1.746568 -1.259910 -0.040437 1 -0.443264 -1.768169 0.765066	-230.2011, 45.3686, 61.9067, 147.4104, 167.3891, 189.3980, 315.2304, 335.2181, 359.4677, 372.5325, 407.4650, 429.6039, 499.3162, 532.1970, 555.8467, 597.6203, 643.8656, 692.1889, 782.8539, 855.6845, 904.1119, 1019.4664, 1117.2722, 1185.2994, 1189.6672, 1247.6992, 1333.1465, 1337.8353, 1522.8713, 1650.7437, 1691.7606, 2234.3606, 2625.9690, 3171.1611, 3776.7366, 3854.5783
IRC	



Compound: sCl 24 + $(H_2O)_2$ Pr4	**Energy (kJ mol^{-1}):** -679.048442818014
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.473365 -0.048274 -0.009183 6 -0.017733 0.015656 -0.396791 8 -0.588033 1.008271 0.399375 8 -1.756684 1.519684 -0.282462 1 -2.456069 0.894736 0.011096 1 -0.100937 0.272677 -1.451227 8 -0.618388 -1.247903 -0.233660 1 -0.451590 -1.552115 0.668792 9 2.116547 -0.920993 -0.801862 9 2.070281 1.138954 -0.129843 9 1.620238 -0.471046 1.264785 8 -3.423651 -0.667016 0.204786 1 -4.198421 -0.854948 -0.333091 1 -2.696323 -1.191175 -0.161751	45.4830, 68.1509, 96.2361, 111.7822, 200.6320, 212.3986, 224.1042, 255.2367, 326.9426, 357.3304, 359.0549, 397.2458, 448.0537, 491.5462, 526.1644, 565.7096, 622.7980, 709.8585, 744.2916, 863.3097, 952.3372, 1042.3365, 1074.2045, 1148.1966, 1196.2764, 1251.1962, 1293.0989, 1358.9790, 1438.9013, 1514.9716, 1617.2477, 3107.5602, 3467.5822, 3706.4459, 3753.9161, 3865.9236

8.10.4 sCI 25 + $(H_2O)_2$

Compound: sCI 25 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -778.151182680016
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.111046 -0.242350 -0.451022 6 -0.319261 0.204891 0.799848 8 0.575408 -0.431904 1.369785 8 1.120026 -1.545860 0.653615 9 -0.884438 1.141948 1.494932 9 -1.929498 0.753446 -0.810346 9 -0.360874 -0.568707 -1.485809 9 -1.858617 -1.293633 -0.091832 8 3.018649 -0.020536 -0.530220 1 2.469097 -0.728816 -0.111137 1 3.419388 -0.408470 -1.312330 8 0.971763 1.712560 -0.356346 1 1.791707 1.193541 -0.556293 1 0.715716 2.156936 -1.170372	40.0825, 56.3618, 104.6947, 124.7390, 139.3793, 203.2420, 215.3984, 255.4641, 258.4817, 270.6400, 290.8050, 315.0485, 329.4540, 367.7848, 474.7718, 484.1919, 516.7047, 573.4577, 595.0829, 616.8202, 678.6174, 729.7337, 775.5858, 897.1599, 919.6383, 1148.1800, 1174.6125, 1237.1290, 1396.7823, 1618.5332, 1663.0453, 1680.6735, 3236.0138, 3341.1214, 3843.7417,81.5127:36,A,3864.2392

Compound: sCI 25 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -778.151865721165
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.071336 -0.436984 -0.252730 6 -0.195585 0.603494 0.504754 8 0.644406 0.301050 1.388751 8 1.223716 -1.028274 1.197705 9 -0.852254 1.710937 0.754235 9 -1.930356 0.240110 -1.038544 9 -0.390157 -1.267841 -1.028562 9 -1.773384 -1.127291 0.642186 8 2.865226 -0.188927 -0.587322 1 2.360559 -0.647889 0.173793 1 3.166402 -0.874471 -1.189704 8 0.827583 1.247575 -0.958306 1 1.697315 0.678420 -0.962383 1 0.405161 1.190257 -1.824314	-198.8784, 46.7101, 59.4403, 154.1929, 180.3588, 225.9582, 267.3994, 284.3814, 305.0015, 352.9306, 366.8464, 375.1442, 413.2466, 466.3781, 489.4181, 524.0339, 590.5112, 604.9577, 620.5837, 681.7673, 768.9943, 815.7543, 922.5824, 949.7419, 1141.7483, 1172.0635, 1196.5290, 1236.0527, 1347.4144, 1540.3012, 1669.2159, 1713.3148, 2389.5730, 2791.1720, 3797.1962, 3855.6133

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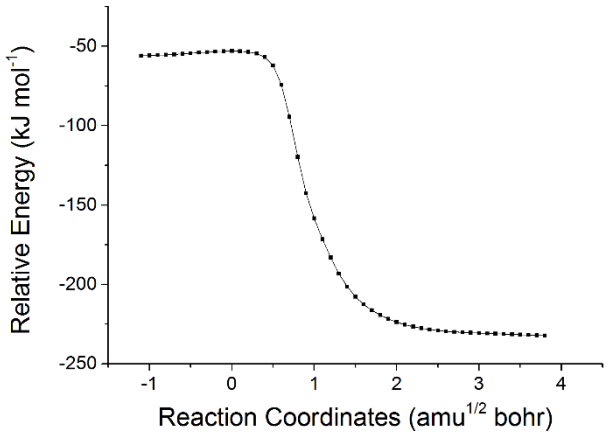
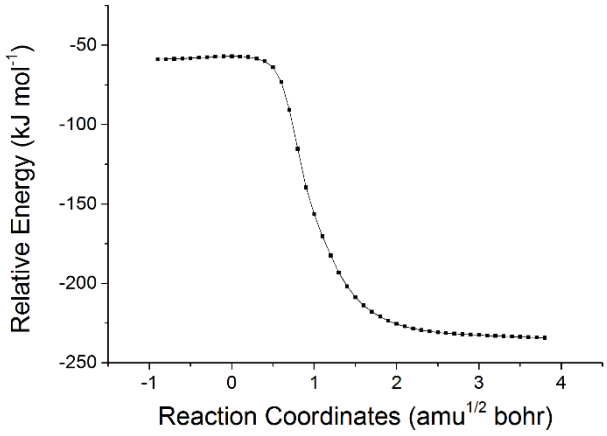
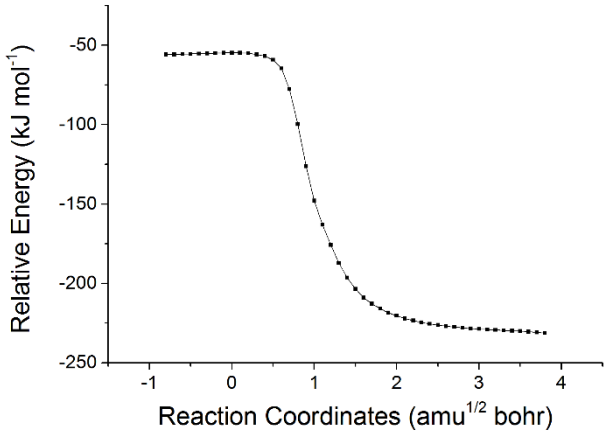


Compound: sCl 25 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -778.232205653240
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.331732 -0.259160 -0.190820 6 -0.039214 0.512746 0.233494 8 0.764673 -0.162432 1.133093 8 1.312123 -1.347541 0.514380 1 2.182508 -1.003043 0.204879 9 -0.474965 1.589770 0.953448 8 0.685330 0.923230 -0.860574 1 0.094400 1.270164 -1.541213 9 -2.075203 0.566046 -0.970916 9 -1.068394 -1.350754 -0.905759 9 -2.056443 -0.598624 0.871114 8 3.488053 -0.006943 -0.504972 1 4.126455 0.403140 0.086804 1 2.895931 0.699771 -0.792911	32.3377, 52.9666, 94.2196, 128.8150, 195.0532, 218.4669, 228.6420, 249.4912, 273.3105, 290.7010, 313.4979, 346.1309, 373.3548, 414.6536, 455.3092, 489.2980, 530.6004, 591.5891, 641.9204, 688.4057, 780.1559, 801.9113, 973.3600, 1055.2043, 1096.2389, 1155.3190, 1174.3793, 1225.3692, 1284.0680, 1391.8185, 1531.8581, 1625.7848, 3408.2526, 3757.6239, 3776.9067, 3869.8559

Compound: sCl 25 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -778.152030386117
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.102056 -0.246402 -0.448061 6 -0.309488 0.215351 0.798177 8 0.581044 -0.419529 1.378511 8 1.132067 -1.536629 0.665104 9 -0.883620 1.150068 1.490200 9 -1.922500 0.745436 -0.815800 9 -0.352326 -0.581202 -1.478943 9 -1.847989 -1.294069 -0.075748 8 2.932636 -0.065549 -0.689559 1 2.410849 -0.746220 -0.192153 1 3.788217 -0.003687 -0.256363 8 0.961724 1.705387 -0.353570 1 1.779495 1.176094 -0.549424 1 0.688847 2.108570 -1.184028	44.2525, 56.9310, 108.9406, 127.2046, 144.0984, 205.2413, 220.0133, 259.9402, 278.6197, 289.1779, 291.1197, 327.8403, 367.6214, 373.9608, 453.8346, 477.7278, 511.0120, 544.8312, 583.1474, 616.4050, 680.1004, 775.2032, 854.8557, 905.2343, 1010.7203, 1147.5637, 1173.6930, 1240.8031, 1394.5360, 1614.3180, 1634.0857, 1665.3915, 3182.2936, 3305.4328, 3836.1632, 3858.2832

Compound: sCl 25 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -778.153124563473
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.084712 -0.399692 -0.287877 6 -0.191557 0.546852 0.565262 8 0.658260 0.151351 1.399623 8 1.215031 -1.162107 1.079200 9 -0.822179 1.637356 0.924134 9 -1.940502 0.364194 -0.992171 9 -0.419363 -1.156160 -1.144925 9 -1.789585 -1.166016 0.542485 8 2.818351 -0.243774 -0.704543 1 2.332416 -0.728241 0.049174 1 3.660685 0.063565 -0.357981 8 0.841237 1.328127 -0.860702 1 1.709802 0.766160 -0.892860 1 0.436348 1.312415 -1.736981	-177.7862, 49.0472, 59.1808, 160.8012, 178.1110, 225.5547, 265.3601, 284.9991, 302.9429, 350.7331, 365.3687, 371.9797, 411.7477, 478.0180, 488.3767, 524.4662, 554.8934, 590.9387, 610.9689, 658.8232, 762.7452, 799.4225, 918.3369, 1066.2885, 1143.3405, 1176.7433, 1228.7899, 1283.7771, 1353.1035, 1546.1413, 1614.5921, 1666.4543, 2456.5473, 2835.4191, 3795.4097, 3851.4800
IRC  	

Compound: sCl 25 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -778.150954513382
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.080992 -0.293421 -0.439963 6 -0.309977 0.296432 0.768099 8 0.558811 -0.280279 1.437111 8 1.142219 -1.451989 0.846038 9 -0.903730 1.292366 1.361635 9 -1.932577 0.628095 -0.892785 9 -0.309351 -0.698009 -1.425552 9 -1.793038 -1.329614 0.028997 8 2.895030 -0.122247 -0.698902 1 2.389433 -0.744109 -0.114572 1 3.785256 -0.065695 -0.342575 8 0.878281 1.626475 -0.616822 1 1.728462 1.123576 -0.720068 1 1.096196 2.456950 -0.181662	44.4745, 66.9528, 96.0815, 125.4516, 153.5415, 200.0214, 219.7523, 260.3854, 275.8252, 281.7944, 289.4425, 326.5408, 354.4326, 368.4141, 467.1720, 478.9558, 512.2091, 570.8623, 586.5908, 615.7412, 664.1888, 775.7265, 811.7557, 899.0429, 990.4887, 1138.0675, 1179.2284, 1248.4219, 1385.5339, 1609.8626, 1639.6982, 1667.4722, 3188.2346, 3302.8218, 3837.7311, 3863.9650

Compound: sCl 25 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -778.152472459163
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.082084 -0.407518 -0.299218 6 -0.198345 0.551416 0.551826 8 0.634511 0.174899 1.410128 8 1.208951 -1.137901 1.126727 9 -0.818533 1.666468 0.875847 9 -1.970688 0.327254 -0.978632 9 -0.403180 -1.149068 -1.152950 9 -1.751044 -1.192463 0.551658 8 2.804368 -0.280419 -0.710283 1 2.322994 -0.734257 0.060595 1 3.676598 -0.023686 -0.399645 8 0.791809 1.255863 -0.967272 1 1.683872 0.744202 -0.952463 1 0.973014 2.181102 -0.761853	-146.3251, 49.3026, 72.0586, 154.6811, 178.9292, 219.8028, 260.3543, 284.4433, 301.4294, 346.7877, 360.6724, 366.8654, 398.8429, 455.9246, 480.5366, 524.7640, 572.1872, 592.4314, 615.8183, 681.7242, 751.1917, 778.9990, 909.6363, 1006.4112, 1144.1584, 1178.5495, 1208.3181, 1237.4715, 1352.2406, 1550.9475, 1624.7314, 1689.1680, 2567.1970, 2888.7471, 3804.3213, 3857.4399
IRC  	

Compound: sCl 25 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -778.234111047535
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.404526 -0.102729 -0.158678 6 0.034254 0.408306 0.152328 8 0.766080 -0.465395 0.988045 8 1.165242 -1.636982 0.246539 1 2.053615 -1.369750 -0.045347 9 -0.113531 1.494110 0.982194 8 0.644104 0.732125 -1.004260 1 1.605443 0.791571 -0.855854 9 -2.113371 0.863791 -0.760818 9 -1.386305 -1.169082 -0.962133 9 -2.029860 -0.437116 0.975584 8 3.370981 0.253816 -0.332380 1 3.626690 0.591064 0.533536 1 4.152231 0.319812 -0.891232	33.9279, 48.3442, 76.1769, 116.7370, 164.3800, 207.5971, 232.5643, 262.9793, 278.8395, 285.3071, 314.5749, 352.1083, 377.7050, 397.3941, 479.3980, 491.5629, 531.8580, 585.8175, 631.6467, 656.0214, 687.7963, 785.5537, 965.8965, 1034.0498, 1076.4672, 1180.9327, 1200.5000, 1231.8247, 1279.5941, 1450.8232, 1474.8038, 1626.3847, 3592.4584, 3661.4694, 3782.2367, 3879.5888

Compound: sCI 25 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -778.151343097919
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.087243 -0.309769 -0.423180 6 -0.300324 0.336446 0.745069 8 0.562981 -0.217347 1.441526 8 1.141377 -1.414420 0.896658 9 -0.890442 1.359501 1.296098 9 -1.936840 0.592432 -0.916534 9 -0.328843 -0.770648 -1.397152 9 -1.800836 -1.316349 0.102686 8 2.962826 -0.076017 -0.560233 1 2.434468 -0.715318 -0.014219 1 3.301488 -0.567780 -1.313216 8 0.878739 1.568034 -0.692410 1 1.724342 1.046292 -0.767222 1 1.110375 2.410320 -0.286886	46.2907, 67.0974, 91.8090, 125.6174, 157.8162, 203.5801, 221.3492, 264.0061, 277.3274, 288.9341, 289.9045, 328.7980, 367.2176, 400.7399, 478.6531, 506.1075, 512.5963, 568.4710, 590.0375, 619.6265, 663.8341, 776.0588, 796.5534, 902.5942, 1034.2265, 1140.0628, 1180.1310, 1242.4727, 1383.1677, 1606.5946, 1647.5553, 1678.8281, 3134.9621, 3275.3006, 3830.4288, 3858.6479

Compound: sCI 25 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -778.153113870118
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.077057 -0.423552 -0.289992 6 -0.213471 0.573107 0.536270 8 0.614289 0.237747 1.414317 8 1.202688 -1.077550 1.192543 9 -0.841564 1.697007 0.803171 9 -1.964096 0.275233 -1.006670 9 -0.380214 -1.189805 -1.110522 9 -1.747493 -1.187118 0.578433 8 2.873625 -0.201596 -0.590203 1 2.368533 -0.672630 0.151143 1 3.159081 -0.873792 -1.215226 8 0.800188 1.222752 -1.014849 1 1.679394 0.693746 -0.977376 1 1.010146 2.146665 -0.830371	-131.8994, 49.7399, 71.5302, 148.2910, 178.8931, 220.1116, 257.5315, 284.2300, 299.6407, 338.1935, 345.6464, 363.6927, 394.7051, 479.8384, 488.8758, 522.9158, 585.5910, 593.2244, 608.6505, 679.4158, 739.0556, 778.5179, 910.2331, 935.9471, 1146.0830, 1180.7008, 1227.9638, 1243.4577, 1355.2067, 1557.3275, 1644.1015, 1693.0530, 2597.1393, 2930.6112, 3800.2592, 3853.4549

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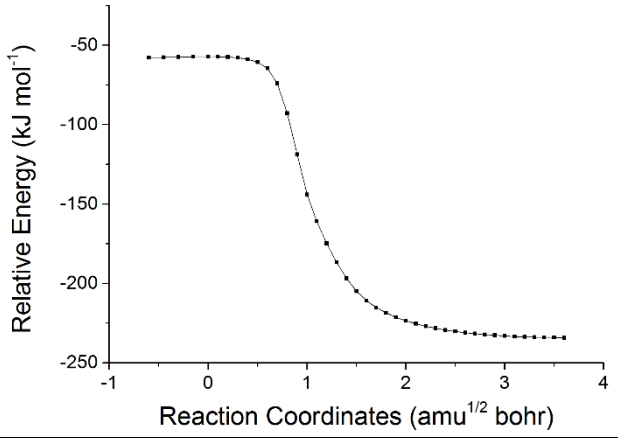

8.10.5 sCl 26 + $(H_2O)_2$

Compound: sCl 26 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -778.155321450549
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.504971 0.099406 0.193399 6 -0.160033 -0.476306 -0.265725 8 0.586751 -1.004163 0.567732 8 1.752981 -1.640438 0.080858 9 -0.001255 -0.619282 -1.534660 9 -2.417557 -0.889230 0.123292 9 -1.438786 0.532881 1.440451 9 -1.895849 1.079132 -0.615166 8 3.287219 0.603792 0.401354 1 2.917263 -0.305750 0.320743 1 4.114254 0.608406 -0.087241 8 0.878010 1.700375 -0.234065 1 1.818974 1.471403 -0.050230 1 0.880874 2.279305 -1.001596	29.4729, 57.0746, 90.7417, 110.8940, 132.9723, 165.3457, 188.1994, 242.3211, 245.6618, 251.7649, 285.3981, 302.2243, 350.6313, 361.6697, 408.5250, 456.8954, 521.4813, 556.2997, 576.4187, 668.3638, 675.6645, 726.7701, 836.6869, 853.3457, 875.4031, 1128.9044, 1186.8392, 1249.0461, 1403.4828, 1632.9929, 1660.5967, 1674.8863, 3334.9174, 3419.1514, 3854.0781, 3865.4630

Compound: sCl 26 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -778.154483796209
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.452057 -0.094944 -0.202984 6 -0.035845 0.328312 0.244444 8 0.643489 0.940770 -0.616381 8 1.899689 1.481311 -0.106517 9 0.026824 0.653674 1.514325 9 -1.969470 -0.968997 0.665102 9 -2.234068 0.992813 -0.218975 9 -1.432751 -0.632623 -1.414317 8 3.030580 -0.790958 -0.439314 1 2.771664 0.195011 -0.357470 1 3.841343 -0.926600 0.058152 8 0.723371 -1.395286 0.379901 1 1.717345 -1.268679 0.095196 1 0.705207 -1.690439 1.298636	-231.7521, 36.0051, 70.1748, 146.3315, 159.4260, 185.6379, 275.1852, 297.2816, 324.5751, 352.2152, 376.7297, 388.5598, 399.7561, 415.8618, 503.1695, 530.5402, 577.9666, 635.6021, 680.1667, 720.5649, 786.4159, 823.5539, 862.7035, 937.3476, 1137.6409, 1181.8605, 1230.4427, 1238.2808, 1358.6367, 1535.1706, 1670.4773, 1707.3520, 2352.8141, 2779.8576, 3800.1789, 3857.8733

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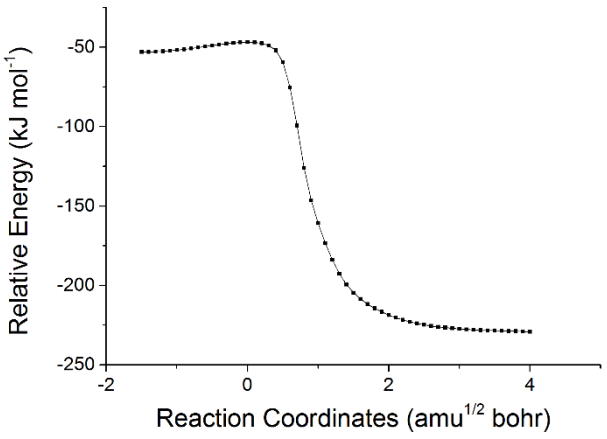
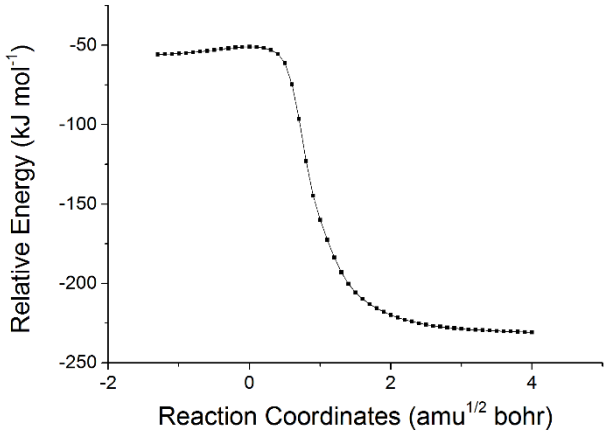


Compound: sCI 26 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -778.234695133756
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.391502 -0.324803 -0.183500 6 -0.060577 0.360168 0.265844 8 0.650426 0.577335 -0.877070 8 1.877358 1.273273 -0.560158 1 2.503994 0.515564 -0.497802 9 -0.415662 1.527793 0.894584 8 0.634214 -0.433231 1.158979 1 0.212620 -0.376145 2.025158 9 -2.119291 -0.605465 0.915204 9 -2.113200 0.467005 -0.974187 9 -1.148361 -1.471151 -0.823439 8 3.269025 -1.063971 -0.100132 1 4.117224 -1.122038 0.349666 1 2.599077 -1.320459 0.546508	41.1071, 60.7539, 94.4583, 129.5898, 168.0954, 191.6362, 221.2917, 237.0399, 249.2516, 304.8284, 316.2066, 339.9198, 370.2838, 386.2925, 400.1450, 519.9118, 527.7303, 588.4687, 604.3415, 728.9488, 739.0615, 825.2194, 938.9418, 1052.5637, 1076.7670, 1161.1253, 1179.2310, 1212.3881, 1326.7694, 1362.8227, 1545.5041, 1626.3435, 3424.4355, 3759.2232, 3792.0834, 3875.4461

Compound: sCI 26 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -778.156341672640
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.505495 0.091967 -0.182594 6 0.145724 -0.463043 0.259704 8 -0.580325 -1.013433 -0.578212 8 -1.759359 -1.639526 -0.100613 9 -0.039231 -0.580917 1.527508 9 1.890669 1.082516 0.615014 9 2.406149 -0.904017 -0.077432 9 1.467986 0.503414 -1.438943 8 -3.304652 0.601187 -0.208372 1 -2.912148 -0.303888 -0.208056 1 -3.817922 0.675253 -1.017456 8 -0.861293 1.702999 0.161215 1 -1.805294 1.458593 0.002872 1 -0.857080 2.277717 0.932501	32.9450, 59.2730, 96.3828, 114.5765, 135.1450, 169.7028, 194.0592, 250.8541, 258.7338, 273.8438, 300.7887, 335.5543, 356.6988, 361.4179, 408.9676, 419.6888, 511.1819, 524.4003, 576.1856, 673.9396, 726.6771, 793.2353, 838.3362, 858.1026, 953.6168, 1129.8197, 1187.6602, 1247.7782, 1403.7621, 1627.8877, 1637.1693, 1664.8016, 3293.5011, 3392.0249, 3847.2631, 3859.1687

Compound: sCl 26 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -778.155935062267
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.456606 0.088286 -0.198395 6 0.036941 -0.328311 0.242080 8 -0.639985 -0.946054 -0.615417 8 -1.893626 -1.493088 -0.108280 9 -0.046269 -0.623819 1.514582 9 1.965682 0.978723 0.656214 9 2.238800 -0.999666 -0.186658 9 1.448326 0.601553 -1.421252 8 -3.088705 0.769786 -0.261179 1 -2.789827 -0.205953 -0.262939 1 -3.460061 0.964938 -1.126053 8 -0.721292 1.424044 0.330129 1 -1.713908 1.278347 0.061623 1 -0.707471 1.754189 1.237248	-216.7111, 40.3464, 71.3754, 145.7554, 159.8329, 190.0347, 275.2563, 296.7082, 321.7700, 352.9757, 365.4023, 383.5055, 400.9371, 423.6081, 502.0856, 530.9374, 569.4630, 584.9973, 673.1975, 718.6764, 776.5858, 821.7894, 865.7069, 1058.9036, 1140.9912, 1183.5082, 1229.8557, 1306.4008, 1365.6796, 1541.4011, 1613.3738, 1666.1703, 2396.9997, 2814.5238, 3796.9692, 3852.1032
IRC	

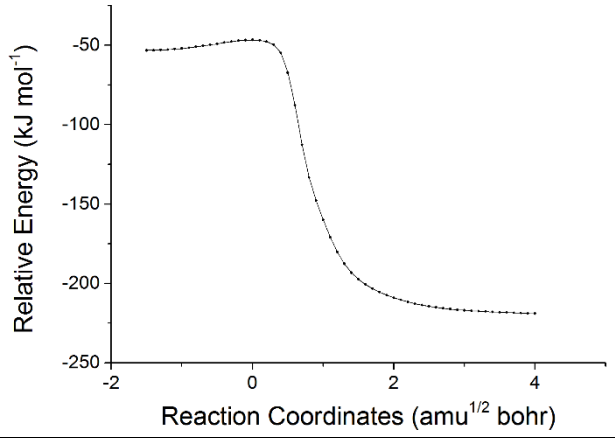


Compound: sCl 26 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -778.235686023368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.378531 -0.337083 -0.171891 6 -0.058616 0.384232 0.252293 8 0.667177 0.532385 -0.893775 8 1.888164 1.250847 -0.604039 1 2.512185 0.498809 -0.471100 9 -0.426818 1.585788 0.801457 8 0.627112 -0.349190 1.201680 1 0.251341 -0.172849 2.072726 9 -2.128952 -0.542988 0.925578 9 -2.085203 0.390208 -1.035037 9 -1.114776 -1.526471 -0.723517 8 3.280512 -1.025707 0.066205 1 3.427652 -1.733253 -0.569030 1 2.529728 -1.301115 0.608085	41.8459, 61.8886, 97.8940, 133.9444, 167.1742, 202.7544, 221.7193, 235.2008, 248.8184, 282.3243, 309.0498, 340.7138, 373.9820, 385.3118, 448.2935, 521.3360, 531.7991, 588.4637, 605.8464, 732.5280, 796.7416, 827.2153, 939.3215, 1050.6581, 1079.8613, 1161.1824, 1181.5318, 1208.9991, 1327.8406, 1357.9245, 1528.8648, 1624.7530, 3406.4916, 3756.1722, 3794.7283, 3870.0375

Compound: sCI 26 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -778.155292325029
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.520553 0.077431 -0.133529 6 0.135438 -0.454670 0.253545 8 -0.530569 -1.060240 -0.597416 8 -1.735393 -1.666024 -0.170800 9 -0.147230 -0.479485 1.505653 9 1.895351 1.053734 0.681438 9 2.401742 -0.932279 -0.020323 9 1.526387 0.507772 -1.390230 8 -3.298053 0.579879 -0.278807 1 -2.896847 -0.320345 -0.267278 1 -4.002248 0.571976 0.375149 8 -0.886250 1.748320 0.139381 1 -1.826386 1.476250 0.011460 1 -0.694596 2.372397 -0.567128	25.7960, 41.9021, 91.7538, 116.0609, 131.6452, 166.6911, 189.2848, 241.5052, 249.2321, 261.3399, 299.9707, 321.0976, 349.3877, 361.8052, 406.4638, 446.2832, 509.0366, 524.6695, 575.3292, 678.4179, 726.8862, 730.8695, 844.2676, 858.9722, 933.6184, 1136.4634, 1190.4264, 1239.2175, 1407.6330, 1630.3118, 1650.7443, 1673.1293, 3312.5611, 3406.4417, 3846.2994, 3859.1966

Compound: sCI 26 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -778.154047110573
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.483665 0.044071 -0.083684 6 -0.005044 -0.255421 0.204566 8 -0.553413 -1.049839 -0.607125 8 -1.871996 -1.524924 -0.202453 9 -0.296320 -0.294613 1.477390 9 1.953513 0.959049 0.758604 9 2.193963 -1.077157 0.059407 9 1.630507 0.489838 -1.337807 8 -3.080035 0.726521 -0.184941 1 -2.743969 -0.245753 -0.204133 1 -3.659142 0.821790 0.576606 8 -0.694641 1.469487 -0.086641 1 -1.730137 1.287986 -0.079072 1 -0.472765 1.740066 -0.987767	-250.6799, 39.0414, 60.9470, 136.9924, 161.6331, 177.9353, 287.5360, 301.9577, 318.5255, 354.5256, 369.5178, 392.4984, 414.7727, 425.6464, 528.2966, 539.3143, 574.3108, 635.7136, 679.6143, 720.4778, 805.9932, 841.1296, 876.5957, 1023.1045, 1148.2582, 1189.5948, 1216.7132, 1332.4466, 1385.5696, 1517.5508, 1651.9311, 1680.8426, 2199.0066, 2688.3510, 3780.5289, 3849.5355

IRC



Compound: sCI 26 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -778.234941477938
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.281619 -0.396869 -0.141349 6 -0.073615 0.502297 0.285331 8 0.679689 0.627928 -0.880580 8 1.863158 1.410381 -0.608218 1 2.514029 0.701364 -0.464738 9 -0.587670 1.698848 0.673107 8 0.589165 -0.024461 1.352062 1 1.313173 -0.592262 1.036499 9 -2.127289 -0.534924 0.882116 9 -1.949836 0.114088 -1.178433 9 -0.840746 -1.623148 -0.487456 8 2.827771 -1.274646 0.090297 1 2.584162 -1.895382 -0.605510 1 3.591648 -1.653679 0.537359	30.8261, 58.0992, 91.0942, 125.3530, 168.5796, 188.2988, 222.2970, 239.3348, 272.1691, 295.7873, 313.8342, 340.1174, 378.3839, 379.9574, 466.4912, 514.4522, 531.0048, 583.5516, 603.2174, 630.9793, 732.1940, 829.7446, 939.0117, 1048.7712, 1086.3898, 1165.0852, 1200.8282, 1208.3361, 1331.2638, 1405.5919, 1457.5082, 1627.6146, 3614.9543, 3656.6230, 3783.3352, 3879.9193

Compound: sCI 26 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -778.154802564593
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.523631 0.070204 -0.117940 6 0.126545 -0.448086 0.244963 8 -0.517977 -1.072454 -0.609207 8 -1.734406 -1.668085 -0.200888 9 -0.192591 -0.438451 1.487670 9 1.887208 1.054233 0.691694 9 2.395072 -0.943889 0.026528 9 1.559768 0.483838 -1.380501 8 -3.302494 0.564233 -0.063406 1 -2.884949 -0.325637 -0.137135 1 -3.976892 0.606944 -0.746286 8 -0.867860 1.766934 0.050317 1 -1.815934 1.508925 -0.029492 1 -0.686495 2.350457 -0.692268	19.4727, 41.9568, 92.4435, 115.0151, 131.1127, 166.1585, 185.4852, 246.9869, 255.5549, 255.9820, 280.3702, 300.0568, 350.8270, 362.2080, 405.1394, 421.3097, 521.6741, 535.5956, 575.1269, 678.9162, 718.8823, 730.9504, 840.7204, 858.5765, 910.2685, 1136.8887, 1190.2595, 1239.3736, 1409.2583, 1630.3548, 1644.9207, 1672.4348, 3327.8774, 3413.8679, 3850.3844, 3863.5024

Compound: sCI 26 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -778.153225068607

Reaction Coordinates:

```
6 -1.482042 -0.041610 -0.082930
6 0.010444 0.247204 0.200130
8 0.556018 1.044842 -0.614002
8 1.877025 1.518238 -0.210042
9 0.304275 0.288980 1.471268
9 -1.956400 -0.952454 0.760697
9 -2.184337 1.084144 0.058772
9 -1.634812 -0.489053 -1.337317
8 3.062989 -0.717905 0.000049
1 2.725841 0.253057 -0.108109
1 3.703589 -0.893273 -0.694674
8 0.686397 -1.465941 -0.099859
1 1.728012 -1.293563 -0.087031
1 0.454186 -1.718206 -1.003343
```

Frequencies (cm^{-1}):

```
-269.4438, 38.7369, 61.8805,
137.6329, 165.4533, 177.4985,
287.8044, 300.9685, 321.0749,
355.1282, 391.5197, 406.9766,
418.2621, 429.1966, 509.3777,
536.6606, 573.7250, 630.1877,
682.9775, 721.9018, 812.5196,
845.7557, 873.0997, 1071.2964,
1151.0672, 1187.7224, 1217.4694,
1320.0152, 1376.8772, 1507.2047,
1621.9928, 1698.8260, 2132.0505,
2622.0161, 3783.7703, 3852.4844
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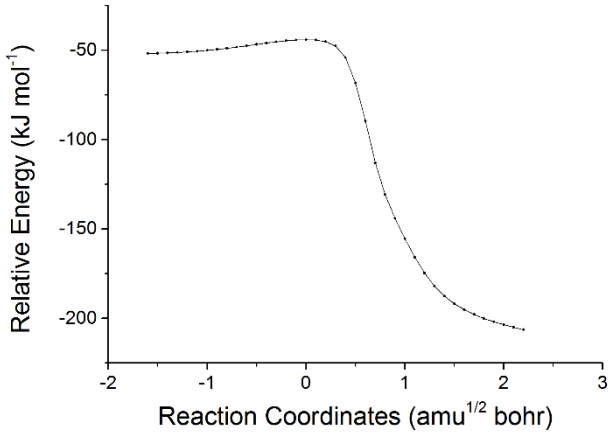
IRC



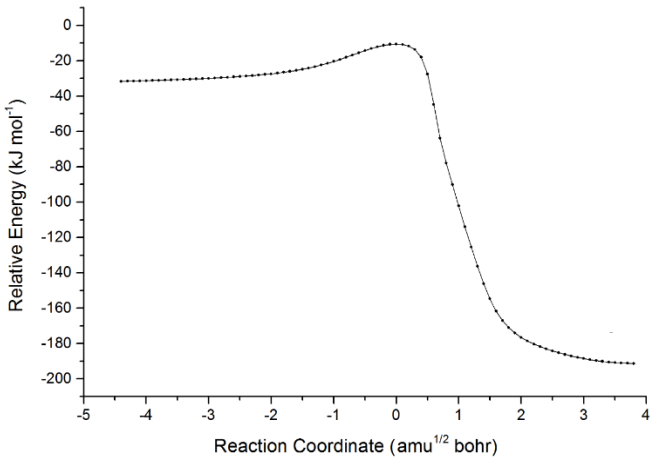
8.11 sCI Reactions with MeOH

Compound: MeOH	**Energy (kJ mol^{-1}):** -115.607115778238
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.667408 -0.020462 0.000000 8 0.748822 0.122098 0.000000 1 1.151097 -0.750378 -0.000000 1 -1.026778 -0.544214 -0.890795 1 -1.026779 -0.544207 0.890799 1 -1.083670 0.984791 -0.000004	290.6856, 1039.0192, 1076.1201, 1170.5975, 1365.7526, 1477.3714, 1498.2111, 1508.8548, 2994.1556, 3039.5029, 3108.4416, 3828.6843

8.11.1 sCI 1 + MeOH

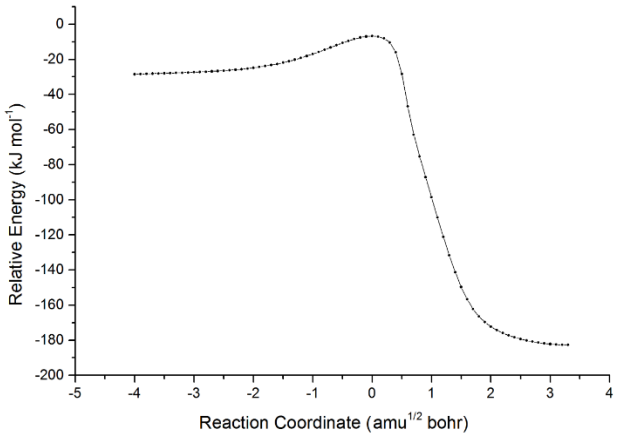
Compound: sCI 1 + MeOH PRC	**Energy (kJ mol^{-1}):** -305.020987250893
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.662111 -0.046788 0.000044 8 1.315288 0.399727 -0.000067 1 0.698704 -0.357599 -0.000052 1 2.893216 -0.640865 -0.889276 1 3.300954 0.835093 0.000016 1 2.893113 -0.640734 0.889478 6 -1.635466 0.998502 0.000005 8 -1.950142 -0.213639 0.000033 8 -0.974471 -1.171188 -0.000023 1 -0.591507 1.299365 -0.000058 1 -2.479754 1.675256 0.000055	24.8880, 82.1748, 110.6320, 111.6029, 135.5092, 259.5276, 549.7940, 665.8058, 696.6622, 879.6470, 1019.2042, 1061.0776, 1138.6918, 1172.9739, 1273.0125, 1420.9590, 1449.4821, 1477.4975, 1497.7786, 1512.0957, 1560.2724, 2992.6031, 3037.4403, 3082.1700, 3095.0315, 3243.6738, 3517.8399

Compound: sCI 1 + MeOH TS1	**Energy (kJ mol^{-1}):** -305.012539571568
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.863745 -0.172056 0.389771 8 0.934811 0.041282 -0.675937 1 0.218702 -0.701416 -0.634231 1 2.400052 -1.106997 0.222573 1 2.571438 0.654242 0.391134 1 1.353139 -0.227500 1.353711 6 -0.701900 1.051055 -0.161035 8 -1.199505 0.166901 0.601952 8 -1.260499 -1.070358 -0.153254 1 -0.936660 1.041876 -1.217190 1 -0.376203 1.963201 0.329508	-303.3420, 135.4580, 151.7227, 188.5069, 331.0013, 453.7042, 543.7435, 799.9595, 865.9194, 1006.5269, 1112.0219, 1165.7576, 1181.7513, 1211.1356, 1251.4969, ,1381.3223, 1464.5139, 1490.1175, 1494.0108, 1518.0904, 1546.2798, 2568.4657, 3021.4453, 3082.0592, 3100.9807, 3116.4553, 3224.8375
IRC	



Compound: sCI 1 + MeOH Pr1	**Energy (kJ mol^{-1}):** -305.089754793660
Reaction Coordinates: 6 1.866681 -0.450981 0.277009 8 0.921620 0.046899 -0.666119 1 -1.363992 -1.344923 -0.391532 1 1.387002 -1.064896 1.042174 1 2.576523 -1.057064 -0.280043 1 2.399568 0.372679 0.762678 6 -0.055601 0.877798 -0.117095 8 -1.003092 0.190929 0.670639 8 -1.879360 -0.542945 -0.220829 1 -0.552119 1.373600 -0.949241 1 0.373190 1.600643 0.586949	**Frequencies (cm^{-1}):** 106.8116, ,132.8786, 193.1857, 247.0967, 336.7449, 481.1437, 625.3832, 875.9852, 931.0861, 997.2289, 1089.2781, 1166.6214, 1175.0153, 1227.8307, 1319.6211, 1377.1010, 1404.1314, 1465.0513, 1483.3431, 1491.0236, 1509.4422, 2998.4938, 3004.6735, 3060.3119, 3105.6338, 3124.8533, 3730.9399

Compound: sCI 1 + MeOH TS2	**Energy (kJ mol^{-1}):** -305.010689091126
Reaction Coordinates: 6 -2.062272 -0.126803 0.198882 8 -0.873223 0.024855 -0.569815 1 -0.214440 -0.747176 -0.352060 1 -1.847455 -0.183951 1.270177 1 -2.707715 0.727406 0.003845 1 -2.578012 -1.040668 -0.100269 6 0.640245 1.001204 0.262268 8 1.540533 0.241828 -0.206971 8 1.213700 -1.115998 0.192501 1 0.218716 0.788854 1.237825 1 0.612990 2.003651 -0.152141	**Frequencies (cm^{-1}):** -314.5301, 101.6876, 161.3604, 201.5254, 339.3872, 430.7475, 527.8844, 805.4684, 867.5779, 1023.6465, 1084.8305, 1162.9890, 1178.4686, 1211.8856, 1228.6814, 1382.1058, 1466.4546, 1494.9678, 1496.1083, 1518.4641, 1588.9879, 2483.6260, 3006.1591, 3068.6532, 3092.7445, 3110.5584, 3214.1642
IRC	



Compound: sCI 1 + MeOH Pr2	**Energy (kJ mol^{-1}):** -305.086315844733
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.116714 -0.273591 0.130007 8 -0.830169 -0.175072 -0.456215 1 1.492242 -1.320331 -0.436822 1 -2.675006 -1.004118 -0.449884 1 -2.647746 0.684065 0.098946 1 -2.055814 -0.610559 1.170591 6 0.028141 0.707631 0.225843 8 1.324359 0.556662 -0.254477 8 1.836333 -0.710029 0.232219 1 -0.011022 0.520149 1.305723 1 -0.215404 1.754062 0.004136	60.9145, 147.5248, 209.1549, 293.1227, 338.1013, 403.9749, 592.9671, 884.4403, 980.1253, 1063.0713, 1112.7765, 1149.6046, 1181.9207, 1223.0636, 1284.8284, 1380.7824, 1419.0086, 1472.8164, 1492.5940, 1494.2584, 1510.0321, 2973.2882, 2985.8560, 3021.2134, 3028.7648, 3121.4429, 3730.7851

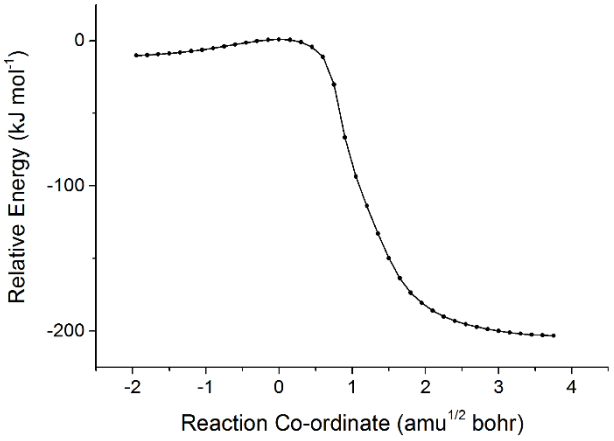
8.11.2 sCI 23 + MeOH

Compound: sCI 23 + MeOH PRC	**Energy (kJ mol^{-1}):** -641.819794756621
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.976708 -0.101676 -0.000009 6 0.996614 1.054995 -0.000301 8 -0.249822 0.916410 -0.000190 8 -0.792449 -0.316205 0.000213 1 1.349980 2.076669 -0.000628 9 1.846753 -0.862233 1.088123 9 1.846623 -0.862894 -1.087664 9 3.216292 0.424173 -0.000243 8 -3.584966 0.541108 0.000387 6 -4.538112 -0.507407 -0.000285 1 -4.454459 -1.141356 -0.889827 1 -5.526454 -0.049380 -0.000250 1 -4.454787 -1.142196 0.888688 1 -2.694655 0.158864 0.000358	7.8778, 13.7557, 25.1694, 81.2882, 84.6164, 111.2334, 128.0235, 216.1099, 246.9664, 334.8528, 479.5373, 509.5491, 535.8498, 587.6098, 593.6590, 759.4478, 800.7172, 884.0324, 930.6324, 1060.9119, 1120.5796, 1157.2830, 1171.8072, 1183.6161, 1242.3480, 1368.3585, 1435.6089, 1476.2118, 1497.0762, 1511.4617, 1558.0757, 2979.1708, 3018.1652, 3089.2369, 3213.6535, 3666.0389

Compound: sCI 23 + MeOH TS1	**Energy (kJ mol^{-1}):** -641.812455653684
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.150706 -0.248514 0.005650 6 -0.071605 0.205229 -0.809726 8 -0.611723 1.344246 -0.747619 8 -0.733833 1.770494 0.616132 1 -0.154234 -0.288556 -1.773672	-238.8203, 43.8051, 115.7554, 142.3150, 155.5798, 189.5276, 207.0024, ,276.0069, 319.3805, 350.2625, 450.7578, 518.3362, 556.3651, 567.6475, 740.0036,

9 2.171590 0.555970 -0.346428 9 1.053301 -0.254276 1.323237 9 1.454370 -1.497428 -0.400749 6 -2.690554 -0.860532 -0.159831 8 -1.391399 -0.737195 0.430712 1 -1.334405 0.156953 0.889988 1 -2.897122 -0.031950 -0.840073 1 -2.719147 -1.804051 -0.699014 1 -3.444072 -0.868249 0.627885	808.7216, 866.5284, 964.4575, 1019.1294, 1049.3368, 1140.5097, 1153.8883, 1176.3217, 1185.9025, 1284.6473, 1345.3465, 1461.2570, 1472.4469, 1494.5943, 1512.0143, 1557.6297, 2991.1165, 3032.5103, 3091.3535, 3130.1032, 3152.3093

IRC



Compound: sCI 23 + MeOH Pr	**Energy (kJ mol^{-1}):** -641.901373422778
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.056705 -0.301665 -0.003500 6 -0.397832 -0.082695 -0.480375 8 -0.714080 1.258866 -0.757921 8 -0.472266 2.067993 0.418501 1 -0.482679 -0.547118 -1.470054 9 1.903483 0.451576 -0.718120 9 1.246603 -0.043594 1.291534 9 1.385379 -1.595895 -0.213342 6 -2.521234 -1.032375 -0.044004 8 -1.230634 -0.673220 0.454765 1 -1.272492 1.909798 0.941578 1 -2.430630 -1.768178 -0.847228 1 -3.059988 -1.473098 0.789745 1 -3.063378 -0.158881 -0.410168	60.3433, 90.3684, 124.3320, 151.2099, 188.2054, 212.0435, 237.2391, 305.6409, 340.8455, 363.2585, 422.9918, 528.8540, 570.8971, 655.1884, 754.2538, 868.8478, 912.9361, 1005.4468, 1038.2480, 1119.0917, 1138.1004, 1176.0669, 1184.7505, 1222.8966, 1280.1943, 1359.9493, 1384.1052, 1403.7418, 1478.3985, 1493.7604, 1507.6477, 3013.0098, 3019.4411, 3075.1426, 3138.0241, 3726.2609

Compound: sCI 23 + MeOH TS2	**Energy (kJ mol^{-1}):** -641.809840895326
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.960039 -0.367008 0.033781 6 0.122443 0.567493 -0.851126 8 -0.143691 1.775553 -0.591170 8 -0.619507 1.888320 0.773109 1 0.227665 0.343139 -1.908782 9 2.222760 0.096404 -0.002129 9 0.603569 -0.516218 1.299182 9 0.954865 -1.586276 -0.548416 6 -2.133213 -1.321958 0.136887 8 -1.682887 -0.076672 -0.411040 1 -1.606554 0.652054 0.300384 1 -2.003882 -2.088661 -0.622590 1 -1.581375 -1.594839 1.034505 1 -3.193516 -1.225657 0.374309	-277.7025, 52.5164, 87.4164, 135.7958, 147.4743, 219.8415, 244.7700, 290.8680, 320.4487, 370.4519, 440.5767, 514.9018, 547.2127, 570.6901, 736.4417, 796.0657, 859.8538, 956.7795, 1013.0329, 1054.6223, 1134.6948, 1157.8251, 1176.4975, 1200.3395, 1281.7528, 1349.0475, 1456.1694, 1477.7089, 1495.4363, ,1506.8177, 1574.5134, 2755.9507, 3037.8079, 3105.9950, 3134.6294, 3150.9265

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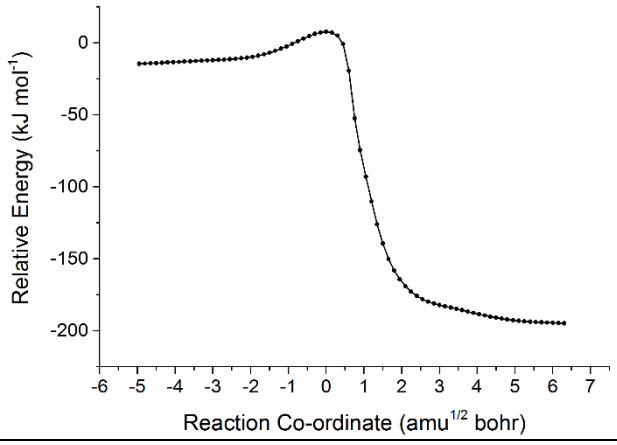

8.11.3 sCI 24 + MeOH

Compound: sCI 24 + MeOH PRC1	**Energy (kJ mol^{-1}):** -641.824942996462
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.702464 -0.317385 0.000001 6 -0.267270 0.153707 -0.000011 8 -0.081319 1.391538 0.000007 8 1.182001 1.890171 -0.000002 1 0.567221 -0.546139 -0.000033 9 -1.920794 -1.080498 -1.085601 9 -2.575951 0.686259 0.000039 9 -1.920758 -1.080548 1.085575 6 3.987682 -0.820759 0.000021 8 2.596940 -0.526234 -0.000035 1 2.443182 0.434526 -0.000022 1 4.483773 -0.424164 0.890025 1 4.483852 -0.424129 -0.889923 1 4.090831 -1.904185 0.000005	18.1908, 34.4140, 66.9668, 84.2489, 109.7187, 124.1555, 174.7514, 207.8882, 243.9959, 388.4638, 395.5289, 429.3178, 556.4368, 560.2631, 620.7028, 699.2395, 891.0590, 945.0049, 957.2409, 1056.3515, 1128.5630, 1140.7914, 1173.1779, 1183.4579, 1280.8269, 1379.4922, 1421.3731, 1477.8260, 1498.3830, 1510.6159, 1557.8223, 3000.7618, 3049.0279, 3103.5151, 3105.0225, 3595.1865

Compound: sCI 24 + MeOH TS1	**Energy (kJ mol^{-1}):** -641.819503461060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.228989 0.036844 -0.016691 6 -0.081692 -0.623835 -0.423002 8 -0.677064 -1.303157 0.463605 8 -1.989265 -1.630824 -0.052192 1 -0.219375 -0.847004 -1.473984 9 2.226195 -0.857648 -0.132697 9 1.206699 0.483418 1.240251 9 1.494590 1.062726 -0.834186 6 -1.732897 1.659385 0.402170 8 -1.479661 0.761487 -0.688621 1 -2.046041 -0.080869 -0.548528 1 -1.570998 1.168913 1.362818 1 -2.766982 1.999803 0.343730 1 -1.062445 2.508280 0.298454	-243.0166, 36.9354, 105.3890, 136.5967, 150.0916, 183.1191, 202.5561, 273.7948, 356.5155, 382.0647, 434.5178, 510.9263, 556.1704, 626.3829, 699.0313, 842.7075, 874.2598, 972.1449, 1093.6682, 1098.0531, 1156.7695, 1179.4347, 1180.7510, 1231.7325, 1265.7809, 1339.2162, 1464.9060, 1477.8580, 1495.2058, 1509.6940, 1543.6809, 2693.1227, 3032.9744, 3096.4649, 3134.2897, 3170.8923

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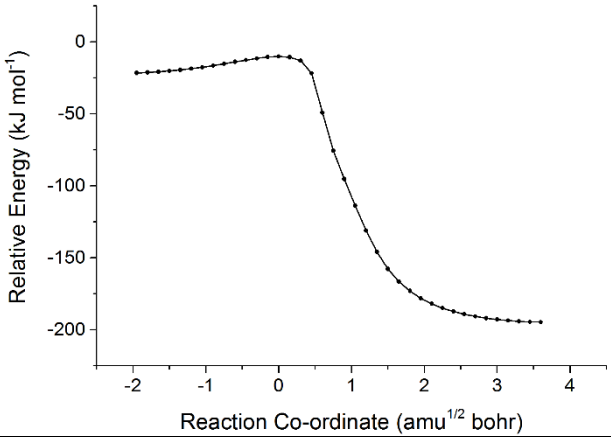

Compound: sCI 24 + MeOH Pr1	**Energy (kJ mol^{-1}):** -641.900575600613
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.077346 -0.234150 -0.016420 6 0.397023 -0.161881 -0.487208 8 1.120044 -0.864566 0.498306 8 2.346263 -1.329349 -0.110191 1 0.458794 -0.690367 -1.437924 9 -1.840623 0.563469 -0.781733 9 -1.541369 -1.486609 -0.135968 9 -1.241862 0.145906 1.262837 6 0.843658 2.057974 0.355278 8 0.867172 1.118444 -0.729322 1 2.958803 -0.610424 0.104143 1 -0.166490 2.428275 0.531427 1 1.236148 1.617870 1.271989 1 1.479588 2.881851 0.043896	61.1974, 99.9853, 120.8446, 175.3253, 192.0609, 226.6944, 232.3815, 305.6868, 353.7993, 357.0616, 405.5817, 529.1777, 562.7402, 651.7204, 731.2299, 869.2845, 929.3750, 956.3906, 1042.2889, 1126.8783, 1165.2849, 1170.3066, 1178.5134, 1221.2817, 1262.6593, 1355.1356, 1386.0573, 1406.5670, 1476.3858, 1500.9000, 1509.1502, 3034.6652, 3094.0915, 3100.0399, 3134.7282, 3734.0248

Compound: sCI 24 + MeOH TS2	**Energy (kJ mol^{-1}):** -641.817837970547
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.246729 -0.152999 -0.014850 6 -0.087939 0.463953 -0.409750 8 -0.388112 1.568790 0.119735 8 -1.780107 1.835183 -0.174680 1 -0.512401 0.177832 -1.365617 9 1.218922 -1.471246 -0.265562 9 2.222144 0.388616 -0.768270 9 1.542659 0.038787 1.265197 6 -2.160149 -1.627810 -0.199932 8 -1.501347 -0.588883 0.526825 1 -1.989149 0.295222 0.387213 1 -1.571607 -2.535336 -0.094325 1 -3.153390 -1.786818 0.221191 1 -2.262298 -1.375899 -1.258594	-225.5585, 40.1970, 100.8561, 103.6552, 163.1262, 184.2740, 200.7893, 274.4572, 346.5777, 380.2987, 428.4281, 494.4856, 553.9362, 609.1866, 696.1118, 844.6004, 876.1550, 1000.2079, 1049.8813, 1073.6859, 1149.3181, 1173.9607, 1179.1282, 1204.5798, 1277.1445, 1335.9007, 1468.1314, 1485.2395, 1496.1987, 1511.5663, 1570.4721, 2775.1052, 3017.4396, 3080.9557, 3130.7253, 3154.6612

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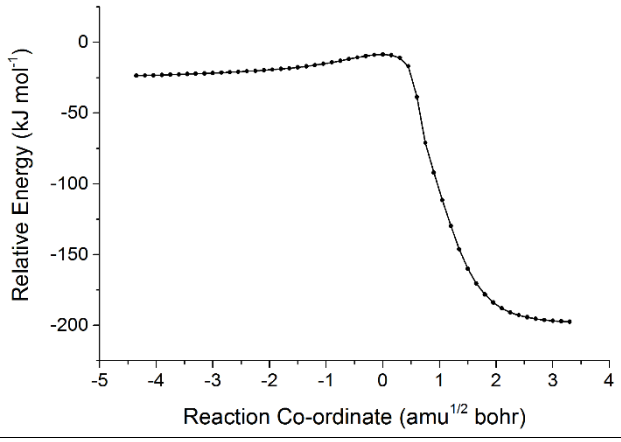

Compound: sCI 24 + MeOH Pr2	**Energy (kJ mol^{-1}):** -641.900995173475
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.140921 -0.070875 -0.025442 6 0.390369 -0.091534 -0.230218 8 0.795574 -1.359801 0.194497 8 2.159133 -1.540207 -0.248752 1 0.593059 0.037779 -1.298686 9 -1.746540 -0.979668 -0.804939 9 -1.491807 -0.301256 1.242750 9 -1.613723 1.144187 -0.373417 6 1.430951 2.061296 -0.178662 8 1.007046 0.896056 0.530933 1 2.647360 -1.258947 0.539414 1 2.015439 2.648362 0.524422 1 2.056613 1.789365 -1.032606 1 0.579747 2.652358 -0.519588	57.8629, 68.4967, 113.4587, 145.8866, 174.8856, 236.2027, .0564, 318.4633, 344.6182, 369.3135, 416.0334, 523.7378, 563.2944, 600.2046, 710.5586, 874.5574, 953.2717, 1005.4349, 1096.5989, 1118.0767, 1151.8004, 1169.1534, 1177.0464, 1226.9317, 1272.1301, 1359.1766, 1388.8027, 1401.1096, 1480.1900, 1494.4337, 1510.4290, 3013.4252, 3022.8458, 3078.2457, 3132.4287, 3731.7653

8.11.4 sCI 25 + MeOH

Compound: sCI 25 + MeOH PRC1	**Energy (kJ mol^{-1}):** -740.991754000359
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.345909 -0.507442 -0.044013 6 0.625157 0.851684 -0.146677 8 -0.223135 1.293586 0.635300 8 -0.649103 0.469357 1.681353 9 0.980931 1.633422 -1.120889 9 2.043850 -0.548257 1.090717 9 0.492606 -1.514647 -0.088400 9 2.194596 -0.607178 -1.072000 8 -2.380149 -0.513216 -0.386899 6 -3.780639 -0.285373 -0.442830 1 -4.331255 -0.968623 0.211071 1 -4.097218 -0.463621 -1.469291 1 -4.040672 0.743369 -0.173975 1 -2.062164 -0.332229 0.510432	13.4464, 24.6617, 45.5949, 55.0213, 91.4055, 120.5258, 153.4675, 186.3622, 223.7360, 286.8126, 294.2847, 363.6197, 481.8579, 499.8008, 579.4303, 601.6396, 627.1066, 673.1296, 778.5503, 913.7607, 1056.2770, 1114.3121, 1156.3328, 1172.9210, 1189.8948, 1224.7012, 1395.9169, 1416.2135, 1477.3762, 1497.2475, 1511.3971, 1608.5151, 2989.7309, 3033.1589, 3096.4651, 3665.396

Compound: sCI 25 + MeOH TS1	**Energy (kJ mol^{-1}):** N/A
Reaction Coordinates: N/A	**Frequencies (cm^{-1}):** N/A

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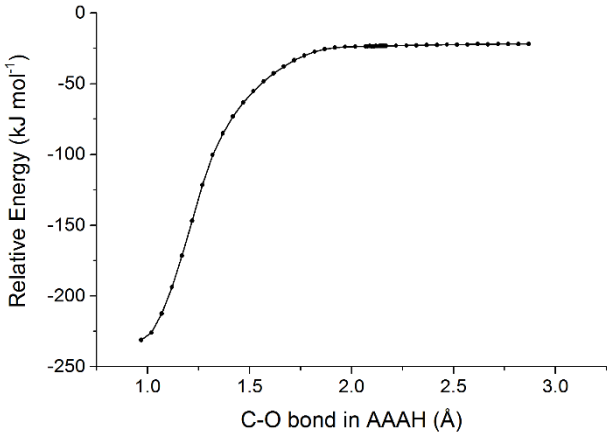

Compound: sCI 25 + MeOH Pr1	**Energy (kJ mol^{-1}):** -741.086414234267
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.143419 -0.203351 -0.157986 6 0.355218 -0.121118 0.283497 8 0.716882 1.129692 0.829131 8 0.469736 2.151148 -0.157813 9 0.498577 -0.935162 1.372468 9 -1.922991 0.388266 0.751186 9 -1.356176 0.367116 -1.344599 9 -1.504495 -1.492389 -0.247342 6 2.503829 -0.784249 -0.483154 8 1.114227 -0.524834 -0.762691 1 1.325266 2.209555 -0.608262 1 2.606413 -1.691707 0.108214 1 2.972764 -0.916680 -1.452615 1 2.960785 0.052604 0.044084	50.7280, 91.7135, 115.4661, 143.9077, 175.5203, 189.7637, 228.0648, 279.0368, 301.0774, 343.7678, 377.1871, 404.5267, 490.8650, 534.0094, 578.3152, 651.8784, 719.7240, 780.8109, 976.3218, 985.8803, 1069.1732, 1120.5552, 1156.4130, 1178.4296, 1186.2852, 1208.0363, 1225.0568, 1353.0381, 1398.3361, 1478.0025, 1493.4508, 1511.1965, 3047.7620, 3118.8728, 3154.7933, 3731.0958

Compound: sCI 25 + MeOH PRC2	**Energy (kJ mol^{-1}):** -740.993837410730
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.929081 -0.620812 -0.234927 6 -0.496165 0.618695 0.577499 8 -0.182377 1.733354 0.147822 8 0.153174 1.822995 -1.219691 9 -0.703493 0.531270 1.857480 9 -2.153690 -0.360273 -0.719156 9 -0.130295 -0.942005 -1.232427 9 -1.017064 -1.660041 0.600950 8 1.994666 0.171217 0.315203 6 2.917818 -0.871055 0.009075 1 1.882285 0.743176 -0.459932 1 2.565636 -1.494846 -0.815822 1 3.014127 -1.486422 0.900852 1 3.899690 -0.463959 -0.243262	8.7072, 46.5863, 71.4762, 97.4421, 106.1329, 151.1997, 166.6269, 198.8084, 241.5571, 290.2502, 301.1464, 367.8671, 479.2797, 504.8591, 573.9102, 587.2462, 621.5557, 661.9547, 776.3573, 904.1488, 1047.7881, 1118.3302, 1138.6682, 1173.3138, 1174.2899, 1238.6741, 1384.8004, 1408.7191, 1477.5542, 1498.1583, 1510.5444, 1615.5861, 3010.9504, 3063.2416, 3114.2077, 3671.1396

Compound: sCI 25 + MeOH TS2	**Energy (kJ mol^{-1}):** -740.993170960665
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.912032 -0.498276 -0.251751 6 0.224113 0.640651 0.542940 8 -0.042847 1.794029 0.143502 8 -0.657774 1.759785 -1.178840 9 0.482013 0.543914 1.818389 9 0.836580 -1.628139 0.462242 9 0.429997 -0.723657 -1.457506 9 2.206117 -0.152187 -0.357672 6 -2.312308 -1.258884 0.017758 8 -1.725805 0.002627 0.354061 1 -2.151755 -1.932718 0.855253 1 -3.384317 -1.121322 -0.131474 1 -1.872395 -1.683438 -0.884327 1 -1.715513 0.625624 -0.431989	-139.5049, 45.0230, 110.9201, 124.5856, 127.9697, 211.7240, 234.6986, 259.1681, 269.3948, 299.0881, 353.7192, 373.6648, 477.4372, 520.0065, 591.1868, 608.4627, 656.8282, 774.8334, 887.3562, 919.3007, 1037.4115, 1130.0942, 1166.9577, 1176.9158, 1178.2235, 1243.7823, 1350.6568, 1454.6869, 1476.6927, 1497.6563, 1508.5865, 1591.4098, 3027.0633, 3066.5636, 3095.9547, 3132.7609
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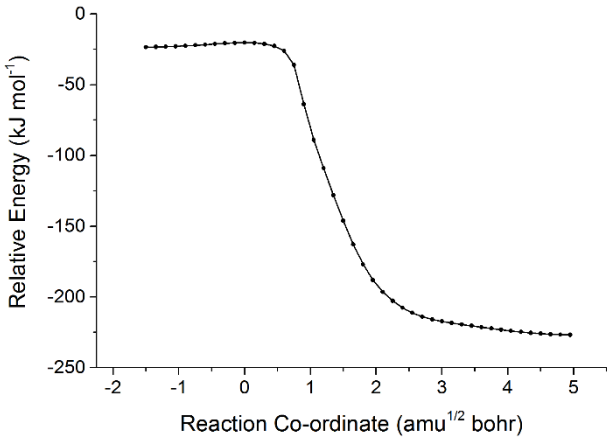	

Compound: sCI 25 + MeOH Pr2	**Energy (kJ mol^{-1}):** -741.084841781096
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.344807 -0.941573 -0.121459 6 0.112414 0.462115 0.425148 8 -0.961502 1.339061 0.593550 8 -1.542744 1.619546 -0.695240 9 0.530358 0.245318 1.708747 9 -1.503957 -1.307551 0.423963 9 -0.478617 -0.930906 -1.452747 9 0.574092 -1.877788 0.186432 6 2.314643 0.392960 -0.558851 8 1.067317 1.074188 -0.322164 1 -0.984830 2.351446 -1.000773 1 2.185348 -0.422482 -1.268434 1 2.731827 0.020531 0.374593 1 2.972709 1.145487 -0.981134	53.5293, 94.1894, 117.9877, 172.1974, 184.4551, 227.5704, 251.8725, 293.5800, 311.8578, 346.8714, 385.0132, 404.2358, 495.8009, 535.1331, 590.8703, 649.2973, 667.2216, 763.0140, 973.6865, 1021.0925, 1090.3159, 1116.6744, 1163.8665, 1176.1525, 1190.3010, 1201.4369, 1229.9396, 1320.1716, 1407.5733, 1485.8850, 1500.9230, 1505.6670, 3051.1521, 3125.5750, 3152.1045, 3720.6253

8.11.5 sCI 26 + MeOH

Compound: sCI 26 + MeOH PRC1	**Energy (kJ mol^{-1}):** -740.999159807260
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.490530 -0.385650 -0.110808 6 0.352908 0.588183 0.182951 8 -0.223060 1.173232 -0.746175 8 -1.277295 2.020177 -0.431860 9 0.090667 0.808213 1.421679 9 2.631497 0.105665 0.394281 9 1.631711 -0.559880 -1.418454 9 1.242669 -1.558110 0.473031 6 -3.154391 -1.296185 -0.266739 8 -2.245899 -0.501111 0.485391 1 -2.363558 0.431126 0.246002 1 -3.008124 -1.176368 -1.344319 1 -4.193753 -1.058374 -0.023763 1 -2.967710 -2.335846 -0.004026	23.4150, 30.2598, 55.7144, 93.4399, 96.9298, 128.3982, 163.7270, 180.7896, 193.8496, 298.6344, 348.4901, 371.8411, 406.8468, 513.5737, 576.3078, 606.4957, 668.9614, 728.7800, 858.6425, 879.7724, 1052.8820, 1112.2481, 1153.0375, 1174.2597, 1175.2901, 1231.5187, 1405.4956, 1405.7647, 1477.6171, 1497.5943, 1511.8428, 1627.0351, 2996.8581, 3043.5378, 3102.7127, 3663.0055

Compound: sCI 26 + MeOH TS1	**Energy (kJ mol^{-1}):** -740.997867488158
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.259490 0.148992 -0.102836 6 0.059196 -0.610304 0.115493 8 0.678664 -1.019101 -0.894231 8 2.007574 -1.470926 -0.516689 9 0.126921 -1.208161 1.270269 9 -2.261522 -0.733491 -0.215233 9 -1.202728 0.879234 -1.214396 9 -1.509496 0.945964 0.934208 6 1.711322 1.877478 -0.137315 8 1.459590 0.746031 0.708515 1 2.061477 -0.003075 0.413809 1 1.599694 1.616308 -1.190411 1 2.726097 2.234749 0.039112 1 1.001370 2.655080 0.131037	-205.1661, 38.2984, 102.6548, 121.0210, 144.8702, 183.0251, 193.0694, 249.3440, 283.4880, 313.9283, 365.6897, 394.5012, 438.0071, 518.7592, 577.9844, 655.4661, 716.1101, 804.1347, 841.3071, 1005.0264, 1037.8971, 1137.6091, 1170.9206, 1179.4643, 1192.0744, 1221.4657, 1363.3945, 1464.4646, 1474.2037, 1496.0565, 1509.8960, 1567.7328, 3017.9730, 3045.0308, 3096.6112, 3135.6940

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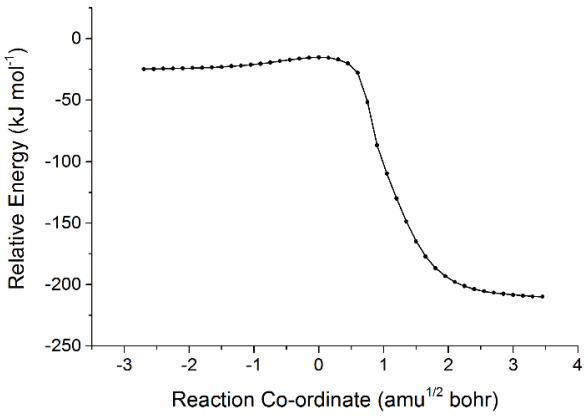
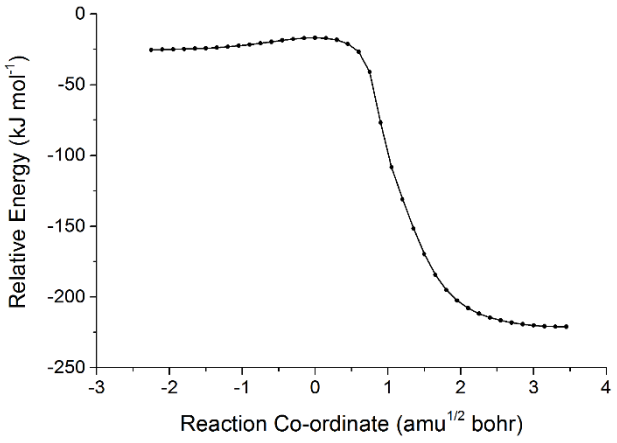


Compound: sCI 26 + MeOH Pr1	**Energy (kJ mol^{-1}):** -741.083786682520
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.162766 -0.094593 -0.145678 6 -0.336932 -0.199013 0.310960 8 -0.989709 -0.731512 -0.802437 8 -2.349799 -1.046730 -0.429102 9 -0.363652 -1.069577 1.347633 9 1.874669 0.510363 0.811497 9 1.684982 -1.300826 -0.366239 9 1.282160 0.628147 -1.273515 6 -0.966001 2.093138 -0.078952 8 -0.862075 0.962079 0.798518 1 -2.836987 -0.340649 -0.878001 1 -0.005667 2.597393 -0.179178 1 -1.327022 1.802088 -1.065158 1 -1.680096 2.760303 0.394142	49.3012, 91.7056, 126.2046, 156.2736, 168.1687, 187.3095, 219.5661, 279.4858, 298.1538, 340.6490, 375.8051, 386.4420, 506.4326, 535.9658, 569.5700, 631.1461, 731.8482, 792.7966, 939.1143, 1040.9147, 1064.8271, 1121.6918, 1172.9430, 1174.9616, 1188.9573, 1201.2160, 1226.1309, 1319.3342, 1396.8534, 1481.1796, 1499.2622, 1511.3160, 3040.3468, 3106.9472, 3143.4978, 3740.4493

Compound: sCI 26 + MeOH PRC2	**Energy (kJ mol^{-1}):** -740.999519026160
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.478552 -0.363963 -0.107978 6 0.302930 0.526805 0.282388 8 -0.096395 1.409091 -0.489724 8 -1.199076 2.162088 -0.104616 9 -0.174435 0.358706 1.466674 9 1.147628 -1.644957 0.055155 9 1.832907 -0.149597 -1.366851 9 2.519460 -0.092485 0.695326 8 -2.108488 -0.523532 -0.567881 6 -3.143139 -1.265147 0.067307 1 -3.232368 -1.014743 1.128483 1 -4.109511 -1.101912 -0.417281 1 -2.885668 -2.318824 -0.021184 1 -2.300880 0.423135 -0.495280	27.2164, 29.1571, 44.1111, 98.3915, 112.5842, 130.8381, 155.6303, 186.9520, 189.4560, 296.7684, 352.8434, 370.3431, 406.8896, 513.4863, 563.0249, 576.8378, 667.3351, 727.7428, 855.7292, 873.3712, 1053.6440, 1116.0326, 1147.1925, 1173.5514, 1174.1936, 1235.5851, 1392.7941, 1416.8320, 1478.0135, 1498.0017, 1511.2876, 1628.5936, 2998.5418, 3046.4055, 3105.3834, 3683.5289

Compound: sCI 26 + MeOH TS2	**Energy (kJ mol^{-1}):** -740.997917500017
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.307922 0.174914 -0.088889 6 -0.030787 -0.497853 0.252216 8 -0.350067 -1.530668 -0.371599 8 -1.745683 -1.865783 -0.135037 9 -0.452090 -0.240559 1.461252 9 1.258492 1.470852 0.227443 9 2.282346 -0.398716 0.633781 9 1.590182 0.043528 -1.376615 8 -1.427798 0.665981 -0.686305 6 -2.123589 1.697954 0.021513 1 -1.953859 -0.183444 -0.649350 1 -3.062137 1.912886 -0.490910 1 -2.331973 1.403900 1.050571 1 -1.495299 2.584383 0.011431	-197.6026, 42.9807, 90.8632, 104.7350, 158.1694, 177.4376, 189.3850, 254.1702, 291.5018, 322.0428, 363.0570, 384.2663, 427.2196, 511.8214, 577.6791, 650.3933, 714.1091, 800.7403, 839.3112, 931.2749, 1039.6013, 1135.8987, 1168.9848, 1175.3687, 1181.7913, 1234.0324, 1363.7070, 1458.9705, 1475.8815, 1496.5038, 1509.9165, 1590.7369, 3030.0270, 3094.6498, 3118.1393, 3138.0592
IRC  	

Compound: sCI 26 + MeOH Pr2	**Energy (kJ mol^{-1}):** -741.087346378048
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.193125 -0.130966 -0.075831 6 -0.360430 -0.102593 0.125412 8 -0.775470 -1.369380 -0.236340 8 -2.208064 -1.455681 -0.094286 9 -0.581278 0.131016 1.458852 9 1.767040 -1.081280 0.664166 9 1.500076 -0.340829 -1.358925 9 1.711964 1.054975 0.288796 6 -1.137958 2.174483 -0.141075 8 -0.976074 0.836339 -0.650734 1 -2.502510 -1.133336 -0.960161 1 -1.617729 2.721975 -0.946229 1 -1.775055 2.172851 0.740006 1 -0.176486 2.627805 0.090227	44.9757, 73.5984, 126.1443, 143.4334, 171.5709, 224.3379, 239.8204, 283.2250, 310.2977, 332.6826, 377.7186, 389.2323, 504.7051, 544.3302, 584.7558, 623.1479, 729.8109, 784.1960, 941.3039, 1035.3797, 1067.2085, 1104.9170, 1170.5624, 1179.6748, 1184.6668, 1202.5637, 1226.4720, 1325.3801, 1408.3648, 1484.1721, 1496.9524, 1509.2122, 3057.9428, 3133.2275, 3152.2286, 3722.1372

9.0 Reaction Coordinates for O_3 + Alkene 19 (Z-2-hexene):

Compound: Z-nPrCHCHMe + O_3 POZ 1.1	**Energy (kJ mol^{-1}):** -460.837557968568
Reaction Coordinates: 6 -1.121781 -0.538109 -0.363984 6 0.232753 -0.546875 0.327289 6 1.034795 0.794899 0.457509 6 0.578645 1.988872 -0.359011 1 0.494529 1.736178 -1.414402 1 -0.381339 2.359445 -0.000790 1 1.304082 2.796003 -0.260311 1 1.103459 1.058865 1.516162 8 2.344914 0.444848 -0.025338 8 2.391771 -0.993450 0.090681 8 1.116566 -1.369861 -0.438096 1 0.137397 -0.982671 1.326232 6 -2.255938 -0.032661 0.532789 1 -2.039288 0.980685 0.879972 6 -3.610000 -0.045420 -0.173926 1 -3.602259 0.598698 -1.055106 1 -3.871797 -1.052492 -0.503622 1 -4.403592 0.304967 0.486573 1 -2.306261 -0.655882 1.429757 1 -1.072146 0.046103 -1.283725 1 -1.339642 -1.566429 -0.662709	**Frequencies (cm^{-1}):** 38.948, 72.4847, 105.2937, 164.8822, 230.6436, 239.7368, 279.2161, 316.6664, 348.6195, 375.3741, 442.7818, 540.8068, 699.172, 709.64, 729.5434, 769.1881, 776.3232, 879.6038, 904.4101, 910.8874, 938.3966, 991.767, 1042.8776, 1050.7188, 1069.8352, 1082.4588, 1125.8977, 1174.0859, 1182.0604, 1260.4194, 1307.2761, 1316.7895, 1330.4913, 1357.2595, 1378.8738, 1393.5233, 1407.2333, 1418.0578, 1424.5298, 1482.8659, 1494.4781, 1496.3118, 1500.79, 1503.2568, 1515.612, 3004.0082, 3015.5799, 3024.3001, 3026.8316, 3032.0696, 3040.9982, 3045.1762, 3075.0331, 3085.8692, 3089.9411, 3105.7869, 3120.3813

Compound: Z-nPrCHCHMe + O_3 POZ 1.2	**Energy (kJ mol^{-1}):** -460.836106562684
Reaction Coordinates: 6 1.115922 -0.133463 0.881547 6 -0.024144 -0.456056 -0.073275 6 -0.975184 0.701068 -0.541078 6 -0.904691 2.031756 0.183359 1 -1.023354 1.903306 1.257684 1 0.042967 2.531407 -0.015346 1 -1.704413 2.681710 -0.170862 1 -0.845754 0.844834 -1.617172 8 -2.289391 0.168586 -0.293777 8 -2.085352 -1.259428 -0.226578 8 -0.919073 -1.348217 0.597030 1 0.353255 -0.961849 -0.964824 6 2.345837 0.493079 0.206530 1 2.997136 0.879482 0.993161 6 3.147812 -0.471737 -0.668413 1 3.489640 -1.331627 -0.089431 1 2.564664 -0.850907 -1.508432 1 4.028600 0.021070 -1.081340 1 2.048601 1.362247 -0.385767 1 0.751437 0.514892 1.677854 1 1.414436 -1.069984 1.359053	**Frequencies (cm^{-1}):** 37.2193, 56.8872, 101.5251, 173.5478, 223.0845, 243.7216, 274.232, 331.4693, 360.8317, 428.7349, 450.8564, 498.3407, 690.9471, 705.9475, 720.3557, 774.6833, 796.4424, 869.8568, 883.6138, 922.9356, 938.172, 983.3939, 1033.3897, 1053.9269, 1067.9226, 1078.4957, 1126.8036, 1158.0882, 1186.4159, 1253.9104, 1296.7583, 1319.7746, 1343.1285, 1367.616, 1379.5591, 1387.5186, 1410.3382, 1420.3002, 1426.7413, 1484.6444, 1492.5918, 1495.4195, 1502.4096, 1507.4404, 1510.3873, 3011.5101, 3021.2721, 3027.1063, 3032.9704, 3036.7599, 3045.3567, 3051.5914, 3082.6199, 3087.4686, 3090.3211, 3106.0429, 3120.4456

Compound: Z-nPrCHCHMe + O_3 POZ 1.3	**Energy (kJ mol^{-1}):** -460.835379640329

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.082344 -0.765306 0.747732 6 -0.113414 -0.575512 -0.183862 6 -0.762243 0.841058 -0.360230 6 -0.420262 1.921456 0.647291 1 -0.581163 1.573729 1.666488 1 0.614394 2.242068 0.535475 1 -1.059040 2.788448 0.480058 1 -0.567907 1.189812 -1.378102 8 -2.172121 0.581339 -0.214910 8 -2.299181 -0.844007 -0.420651 8 -1.198949 -1.347933 0.338733 1 0.125518 -0.961758 -1.179092 6 2.440464 -0.746627 0.035209 1 2.444866 -1.526315 -0.731472 6 2.830923 0.588831 -0.597128 1 2.117058 0.904239 -1.360573 1 2.890166 1.380682 0.151653 1 3.807168 0.518446 -1.077842 1 3.205194 -1.032946 0.760483 1 1.063339 -0.032847 1.554882 1 0.955543 -1.742155 1.218589	52.0129, 65.084, 107.3971, 200.4115, 235.3546, 263.4272, 287.4092, 312.0389, 363.9057, 418.9515, 448.5108, 492.7171, 704.2367, 711.8973, 742.9885, 775.6002, 782.151, 863.2286, 890.9248, 906.9946, 939.161, 983.96, 1024.4982, 1061.6543, 1074.8534, 1088.0413, 1113.6252, 1168.6002, 1171.1125, 1258.0319, 1303.6455, 1313.9805, 1347.5815, 1359.7989, 1384.8538, 1388.0197, 1407.6493, 1418.1513, 1423.664, 1483.5155, 1491.1066, 1495.6467, 1501.6827, 1507.1584, 1508.8499, 3003.5691, 3017.3449, 3023.5438, 3025.4074, 3038.9907, 3045.5772, 3050.0117, 3079.575, 3084.8392, 3087.7054, 3108.0303, 3121.226

Compound: Z-nPrCHCHMe + O_3 POZ 1.4	**Energy (kJ mol^{-1}):** -460.836020241809
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.133719 -0.112207 0.887399 6 0.382025 -0.306583 0.948607 6 1.311485 0.761509 0.287040 1 2.199931 0.860326 0.916664 6 0.747866 2.132032 -0.019944 1 1.515259 2.750625 -0.483615 1 -0.108805 2.084540 -0.687092 1 0.442886 2.619294 0.906340 8 1.703842 0.126179 -0.929954 8 1.940887 -1.205797 -0.474608 8 0.714038 -1.514942 0.242953 1 0.687066 -0.410027 1.994340 1 -1.359414 0.869728 1.314415 1 -1.585511 -0.837902 1.569165 6 -1.792664 -0.259863 -0.487279 1 -1.617529 -1.270155 -0.856284 6 -3.293773 0.020178 -0.434042 1 -3.499371 1.041837 -0.106850 1 -3.753732 -0.112281 -1.413804 1 -3.797299 -0.654954 0.261088 1 -1.320934 0.405051 -1.212190	42.1469, 61.6395, 124.9634, 190.1755, 206.8156, 239.5467, 259.0921, 309.9882, 321.3051, 360.9409, 487.4827, 563.7309, 702.9958, 722.2468, 728.7876, 749.5498, 772.7737, 861.2098, 879.0835, 915.0883, 931.258, 966.7982, 1016.1017, 1048.2755, 1088.0921, 1104.0885, 1129.5336, 1146.9616, 1196.3136, 1264.0522, 1302.7596, 1316.3585, 1343.7902, 1356.3529, 1376.5214, 1401.0992, 1410.2455, 1416.6881, 1426.267, 1480.5999, 1491.2326, 1495.5364, 1500.692, 1504.6952, 1516.8108, 2998.4199, 3014.9855, 3019.0011, 3026.0948, 3037.881, 3047.438, 3050.5317, 3063.3617, 3087.0294, 3091.004, 3106.5054, 3134.0462

Compound: Z-nPrCHCHMe + O_3 POZ 1.5	**Energy (kJ mol^{-1}):** -460.832205691173
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.226384 -0.037295 1.179951 6 0.264360 -0.381062 0.998766 6 1.249851 0.655594 0.351423 1 2.169023 0.639088 0.943237 6 0.797378 2.085039 0.152562	55.5038, 78.218, 141.3259, 212.1718, 218.9934, 241.0355, 288.4844, 320.62, 345.5188, 385.8574, 496.3699, 548.6433, 686.8443, 692.9598, 713.2084, 755.1195, 793.715, 857.7593, 882.028, 902.5268,

1 1.596254 2.661865 -0.312236 1 -0.088089 2.149027 -0.473207 1 0.578442 2.540370 1.118762 8 1.536397 0.075603 -0.921956 8 1.616793 -1.311890 -0.583412 8 0.375061 -1.521256 0.132379 1 0.680632 -0.639729 1.976314 1 -1.306608 1.023258 1.431166 1 -1.567341 -0.574969 2.066643 6 -2.192336 -0.386441 0.035928 1 -3.203519 -0.245136 0.426184 6 -2.047099 0.414392 -1.256203 1 -1.066045 0.278331 -1.709712 1 -2.793469 0.093781 -1.984353 1 -2.201484 1.482031 -1.084422 1 -2.098414 -1.448921 -0.189031	932.7809, 968.411, 1007.4916, 1064.3041, 1097.2506, 1110.9046, 1126.8158, 1140.2601, 1189.6313, 1266.6519, 1310.0529, 1326.6873, 1350.3043, 1373.3089, 1391.327, 1397.8913, 1407.2115, 1420.2235, 1426.4725, 1483.3395, 1489.37, 1494.8954, 1501.7504, 1510.5151, 1515.8499, 2999.7304, 3019.714, 3022.4371, 3024.7252, 3033.8881, 3049.4097, 3055.6765, 3067.0215, 3083.2235, 3103.678, 3104.1707, 3144.0685

Compound: Z-nPrCHCHMe + O_3 POZ 1.6	**Energy (kJ mol^{-1}):** -460.834785257852
Reaction Coordinates: 6 -1.057500 0.729065 0.907881 6 0.241824 -0.072684 0.993101 6 1.493107 0.441523 0.200429 1 2.366429 0.317918 0.846514 6 1.472555 1.843730 -0.370184 1 2.399408 2.034814 -0.909793 1 0.637528 1.998841 -1.048670 1 1.404752 2.569964 0.440044 8 1.599389 -0.494753 -0.873509 8 1.265968 -1.717288 -0.211856 8 0.015488 -1.377842 0.438935 1 0.533889 -0.174241 2.042621 1 -0.812235 1.754363 1.194833 1 -1.727990 0.361829 1.688570 6 -1.797221 0.706056 -0.443704 1 -1.083760 0.577656 -1.258185 6 -2.865084 -0.384371 -0.541816 1 -3.624756 -0.257698 0.232671 1 -3.369845 -0.348969 -1.508311 1 -2.427023 -1.374636 -0.425984 1 -2.269242 1.679308 -0.597112	**Frequencies (cm^{-1}):** 53.9463, 81.8826, 98.6364, 186.8291, 216.5437, 235.8303, 260.8345, 328.7673, 340.0628, 390.8576, 484.2065, 538.7441, 690.4021, 715.7206, 743.2424, 754.5736, 792.8338, 838.8131, 882.4191, 927.0171, 933.3885, 970.3373, 1009.8588, 1056.5343, 1098.4436, 1104.5378, 1120.1766, 1143.5161, 1183.0474, 1265.2237, 1294.83, 1332.3695, 1344.7826, 1368.9898, 1371.3179, 1398.9172, 1407.6984, 1414.567, 1425.261, 1481.9066, 1490.3458, 1497.4351, 1500.707, 1505.337, 1510.8259, 2999.3866, 3020.6529, 3023.3431, 3024.7081, 3032.6834, 3048.2745, 3054.6614, 3064.5331, 3083.4481, 3105.5069, 3107.2414, 3132.8711

Compound: Z-nPrCHCHMe + O_3 POZ 1.7	**Energy (kJ mol^{-1}):** -460.838907230968
Reaction Coordinates: 6 -1.120737 0.446122 0.031088 6 0.156615 -0.192147 0.548928 6 1.489968 0.631014 0.442403 6 1.437432 2.006089 -0.192119 1 1.009482 1.968344 -1.191869 1 0.844342 2.683300 0.422484 1 2.443945 2.417003 -0.263887 1 1.934340 0.690894 1.439594 8 2.319947 -0.192460 -0.386393 8 1.846089 -1.517628 -0.096024 8 0.426913 -1.355515 -0.244743 1 0.027242 -0.500209 1.591072	**Frequencies (cm^{-1}):** 35.6126, 91.4126, 96.3025, 130.1509, 230.4861, 243.5905, 269.4801, 318.4774, 330.8075, 394.7308, 462.9515, 511.7362, 696.2069, 707.6496, 744.2381, 766.5846, 813.6744, 860.4237, 901.2798, 910.8162, 936.8625, 965.9902, 1033.259, 1058.4691, 1079.2329, 1086.8243, 1131.0209, 1166.6998, 1186.2225, 1267.2408, 1303.1785, 1329.2183, 1333.2457, 1350.7037, 1378.1989, 1391.2298,

6 -2.354820 -0.442675 0.208744 1 -2.457779 -0.706208 1.265447 6 -3.636741 0.228415 -0.279660 1 -3.574391 0.472387 -1.341929 1 -4.500511 -0.422282 -0.140417 1 -3.830123 1.156911 0.261887 1 -2.202758 -1.380993 -0.327642 1 -1.272287 1.385854 0.569844 1 -0.995409 0.698919 -1.023604	1412.1749, 1416.7418, 1425.4011, 1472.7152, 1489.345, 1494.4656, 1501.0371, 1503.8103, 1510.2316, 2999.7183, 3014.0435, 3019.2096, 3022.2347, 3024.4684, 3045.2773, 3050.4671, 3067.6673, 3083.7122, 3088.3077, 3105.2793, 3122.7565

Compound: Z-nPrCHCHMe + O_3 POZ 1.8	**Energy (kJ mol^{-1}):** -460.837301804984
Reaction Coordinates: 6 -1.001322 1.011421 -0.016420 6 0.039248 0.051897 0.541362 6 1.551266 0.459106 0.402708 6 1.894462 1.681795 -0.425013 1 1.470013 1.617694 -1.425092 1 1.527739 2.585912 0.060850 1 2.976652 1.769984 -0.516621 1 1.973882 0.549777 1.407190 8 2.141342 -0.672257 -0.252943 8 1.266394 -1.758297 0.102451 8 -0.023062 -1.190091 -0.169281 1 -0.162473 -0.142321 1.599277 6 -2.456519 0.664402 0.327222 1 -3.067975 1.543494 0.109410 6 -3.034316 -0.538054 -0.419415 1 -2.493927 -1.455367 -0.191246 1 -4.081443 -0.687307 -0.152774 1 -2.984965 -0.387596 -1.499535 1 -2.537586 0.502525 1.406360 1 -0.775840 1.997588 0.396603 1 -0.878378 1.087363 -1.098896	**Frequencies (cm^{-1}):** 40.5973, 52.1554, 114.778, 170.1481, 234.3853, 238.2571, 289.2327, 310.9242, 349.5532, 436.2094, 453.9807, 471.7531, 700.5729, 704.8694, 759.786, 763.8367, 815.3215, 839.6193, 892.166, 904.2976, 935.1857, 970.8688, 1029.2065, 1059.4215, 1079.8238, 1093.7536, 1119.8338, 1166.0969, 1174.8516, 1262.1076, 1302.6176, 1323.514, 1344.5134, 1357.073, 1383.7776, 1389.1233, 1410.5967, 1420.8624, 1425.2182, 1470.1043, 1489.6054, 1490.8503, 1500.9451, 1503.3915, 1509.2814, 2999.5951, 3009.7657, 3023.1989, 3024.1706, 3028.8961, 3042.0954, 3045.1979, 3067.5681, 3083.624, 3104.4272, 3108.2737, 3121.5455

Compound: Z-nPrCHCHMe + O_3 POZ 1.9	**Energy (kJ mol^{-1}):** -460.837921232771
Reaction Coordinates: 6 -1.033426 0.771484 -0.444757 6 -0.033953 -0.075453 0.325896 6 1.409421 0.506988 0.540383 6 1.740306 1.857488 -0.062265 1 1.555686 1.872884 -1.134515 1 1.146047 2.638725 0.411727 1 2.791232 2.088733 0.108633 1 1.619264 0.510644 1.613440 8 2.252951 -0.462871 -0.094454 8 1.501115 -1.680847 0.039896 8 0.206068 -1.272794 -0.425913 1 -0.432848 -0.351165 1.304915 6 -2.408686 0.114597 -0.631936 1 -2.283921 -0.835833 -1.154084 6 -3.192167 -0.105571 0.662244 1 -3.330177 0.831565 1.206382 1 -4.181505 -0.511623 0.449461 1 -2.692699 -0.808327 1.330058 1 -2.993888 0.753247 -1.297524	**Frequencies (cm^{-1}):** 33.6793, 51.2911, 115.7119, 161.2212, 226.8324, 239.8884, 252.4029, 331.1168, 364.5095, 445.1779, 467.3375, 473.5028, 692.2857, 704.2341, 736.0101, 767.908, 829.8723, 863.0432, 876.9552, 907.9091, 937.108, 969.6548, 1016.431, 1066.861, 1071.4745, 1089.6467, 1133.3733, 1155.0073, 1182.0106, 1265.4829, 1294.1006, 1330.2961, 1343.6342, 1359.347, 1381.0557, 1388.9842, 1412.6351, 1419.2421, 1428.8466, 1472.622, 1489.5686, 1493.1329, 1502.352, 1503.9998, 1509.2324, 3009.245, 3019.2527, 3022.5748, 3027.2603, 3034.9279, 3045.1522, 3057.1554, 3074.1859, 3084.2441, 3090.6747, 3105.073, 3122.2791

1 -1.155635 1.717697 0.090244 1 -0.611586 1.008357 -1.422358	

Compound: Z-nPrCHCHMe + O_3 POZ 2.1	**Energy (kJ mol^{-1}):** -460.836825517089
Reaction Coordinates: 6 -1.123073 -0.572910 -0.294926 6 0.206462 -0.576014 0.448597 6 0.997379 0.763018 0.540401 6 0.714945 1.810950 -0.523542 1 0.882981 1.411616 -1.521726 1 -0.310384 2.173965 -0.460888 1 1.382520 2.658684 -0.373795 1 0.903011 1.187582 1.540022 8 2.350201 0.299950 0.470473 8 2.261467 -0.654541 -0.588167 8 1.141907 -1.486217 -0.170639 1 0.056766 -0.959621 1.461089 6 -2.260777 0.076811 0.498222 1 -2.012801 1.115196 0.734073 6 -3.595078 0.034041 -0.244641 1 -3.535780 0.568927 -1.194299 1 -3.890044 -0.993857 -0.463129 1 -4.391102 0.490427 0.344482 1 -2.362917 -0.434808 1.459662 1 -1.007862 -0.092124 -1.267808 1 -1.382145 -1.614901 -0.495685	**Frequencies (cm^{-1}):** 36.162, 74.9152, 118.9849, 167.7623, 232.9146, 241.4672, 278.0419, 282.3931, 317.9232, 400.1283, 487.4624, 524.91, 693.1138, 715.2169, 741.4108, 762.9785, 799.6674, 884.4089, 901.6045, 917.2983, 923.1126, 966.9476, 1033.4842, 1045.1026, 1064.6324, 1079.0489, 1112.3541, 1154.1743, 1175.9673, 1257.0357, 1298.9524, 1302.2695, 1325.939, 1345.3009, 1371.3401, 1388.4037, 1403.0642, 1415.4553, 1417.9085, 1485.2828, 1493.9771, 1498.2707, 1500.8873, 1502.035, 1514.7887, 3010.6987, 3023.2272, 3024.1123, 3030.7125, 3037.8403, 3047.3241, 3072.5693, 3074.1197, 3084.6949, 3088.943, 3108.5423, 3124.7335

Compound: Z-nPrCHCHMe + O_3 POZ 2.2	**Energy (kJ mol^{-1}):** -460.835316682541
Reaction Coordinates: 6 -1.093420 -0.262975 -0.853654 6 -0.008623 -0.511420 0.188256 6 0.892415 0.691868 0.603309 6 0.994313 1.855591 -0.369039 1 1.347157 1.522964 -1.343232 1 0.033301 2.352415 -0.497452 1 1.701802 2.585072 0.023468 1 0.617337 1.041006 1.598864 8 2.160719 0.052270 0.783209 8 2.205887 -0.798946 -0.363621 8 0.935429 -1.500784 -0.281988 1 -0.443993 -0.943658 1.090326 6 -2.322380 0.493529 -0.325744 1 -2.930409 0.785880 -1.184504 6 -3.192410 -0.310242 0.642973 1 -3.536559 -1.237530 0.181213 1 -2.659487 -0.575615 1.556849 1 -4.074022 0.260360 0.936876 1 -2.015143 1.428199 0.151070 1 -0.662657 0.262009 -1.706525 1 -1.412973 -1.239525 -1.224358	**Frequencies (cm^{-1}):** 34.8554, 61.5663, 107.7585, 175.5085, 230.7504, 235.1552, 276.8558, 299.8836, 342.6403, 449.1067, 467.7461, 509.1442, 684.4613, 713.2461, 743.2765, 764.6933, 809.2068, 868.7478, 890.5555, 918.3707, 926.8275, 961.6469, 1022.2112, 1041.6414, 1068.7458, 1071.9147, 1111.2419, 1150.9834, 1169.1813, 1249.9595, 1292.8466, 1301.4716, 1332.054, 1365.1436, 1371.9977, 1377.5253, 1408.1938, 1416.8844, 1419.985, 1486.9025, 1492.6706, 1496.4173, 1501.9924, 1507.0256, 1509.5341, 3017.999, 3026.7118, 3033.6315, 3045.1573, 3047.5327, 3050.0416, 3072.0109, 3080.4288, 3086.8175, 3089.5242, 3109.0131, 3124.2919

Compound: Z-nPrCHCHMe + O_3 POZ 2.3	**Energy (kJ mol^{-1}):** -460.833906480307

Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.110504 -0.916158 0.591423 6 -0.096490 -0.628117 -0.300116 6 -0.664567 0.805459 -0.391370 6 -0.620788 1.651914 0.868712 1 -1.050677 1.120984 1.715667 1 0.402679 1.931129 1.114210 1 -1.191720 2.565437 0.706260 1 -0.235281 1.334507 -1.241872 8 -2.006290 0.512816 -0.797452 8 -2.383966 -0.495030 0.136241 8 -1.214095 -1.393643 0.189165 1 0.111630 -0.969633 -1.319343 6 2.471971 -0.671062 -0.072245 1 2.516726 -1.237961 -1.006607 6 2.829034 0.789957 -0.346222 1 2.140600 1.258857 -1.050723 1 2.819756 1.379738 0.572241 1 3.828676 0.867835 -0.775023 1 3.238188 -1.102556 0.575448 1 1.027747 -0.360674 1.527054 1 1.048502 -1.972755 0.857948	49.232, 61.7998, 112.6636, 203.3084, 213.5032, 234.023, 244.7358, 281.2131, 325.2454, 431.2508, 454.0236, 499.9547, 687.2207, 710.4225, 767.7109, 773.1331, 784.9608, 862.9297, 889.862, 909.0727, 917.3788, 986.7449, 1007.7761, 1058.4885, 1075.475, 1084.7217, 1108.5468, 1159.9822, 1168.3074, 1250.9781, 1294.4317, 1303.2885, 1342.3428, 1361.2128, 1373.7395, 1388.3761, 1403.8698, 1416.7605, 1419.2571, 1484.3954, 1489.8679, 1496.9559, 1499.7989, 1506.5625, 1508.0014, 2999.8692, 3015.5468, 3026.5406, 3035.9107, 3049.0371, 3050.328, 3075.2039, 3079.356, 3086.0766, 3088.969, 3112.6436, 3127.198

Compound: Z-nPrCHCHMe + O_3 POZ 2.4	**Energy (kJ mol^{-1}):** -460.833953868328
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.090674 0.092572 0.895781 6 0.395500 -0.265716 1.011722 6 1.455927 0.681906 0.350081 1 2.244842 0.884428 1.076383 6 0.965458 1.991640 -0.241471 1 1.809351 2.529179 -0.672101 1 0.226202 1.833785 -1.022676 1 0.528727 2.624484 0.532597 8 2.088607 -0.152259 -0.638185 8 1.107850 -1.176270 -0.896752 8 0.708761 -1.539459 0.435145 1 0.645387 -0.380636 2.067353 1 -1.216287 1.141046 1.180778 1 -1.612929 -0.485047 1.663305 6 -1.779697 -0.175783 -0.445447 1 -1.648288 -1.226240 -0.706176 6 -3.270161 0.158328 -0.393287 1 -3.435490 1.213568 -0.165207 1 -3.753636 -0.053337 -1.347485 1 -3.780604 -0.428192 0.373450 1 -1.307142 0.393196 -1.246163	45.2224, 72.7514, 114.4477, 177.6954, 230.8736, 244.9856, 271.6184, 288.62, 345.0578, 387.4363, 483.5636, 589.1661, 697.0923, 714.3394, 743.4368, 753.981, 796.5554, 861.8089, 878.0377, 914.002, 932.6289, 946.6018, 1019.6941, 1052.1802, 1065.824, 1091.3801, 1112.5786, 1143.372, 1166.332, 1260.3414, 1301.8163, 1310.2803, 1327.9277, 1350.9427, 1368.4973, 1392.1437, 1408.6687, 1413.5334, 1419.7074, 1479.0584, 1491.7515, 1495.5036, 1500.3559, 1501.3601, 1514.0871, 3014.6854, 3019.6954, 3039.0221, 3041.5225, 3044.9233, 3050.3108, 3063.4671, 3064.6558, 3087.4393, 3091.904, 3100.4367, 3132.8051

Compound: Z-nPrCHCHMe + O_3 POZ 2.5	**Energy (kJ mol^{-1}):** -460.830310216407
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.044999 -0.047322 1.248122 6 0.423731 -0.454922 1.026299 6 1.405371 0.494254 0.280852 1 2.389084 0.373656 0.740401 6 1.062526 1.969985 0.213454	34.9176, 107.4512, 137.78, 201.5538, 232.4066, 237.0645, 258.373, 306.298, 362.3561, 396.7007, 469.155, 546.8767, 684.0764, 696.9104, 737.9259, 764.0834, 810.4058, 857.9323, 879.3478, 897.6033,

1 1.833080 2.498381 -0.346686 1 0.105129 2.145705 -0.268145 1 1.035071 2.393724 1.219250 8 1.528790 -0.082233 -1.036934 8 0.561716 -1.171937 -1.067914 8 0.578223 -1.661235 0.276441 1 0.859662 -0.688527 1.998754 1 -1.068482 0.992394 1.585981 1 -1.382441 -0.639456 2.101515 6 -2.068000 -0.264102 0.119903 1 -3.052811 -0.262645 0.594023 6 -2.083780 0.756532 -1.016879 1 -1.160299 0.742905 -1.592639 1 -2.899967 0.536890 -1.706661 1 -2.242252 1.769679 -0.640113 1 -1.934697 -1.266022 -0.288936	933.5672, 959.2135, 1005.1324, 1055.1425, 1076.412, 1109.0815, 1122.096, 1133.0502, 1174.245, 1253.4865, 1303.5879, 1322.3272, 1341.8073, 1365.4569, 1391.6671, 1399.2289, 1404.5356, 1416.2732, 1419.6103, 1480.9449, 1491.7975, 1492.7896, 1501.1578, 1507.4035, 1516.929, 3016.256, 3022.6773, 3024.9585, 3028.0164, 3040.2184, 3048.5222, 3065.2298, 3066.7047, 3082.1267, 3097.7317, 3111.0191, 3144.6847

Compound: Z-nPrCHCHMe + O_3 POZ 2.6	**Energy (kJ mol^{-1}):** -460.831697748487
Reaction Coordinates: 6 -0.986063 0.883725 0.818809 6 0.239945 -0.013586 1.030104 6 1.580011 0.387884 0.312842 1 2.365749 0.496255 1.061905 6 1.563066 1.609978 -0.589742 1 2.547142 1.731115 -1.040846 1 0.829000 1.517849 -1.386537 1 1.346117 2.513020 -0.018061 8 1.940272 -0.802413 -0.405121 8 0.665153 -1.397974 -0.693392 8 0.036474 -1.369858 0.602491 1 0.435304 -0.096978 2.100144 1 -0.657326 1.918965 0.932615 1 -1.668566 0.702733 1.652609 6 -1.771480 0.713819 -0.496474 1 -1.096155 0.461668 -1.313261 6 -2.878899 -0.339192 -0.419675 1 -3.606355 -0.083749 0.354059 1 -3.415393 -0.407637 -1.367098 1 -2.475603 -1.323824 -0.189028 1 -2.218586 1.676767 -0.753521	**Frequencies (cm^{-1}):** 31.2129, 83.6219, 92.0386, 185.452, 230.1795, 245.3043, 255.242, 319.0572, 364.3211, 402.1964, 482.8143, 561.5183, 696.1415, 708.7014, 741.3165, 782.9886, 794.8489, 847.0201, 883.9664, 922.8059, 923.8953, 945.2347, 1011.6542, 1061.2996, 1069.0551, 1090.1012, 1116.7535, 1133.2588, 1156.0798, 1254.3926, 1294.0984, 1309.8471, 1328.7071, 1363.7714, 1372.3483, 1389.1947, 1402.7893, 1413.8001, 1418.5884, 1483.5084, 1489.3688, 1498.747, 1499.9798, 1504.0127, 1511.4038, 3022.2433, 3023.936, 3029.444, 3043.61, 3046.7495, 3057.1885, 3064.2738, 3069.774, 3087.7086, 3102.1269, 3109.5779, 3131.8973

Compound: Z-nPrCHCHMe + O_3 POZ 2.7	**Energy (kJ mol^{-1}):** -460.838017085097
Reaction Coordinates: 6 -1.055534 0.445857 0.018615 6 0.165045 -0.171947 0.687238 6 1.527963 0.590329 0.524307 6 1.511209 1.870113 -0.294222 1 1.148509 1.691435 -1.304620 1 0.882994 2.628666 0.173724 1 2.523854 2.266126 -0.357869 1 1.963855 0.776509 1.506584 8 2.386876 -0.397345 -0.067706 8 1.464223 -1.197642 -0.826946 8 0.457537 -1.477784 0.160595 1 -0.035851 -0.346026 1.746181	**Frequencies (cm^{-1}):** 34.4059, 91.1409, 98.7369, 138.4464, 240.1534, 251.6336, 275.2791, 288.9038, 339.6836, 422.0858, 485.4395, 523.0826, 695.1361, 716.6446, 750.9395, 764.1281, 818.552, 866.5984, 902.94, 914.2651, 930.2283, 945.8197, 1029.5484, 1054.4214, 1061.6614, 1079.7311, 1115.2273, 1147.3445, 1170.3333, 1264.5409, 1279.3543, 1308.6725, 1324.9493, 1339.9725, 1377.6909,

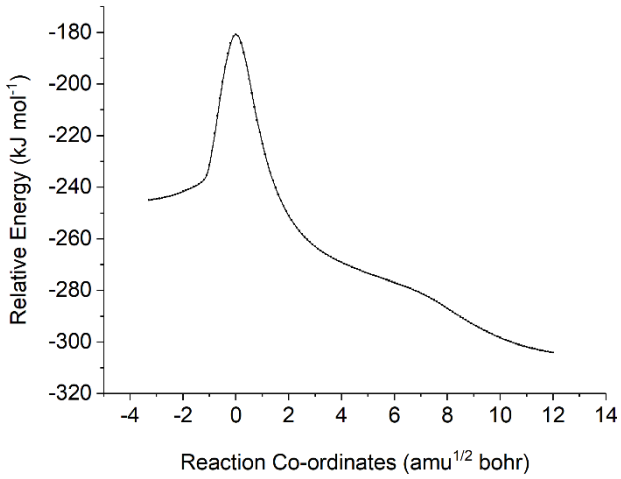
6 -2.341246 -0.333639 0.302181 1 -2.509343 -0.369569 1.383009 6 -3.563544 0.272638 -0.384169 1 -3.439654 0.286967 -1.468707 1 -4.465189 -0.299024 -0.162082 1 -3.734036 1.300771 -0.057730 1 -2.211011 -1.367412 -0.023173 1 -1.171496 1.474329 0.372105 1 -0.885071 0.499293 -1.058659	1382.8359, 1404.5677, 1414.2975, 1416.9042, 1473.227, 1492.5389, 1495.3723, 1500.7769, 1501.4716, 1510.7999, 3009.1262, 3018.8386, 3021.9144, 3041.3793, 3043.551, 3051.0353, 3062.1026, 3069.047, 3082.9145, 3087.3758, 3103.9629, 3122.4961

Compound: Z-nPrCHCHMe + O_3 POZ 2.8	**Energy (kJ mol^{-1}):** -460.835999996184
Reaction Coordinates: 6 -0.946790 0.978874 -0.162207 6 0.018629 0.095097 0.619089 6 1.544425 0.453252 0.511065 6 1.938798 1.515183 -0.502253 1 1.606998 1.250226 -1.504347 1 1.521243 2.487599 -0.241489 1 3.023970 1.608575 -0.512219 1 1.934160 0.706737 1.497598 8 2.147499 -0.809364 0.200320 8 1.145054 -1.419680 -0.626004 8 -0.026239 -1.283870 0.201428 1 -0.271892 0.069359 1.671661 6 -2.427502 0.763831 0.179020 1 -2.995434 1.575865 -0.281769 6 -3.022512 -0.571335 -0.269315 1 -2.546271 -1.418116 0.222304 1 -4.089510 -0.607456 -0.045183 1 -2.902747 -0.711444 -1.345215 1 -2.562363 0.881378 1.259132 1 -0.697770 2.020966 0.052775 1 -0.781172 0.830202 -1.231596	**Frequencies (cm^{-1}):** 29.2535, 50.3637, 111.8816, 185.3227, 239.148, 250.6046, 270.4443, 303.2271, 360.7711, 438.8722, 465.9833, 507.4816, 700.5774, 713.4244, 752.7643, 773.1261, 816.2607, 854.3219, 889.9344, 912.5849, 929.5527, 945.6062, 1021.6995, 1059.1172, 1067.4938, 1084.8484, 1104.4466, 1138.4125, 1167.2081, 1256.5511, 1282.9473, 1303.1817, 1323.6388, 1358.5971, 1375.3626, 1387.3372, 1403.9084, 1413.9138, 1423.5572, 1469.2936, 1490.1823, 1493.4519, 1499.9525, 1501.4611, 1507.4907, 3004.2994, 3021.1638, 3028.8682, 3036.4972, 3039.8394, 3046.0773, 3063.5652, 3067.8002, 3083.538, 3105.8485, 3106.3269, 3122.9146

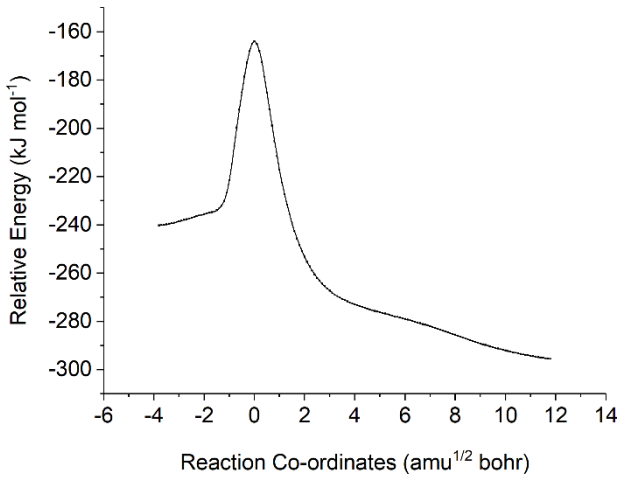
Compound: Z-nPrCHCHMe + O_3 POZ 2.9	**Energy (kJ mol^{-1}):** -460.837194932358
Reaction Coordinates: 6 -0.978680 0.558853 -0.575958 6 -0.045664 -0.071537 0.451015 6 1.376821 0.576266 0.604127 6 1.686752 1.784418 -0.263323 1 1.581715 1.553125 -1.321505 1 1.030625 2.621161 -0.021365 1 2.713228 2.099995 -0.081376 1 1.561728 0.809478 1.653441 8 2.267081 -0.514891 0.317391 8 1.495970 -1.319337 -0.592579 8 0.254889 -1.438799 0.122220 1 -0.526482 -0.127904 1.427650 6 -2.363340 -0.099243 -0.635700 1 -2.240962 -1.172123 -0.796940 6 -3.237733 0.146201 0.594710 1 -3.383969 1.214583 0.768984 1 -4.222367 -0.304370 0.466143 1 -2.806014 -0.281697 1.500712 1 -2.880441 0.283580 -1.518384	**Frequencies (cm^{-1}):** 32.6383, 53.4905, 115.0577, 173.4115, 240.0102, 245.66, 259.299, 297.3144, 384.8848, 450.6564, 464.7435, 519.9367, 693.3218, 716.6317, 736.0651, 761.5755, 832.0535, 869.2336, 877.5553, 912.668, 934.5285, 949.1055, 1010.3893, 1060.1545, 1067.3166, 1071.8957, 1115.2816, 1147.571, 1153.6271, 1258.3962, 1279.8941, 1311.1811, 1313.6319, 1360.1354, 1379.0373, 1380.6612, 1409.1157, 1414.2381, 1418.2287, 1473.0116, 1492.9324, 1493.8292, 1501.2724, 1504.0143, 1508.5918, 3020.0996, 3022.7671, 3027.9496, 3043.3898, 3052.8339, 3055.8117, 3066.1067, 3079.0734,

1 -1.094234 1.621801 -0.345993 1 -0.505277 0.496836 -1.556848	3083.4039, 3088.3884, 3103.6215, 3123.0595

Compound: Z-nPrCHCHMe + O_3 TS_{ANTI} 1.8	**Energy (kJ mol^{-1}):** -460.810082341262
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.061521 -1.032026 -0.074233 6 -0.051557 0.025697 -0.411962 6 1.722041 -0.542484 -0.446004 6 1.985680 -1.451508 0.745401 1 1.862553 -0.903900 1.678384 1 1.338595 -2.328881 0.748843 1 3.019549 -1.795972 0.694147 1 1.591755 -1.067534 -1.407722 8 2.357838 0.568266 -0.513963 8 0.961122 1.895264 0.118986 8 0.119763 0.961999 0.539161 1 -0.083145 0.450399 -1.411717 6 -2.504298 -0.652621 -0.457861 1 -2.537110 -0.404139 -1.522051 6 -3.096536 0.492046 0.361603 1 -2.537385 1.418575 0.231736 1 -4.127696 0.683523 0.063704 1 -3.096457 0.254290 1.426837 1 -3.122181 -1.545085 -0.336112 1 -0.780429 -1.939260 -0.612380 1 -1.000688 -1.260879 0.991191	-443.0757, 46.938, 93.9573, 109.4862, 157.5493, 183.1382, 207.4873, 248.0385, 295.7406, 346.8906, 353.9159, 473.9063, 485.8969, 519.0053, 609.0184, 617.9605, 784.7679, 831.8833, 859.545, 889.8319, 953.8594, 991.7382, 1034.3045, 1061.605, 1072.9304, 1115.768, 1121.3027, 1156.4795, 1170.1854, 1220.1112, 1281.3321, 1293.0268, 1311.0719, 1349.1036, 1381.4353, 1398.4263, 1414.5024, 1424.0805, 1433.8192, 1475.2488, 1482.4362, 1490.3842, 1497.9018, 1501.4444, 1506.7205, 2907.5882, 3019.3098, 3031.3203, 3034.3937, 3037.5204, 3051.5547, 3078.2476, 3090.3328, 3095.0566, 3099.6652, 3115.206, 3117.9454
IRC	



Compound: Z-nPrCHCHMe + O_3 TS_{SYN} 1.8	**Energy (kJ mol^{-1}):** -460.804572109195
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.673677 0.921141 -0.346591 6 0.047883 0.122132 0.707369 6 1.891503 0.045523 0.293961 6 2.289100 1.469540 -0.095401	-467.6136, 49.3856, 82.835, 108.871, 177.6914, 214.7649, 256.9756, 271.3339, 291.0365, 318.2738, 374.4216, 437.4078,

1 1.956277 2.203643 0.639078 1 1.909435 1.727793 -1.080929 1 3.378775 1.503328 -0.133483 1 2.258224 -0.239064 1.294337 8 1.950225 -0.858703 -0.612289 8 0.109262 -1.744624 -0.455227 8 -0.105402 -1.216401 0.735566 1 -0.032383 0.492129 1.727482 6 -2.176337 1.083263 -0.038491 1 -2.295740 1.519800 0.957731 6 -3.011816 -0.190809 -0.149233 1 -2.713989 -0.941880 0.581799 1 -4.066430 0.031440 0.017604 1 -2.914880 -0.639527 -1.138571 1 -2.561884 1.827609 -0.739577 1 -0.227785 1.913226 -0.381977 1 -0.522229 0.454601 -1.317576	483.3718, 536.5451, 585.38, 674.6698, 776.4817, 841.3679, 878.1107, 900.2474, 943.783, 985.5339, 1001.8101, 1057.0774, 1071.7602, 1083.9055, 1104.3304, 1162.5466, 1184.8028, 1196.1274, 1269.7079, 1295.4282, 1340.6757, 1359.94, 1382.935, 1390.8515, 1423.8786, 1427.8123, 1439.1192, 1475.9492, 1486.024, 1488.1217, 1499.893, 1502.6855, 1508.2353, 2909.4351, 3010.0925, 3033.5478, 3033.7161, 3039.5337, 3075.5115, 3091.434, 3092.4492, 3101.339, 3106.9179, 3124.4023, 3130.5275
IRC  	

10.0 Example MESMER Input File for O_3 + 1-Propene:

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<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <me:title>MeCHCH2 + O3 R1_f</me:title>
  <moleculeList convention="">
    <molecule id="N2">
      <atomArray>
        <atom id="a1" elementType="N" />
        <atom id="a2" elementType="N" />
      </atomArray>
      <bondArray>
        <bond atomRefs2="a2 a1" order="3" />
      </bondArray>
      <propertyList>
        <property dictRef="me:epsilon">
          <scalar>48.0</scalar>
        </property>
        <property dictRef="me:sigma">
          <scalar>3.90</scalar>
        </property>
        <property dictRef="me:MW">
          <scalar units="amu">28.0</scalar>
        </property>
      </propertyList>
      <metadata name="copiedFrom" content="C:\Mesmer-5.2/librarymols.xml"
timestamp="20190613_164702" />
```

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  </molecule>
  <molecule id="Canti">
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      <atom id="a2" elementType="C" spinMultiplicity="2" x3="0.958332" y3="0.105026" z3="-
0.385106" />
      <atom id="a3" elementType="H" x3="0.536037" y3="-0.090929" z3="-1.361383" />
      <atom id="a4" elementType="O" x3="0.400476" y3="0.976339" z3="0.330402" />
      <atom id="a5" elementType="O" spinMultiplicity="2" x3="-0.826700" y3="1.434854"
z3="-0.130168" />
      <atom id="a6" elementType="H" x3="3.011534" y3="-0.346947" z3="-0.607012" />
      <atom id="a7" elementType="H" x3="2.037337" y3="-1.608719" z3="0.138469" />
      <atom id="a8" elementType="H" x3="2.469683" y3="-0.163904" z3="1.085429" />
      <atom id="a9" elementType="C" x3="-1.874516" y3="-0.546271" z3="0.078546" />
      <atom id="a10" elementType="H" x3="-2.271882" y3="-0.198727" z3="1.040808" />
      <atom id="a11" elementType="H" x3="-2.454921" y3="-0.266176" z3="-0.810583" />
      <atom id="a12" elementType="O" x3="-0.950841" y3="-1.348998" z3="0.020012" />
    </atomArray>
    <bondArray>
      <bond atomRefs2="a3 a2" order="1" />
      <bond atomRefs2="a11 a9" order="1" />
      <bond atomRefs2="a6 a1" order="1" />
      <bond atomRefs2="a2 a1" order="1" />
      <bond atomRefs2="a2 a4" order="1" />
      <bond atomRefs2="a5 a4" order="1" />
      <bond atomRefs2="a12 a9" order="2" />
      <bond atomRefs2="a9 a10" order="1" />
      <bond atomRefs2="a1 a7" order="1" />
      <bond atomRefs2="a1 a8" order="1" />
    </bondArray>
    <propertyList>
      <property title="program">
```

```
        <scalar>Gaussian 09, Revision D.01</scalar>
      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
      <property title="method">
        <scalar>B3LYP</scalar>
      </property>
      <property title="File Format">
        <scalar>g03</scalar>
      </property>
      <property title="Energy" dictRef="me:ZPE">
        <scalar units="kJ/mol" convention="computational"
zeroPointVibEnergyAdded="true">-266.76</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">62.13 97.23 140.26 151.44 304.11 314.85 337.33 380.87 561.43
573.63 866.80 897.83 973.51 1066.90 1149.08 1168.96 1251.17 1351.78 1408.32 1454.16
1464.08 1508.28 1579.47 1689.46 2956.35 3020.80 3031.27 3081.66 3140.65
3197.87</array>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
        <array units="cm-1">0.175 0.094 0.066</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>1</scalar>
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    </propertyList>
  </molecule>
  <molecule id="Cfa1">
    <atomArray>
      <atom id="a1" elementType="C" x3="-1.628628" y3="1.178988" z3="0.019416" />
      <atom id="a2" elementType="C" x3="-2.014980" y3="-0.263196" z3="0.043493" />
```

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      <atom id="a3" elementType="H" x3="-3.099230" y3="-0.463665" z3="0.154371" />
      <atom id="a4" elementType="O" x3="-1.252698" y3="-1.199519" z3="-0.046059" />
      <atom id="a5" elementType="H" x3="-2.182262" y3="1.678699" z3="-0.780919" />
      <atom id="a6" elementType="H" x3="-1.959522" y3="1.646138" z3="0.951932" />
      <atom id="a7" elementType="H" x3="-0.555607" y3="1.321104" z3="-0.111564" />
      <atom id="a8" elementType="C" spinMultiplicity="2" x3="1.459277" y3="-1.055111"
z3="-0.183656" />
      <atom id="a9" elementType="H" x3="1.514456" y3="-1.979499" z3="0.373492" />
      <atom id="a10" elementType="H" x3="1.142293" y3="-0.980298" z3="-1.214471" />
      <atom id="a11" elementType="O" x3="1.809286" y3="-0.028010" z3="0.433852" />
      <atom id="a12" elementType="O" spinMultiplicity="2" x3="1.724144" y3="1.179208"
z3="-0.218837" />
    </atomArray>
    <bondArray>
      <bond atomRefs2="a10 a8" order="1" />
      <bond atomRefs2="a5 a1" order="1" />
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      <bond atomRefs2="a8 a9" order="1" />
      <bond atomRefs2="a8 a11" order="1" />
      <bond atomRefs2="a7 a1" order="1" />
      <bond atomRefs2="a4 a2" order="2" />
      <bond atomRefs2="a1 a2" order="1" />
      <bond atomRefs2="a1 a6" order="1" />
      <bond atomRefs2="a2 a3" order="1" />
    </bondArray>
    <propertyList>
      <property title="program">
        <scalar>Gaussian 09, Revision D.01</scalar>
      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
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<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

<scalar>g03</scalar>

</property>

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<scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="true">-259.95</scalar>

</property>

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">51.09 82.24 90.25 109.08 128.39 181.09 202.48 519.04 532.84 678.81 782.70 865.13 896.38 992.85 1143.64 1149.84 1235.54 1389.74 1413.67 1423.72 1467.81 1478.41 1567.37 1779.24 2890.17 3004.47 3062.78 3101.24 3132.86 3276.84</array>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.177 0.065 0.049</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

</propertyList>

</molecule>

<molecule id="Cfa2">

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<atom id="a2" elementType="C" x3="-2.440784" y3="0.188467" z3="0.000015" />

<atom id="a3" elementType="H" x3="-3.534865" y3="0.363110" z3="0.000049" />

<atom id="a4" elementType="O" x3="-1.686882" y3="1.132770" z3="-0.000001" />

<atom id="a5" elementType="H" x3="-2.444380" y3="-1.746527" z3="-0.875108" />

<atom id="a6" elementType="H" x3="-2.444331" y3="-1.746540" z3="0.875111" />

<atom id="a7" elementType="H" x3="-0.937189" y3="-1.348876" z3="-0.000038" />

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      <atom id="a8" elementType="C" spinMultiplicity="2" x3="1.565528" y3="1.042583" z3="-
0.000006" />
      <atom id="a9" elementType="H" x3="2.454020" y3="1.663367" z3="0.000053" />
      <atom id="a10" elementType="H" x3="0.539327" y3="1.388502" z3="-0.000047" />
      <atom id="a11" elementType="O" x3="1.702666" y3="-0.203437" z3="-0.000027" />
      <atom id="a12" elementType="O" spinMultiplicity="2" x3="2.951301" y3="-0.738689"
z3="0.000024" />
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      <bond atomRefs2="a1 a2" order="1" />
      <bond atomRefs2="a1 a6" order="1" />
      <bond atomRefs2="a8 a9" order="1" />
      <bond atomRefs2="a4 a2" order="2" />
      <bond atomRefs2="a2 a3" order="1" />
    </bondArray>
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        <scalar>Gaussian 09, Revision C.01</scalar>
      </property>
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      </property>
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712.47 778.05 891.42 901.18 997.48 1137.40 1140.19 1255.84 1384.28 1409.26 1426.42
1461.30 1469.91 1544.73 1792.50 2893.97 3022.66 3072.25 3098.31 3137.99
3251.02</array>
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  </molecule>
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z3="0.612757" />
      <atom id="a3" elementType="H" x3="-1.657196" y3="0.454777" z3="1.600228" />
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      <atom id="a5" elementType="O" spinMultiplicity="2" x3="-0.164546" y3="-1.328994"
z3="-0.604524" />
      <atom id="a6" elementType="H" x3="-0.524243" y3="1.411419" z3="-0.910582" />
      <atom id="a7" elementType="H" x3="-2.169283" y3="1.847171" z3="-0.372369" />
      <atom id="a8" elementType="H" x3="-1.860722" y3="0.392913" z3="-1.393197" />
      <atom id="a9" elementType="C" x3="2.029503" y3="-0.043452" z3="-0.167678" />
      <atom id="a10" elementType="H" x3="2.334801" y3="-0.918443" z3="0.427315" />
      <atom id="a11" elementType="H" x3="2.130582" y3="-0.146991" z3="-1.259248" />
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      <bond atomRefs2="a4 a2" order="1" />
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      </property>
      <property title="basis">
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      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
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</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.160 0.084 0.068</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

</propertyList>

</molecule>

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<atom id="a3" elementType="C" x3="1.278183" y3="0.219838" z3="0.000000" />

<atom id="a4" elementType="H" x3="2.233452" y3="-0.287527" z3="-0.000000" />

<atom id="a5" elementType="H" x3="1.300084" y3="1.303347" z3="-0.000000" />

<atom id="a6" elementType="H" x3="0.166634" y3="-1.537973" z3="-0.000000" />

<atom id="a7" elementType="H" x3="-1.180079" y3="1.250999" z3="-0.000004" />

<atom id="a8" elementType="H" x3="-1.803043" y3="-0.153849" z3="-0.876177" />

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</atomArray>

<bondArray>

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<bond atomRefs2="a1 a9" order="1" />

<bond atomRefs2="a2 a3" order="2" />

<bond atomRefs2="a2 a6" order="1" />

<bond atomRefs2="a3 a4" order="1" />

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    </bondArray>
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      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
      <property title="method">
        <scalar>B3LYP</scalar>
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      </property>
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        <scalar units="kJ/mol" convention="computational"
zeroPointVibEnergyAdded="true">0.00</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">204.95 425.86 592.52 924.20 947.72 950.30 1027.49 1075.02
1192.56 1330.73 1409.89 1452.59 1479.59 1494.42 1708.03 3014.16 3054.98 3090.02
3122.29 3128.63 3208.66</array>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
        <array units="cm-1">1.575 0.311 0.272</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor" default="true">
        <scalar>1</scalar>
      </property>
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    </propertyList>
    <me:DOSCMethod xsi:type="QMRotors" />
  </molecule>
  <molecule id="O3" spinMultiplicity="1" default="true">
    <atomArray>
      <atom id="a1" elementType="O" x3="0.000000" y3="-0.000000" z3="0.429077" />
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839.02 906.08 933.04 962.74 994.90 1078.86 1146.02 1166.37 1235.20 1332.60 1351.33

1390.43 1416.35 1486.57 1500.25 1512.18 3023.49 3037.84 3039.65 3100.11 3104.12 3113.69</array>
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<me:DistributionCalcMethod default="true" name="Boltzmann" />
<me:energyTransferModel name="ExponentialDown" default="true" />
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<atom id="a3" elementType="C" x3="-0.319630" y3="1.177145" z3="0.070401" />
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  <atom id="a11" elementType="H" x3="1.641410" y3="-0.162621" z3="-1.426001" />
  <atom id="a12" elementType="H" x3="2.619423" y3="-0.740974" z3="-0.066630" />
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  <property title="basis">
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  </property>
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835.09 904.91 934.15 954.79 1002.13 1062.49 1110.89 1165.63 1241.22 1308.39 1345.08
1380.99 1411.28 1486.88 1496.36 1506.91 3029.38 3033.44 3063.31 3095.20 3110.69
3116.89</array>
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      <property title="Symmetry Number" dictRef="me:symmetryNumber">
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      <property dictRef="me:frequenciesScaleFactor" default="true">
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    </propertyList>
    <me:DOSCMethod xsi:type="QMRotors" />
    <me:DistributionCalcMethod default="true" name="Boltzmann" />
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      <atom id="a3" elementType="C" x3="0.971533" y3="1.353841" z3="-0.316182" />
      <atom id="a4" elementType="H" x3="0.531213" y3="1.938242" z3="-1.112426" />
      <atom id="a5" elementType="H" x3="1.068868" y3="1.835740" z3="0.648039" />
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      <atom id="a7" elementType="H" x3="2.105661" y3="-0.251830" z3="1.477924" />
      <atom id="a8" elementType="H" x3="1.478727" y3="-1.680958" z3="0.645647" />
      <atom id="a9" elementType="H" x3="3.055910" y3="-1.045358" z3="0.210847" />
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    <property title="method">
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741.88 925.19 952.25 956.03 1008.94 1069.60 1163.20 1192.11 1196.83 1325.78 1407.21
1449.56 1477.89 1493.02 1667.02 3019.25 3064.56 3098.95 3134.08 3139.23
3220.60</array>
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    <property dictRef="me:sigma" default="true">
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<property dictRef="me:frequenciesScaleFactor" default="true">
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<atom id="a3" elementType="C" x3="0.975341" y3="1.340484" z3="0.275489" />
<atom id="a4" elementType="H" x3="1.047800" y3="1.810920" z3="-0.697473" />
<atom id="a5" elementType="H" x3="0.511754" y3="1.915285" z3="1.063783" />
<atom id="a6" elementType="H" x3="1.389971" y3="-0.298113" z3="1.496664" />
<atom id="a7" elementType="H" x3="3.146442" y3="-0.982935" z3="-0.233810" />
<atom id="a8" elementType="H" x3="1.600609" y3="-1.696077" z3="-0.641658" />
<atom id="a9" elementType="H" x3="2.155223" y3="-0.253003" z3="-1.505010" />
<atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.736533" y3="0.801348" z3="-0.451900" />
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<property title="basis">

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</property>

<property title="method">

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</property>

<property title="File Format">

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</property>

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    <me:DistributionCalcMethod default="true" name="Boltzmann" />
    <me:energyTransferModel name="ExponentialDown" default="true" />
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      <atom id="a5" elementType="H" x3="-0.106096" y3="1.573175" z3="-1.084563" />
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      <atom id="a7" elementType="H" x3="2.797103" y3="-0.533157" z3="0.389879" />
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z3="-0.019875" />
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</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

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<property dictRef="me:frequenciesScaleFactor" default="true">

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</molecule>

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<atom id="a9" elementType="H" x3="-1.396042" y3="0.333887" z3="-1.538607" />

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zeroPointVibEnergyAdded="true">-156.71</scalar>
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848.66 897.37 947.79 1017.56 1051.81 1112.74 1170.13 1222.41 1267.65 1317.82 1398.67
1451.48 1477.75 1481.97 1499.91 2891.63 3032.51 3092.50 3106.45 3118.82
3224.46</array>
      </property>
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      <atom id="a6" elementType="H" x3="-0.899090" y3="0.060505" z3="-1.547828" />
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873.65 884.71 988.54 989.69 1062.21 1090.56 1182.05 1229.85 1265.85 1351.31 1392.08
1451.36 1479.27 1483.45 1501.20 2912.54 3029.00 3091.75 3104.88 3115.75
3224.03</array>
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      <property dictRef="me:frequenciesScaleFactor" default="true">
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      <atom id="a3" elementType="C" x3="-0.481983" y3="1.364071" z3="0.249512" />
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      <atom id="a7" elementType="H" x3="-1.849166" y3="-1.578058" z3="-0.436073" />
      <atom id="a8" elementType="H" x3="-1.924197" y3="-0.119125" z3="-1.434144" />
      <atom id="a9" elementType="H" x3="-3.071437" y3="-0.358797" z3="-0.108116" />
      <atom id="a10" elementType="O" spinMultiplicity="2" x3="1.461418" y3="0.617093"
z3="-0.613638" />
      <atom id="a11" elementType="O" x3="1.635810" y3="-0.360818" z3="0.205516" />
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743.36 919.21 949.34 962.03 990.92 1054.68 1085.52 1117.27 1199.16 1300.89 1407.93
1445.11 1476.59 1492.81 1591.48 3019.96 3076.47 3109.70 3154.11 3165.25
3245.18</array>
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      <property dictRef="me:frequenciesScaleFactor" default="true">
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      <atom id="a5" elementType="H" x3="-0.529152" y3="1.793872" z3="-0.840672" />
      <atom id="a6" elementType="H" x3="-1.234267" y3="-0.003310" z3="1.545558" />
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z3="0.645224" />
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<property title="File Format">

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</property>

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<scalar units="cm-1">214.98</scalar>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

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</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

<property dictRef="me:frequenciesScaleFactor" default="true">

<scalar>1</scalar>

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</propertyList>

<me:DOSCMethod xsi:type="QMRotors" />

</molecule>

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  <atom id="a3" elementType="C" x3="0.296814" y3="1.113797" z3="0.488690" />
  <atom id="a4" elementType="H" x3="-0.100018" y3="2.072517" z3="0.158989" />
  <atom id="a5" elementType="H" x3="0.825170" y3="1.214993" z3="1.439952" />
  <atom id="a6" elementType="H" x3="-1.218772" y3="-0.047703" z3="1.526952" />
  <atom id="a7" elementType="H" x3="-1.277398" y3="0.095444" z3="-1.546414" />
  <atom id="a8" elementType="H" x3="-2.363395" y3="-0.889421" z3="-0.556673" />
  <atom id="a9" elementType="C" x3="-0.743890" y3="-0.000174" z3="0.545489" />
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<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>B3LYP</scalar>

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<property title="File Format">

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</property>

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</property>

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<scalar units="cm-1">147.80</scalar>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

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</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

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</property>

<property dictRef="me:frequenciesScaleFactor" default="true">

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<me:DOSCMethod xsi:type="QMRotors" />

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    <atom id="a5" elementType="H" x3="-0.133667" y3="2.081572" z3="-0.334133" />
    <atom id="a6" elementType="H" x3="0.636947" y3="0.072052" z3="-1.487915" />
    <atom id="a7" elementType="H" x3="2.136289" y3="-0.003363" z3="1.195784" />
    <atom id="a8" elementType="H" x3="2.625909" y3="-0.866339" z3="-0.268922" />
    <atom id="a9" elementType="C" x3="0.677520" y3="0.040398" z3="-0.394185" />
    <atom id="a10" elementType="O" x3="-1.511611" y3="0.632049" z3="-0.109715" />
    <atom id="a11" elementType="O" x3="0.018055" y3="-1.131655" z3="0.081309" />
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      </property>
      <property title="method">
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1415.52 1485.35 1489.78 1502.14 3004.83 3019.35 3042.65 3106.74 3109.95
3117.97</array>
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      <atom id="a7" elementType="H" x3="0.965329" y3="-0.573860" z3="-1.499174" />
      <atom id="a8" elementType="H" x3="1.942306" y3="-1.617141" z3="-0.438116" />
      <atom id="a9" elementType="H" x3="2.387497" y3="0.079938" z3="-0.677500" />
      <atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.491250" y3="-0.326126"
z3="-0.549136" />
      <atom id="a11" elementType="O" spinMultiplicity="2" x3="-0.299553" y3="1.391748"
z3="-0.474450" />
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      </property>
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      <property title="Energy" dictRef="me:ZPE">
        <scalar units="kJ/mol" convention="computational"
zeroPointVibEnergyAdded="true">-161.14</scalar>
      </property>
      <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
        <array units="cm-1">156.66 188.42 296.57 306.33 344.35 527.31 563.61 702.29
871.60 883.89 939.20 1020.93 1086.14 1147.21 1186.07 1222.88 1223.60 1375.65 1398.52
1429.40 1471.58 1495.34 1539.20 2919.34 2983.64 3034.73 3105.23 3132.48
3154.73</array>
      </property>
      <property title="ImaginaryFrequency" dictRef="me:imFreqs">
        <scalar units="cm-1">444.86</scalar>
      </property>
      <property title="Rotational Constants" dictRef="me:rotConsts">
        <array units="cm-1">0.156 0.129 0.098</array>
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
        <scalar>1</scalar>
```

```
      </property>
      <property dictRef="me:frequenciesScaleFactor" default="true">
        <scalar>1</scalar>
      </property>
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  </molecule>
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      </reactant>
      <reactant>
        <molecule ref="O3" role="excessReactant" />
      </reactant>
    </reactantList>
    <productList>
      <product>
        <molecule ref="PRC1" role="modelled" />
      </product>
    </productList>
    <rateParameters reactionType="arrhenius" reversible="true">
      <A>1.000e-010</A>
      <n>0</n>
      <E>0</E>
    </rateParameters>
    <me:MCRCMethod xsi:type="MesmerILT">
    <me:excessReactantConc>1.0E16</me:excessReactantConc>
    <me:TInfinity default="true">298</me:TInfinity>
```

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</reaction>
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  <reactantList>
    <reactant>
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    <reactant>
      <molecule ref="O3" role="excessReactant" />
    </reactant>
  </reactantList>
  <productList>
    <product>
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    </product>
  </productList>
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    <A>1.000e-010</A>
    <n>0</n>
    <E>0</E>
  </rateParameters>
  <me:MCRCMethod xsi:type="MesmerILT">
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  <me:TInfinity default="true">298</me:TInfinity>
</reaction>
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    <reactant>
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    </reactant>
  </reactantList>
  <productList>
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    <product>
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    </product>
  </productList>
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    <molecule ref="TSozo1" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
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    <reactant>
      <molecule ref="PRC2" role="modelled" />
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  </reactantList>
  <productList>
    <product>
      <molecule ref="POZ2" role="modelled" />
    </product>
  </productList>
  <me:transitionState>
    <molecule ref="TSozo2" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
</reaction>
<reaction id="R5" reversible="true">
  <reactantList>
    <reactant>
      <molecule ref="POZ1" role="modelled" />
```

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    </reactant>
  </reactantList>
  <productList>
    <product>
      <molecule ref="POZ2" role="modelled" />
    </product>
  </productList>
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  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
</reaction>
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      <molecule ref="POZ1" role="modelled" />
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  <productList>
    <product>
      <molecule ref="POZ2" role="modelled" />
    </product>
  </productList>
  <me:transitionState>
    <molecule ref="TSpoz2" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
</reaction>
<reaction id="R7">
```

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  </productList>
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  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
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      <molecule ref="POZ1" role="modelled" />
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  </reactantList>
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    <product>
      <molecule ref="Canti" role="sink" />
    </product>
  </productList>
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    <molecule ref="TSanti" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
```

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  <me:tunneling>Eckart</me:tunneling>
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      <molecule ref="POZ2" role="modelled" />
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  </reactantList>
  <productList>
    <product>
      <molecule ref="Cfa2" role="sink" />
    </product>
  </productList>
  <me:transitionState>
    <molecule ref="TSfa2" role="transitionState" />
  </me:transitionState>
  <me:MCRCMethod name="SimpleRRKM" />
  <me:tunneling>Eckart</me:tunneling>
</reaction>
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    <reactant>
      <molecule ref="POZ2" role="modelled" />
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  </reactantList>
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    <product>
      <molecule ref="Csyn" role="sink" />
    </product>
  </productList>
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```

```
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    <me:tunneling>Eckart</me:tunneling>
  </reaction>
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 <me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
   <me:PTpair units="Torr" P="760" T="200." precision="d" default="true" bathGas="N2" />
   <me:PTpair units="Torr" P="760" T="275." precision="d" default="true" bathGas="N2" />
   <me:PTpair units="Torr" P="760" T="298." precision="d" default="true" bathGas="N2" />
   <me:PTpair units="Torr" P="760" T="325." precision="d" default="true" bathGas="N2" />
   <me:PTpair units="Torr" P="760" T="400." precision="d" default="true" bathGas="N2" />
  </me:PTs>
 </me:conditions>
 <me:modelParameters>
  <me:grainSize units="cm-1">50</me:grainSize>
  <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
 </me:modelParameters>
 <me:control>
  <!--<me:calcMethod xsi:type="me:marquardt">
  <me:MarquardtIterations>50</me:MarquardtIterations>
  <me:MarquardtTolerance>0.1</me:MarquardtTolerance>
  </me:calcMethod>-->
  <me:printSpeciesProfile />
  <me:testRateConstants />
  <me:printGrainedSpeciesProfile />
  <me:eigenvalues>3</me:eigenvalues>
  <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not
shown-->
  <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
```

```
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
    <me:ForceMacroDetailedBalance default="true">true</me:ForceMacroDetailedBalance>
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>MeCHCH2 + O3 R1_f</dc:title>
    <dc:source>R1_f.xml</dc:source>
    <dc:creator>Mesmer v5.2</dc:creator>
    <dc:date>20190613_180524</dc:date>
    <dc:contributor>c1675612</dc:contributor>
  </metadataList>
</me:mesmer>
```