Ambient-pressure Alkoxycarbonylation for Sustainable Synthesis of Ester

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Supplementary Table 1 Representative recent cases of alkoxycarbonylation of alkenes via heterogenous catalysis (Entry 1-7) and homogeneous catalysis (Entry 8-15).

Entry	Substrate	n_{Sub} (mmol)	Catalyst			Nucleophile	Solvent	condition			Yield (%)	**TOF (h^{-1})**	Reactor V (ml)	**CO utilization** (%)	**CO efficiency** ($mmol_{COO}$·mol_{CO}^{-1}·h^{-1})	Reference
			Metal	**Ligand**	**Promoters**			CO (bar)	T/°C	t/h						
1	styrene	0.188	**Ru/NbO_x**			MeOH		1.6	170	16	71	**4.1**	14.0	14.8	**9.2**	**this work**
2	styrene	1.88				MeOH		1.6	170	10	60	**8.4**	14	62.4	**62.4**	
3	ethylene	0.57						1	170	1	33.6	**33.8**	14	33.6	**336**	
4	ethylene	1.13				MeOH		1	170	2	22.5	**22.7**	14	45.0	**225**	
5	styrene	0.5	**Ru/CeO_2**			MeOH		2	165	14	80	**1.4**	46	10.8	**7.7**	Chin. J. Catal. , 2020, 41, 963-969.
6	ethylene	7.5	**Ru/CeO_2**			MeOH		7	165	8	62	**19.6**	46	35.8	**44.7**	J. Am. Chem. Soc. , 2018, 140, 4172-4181.
7	styrene	5	**Pd/LSI**	**TPPTS–OTPPTS**		MeOH	toluene	30	80	3.5	92.7	**82.9**	46	8.1	**23**	Catal. Sci. Technol., 2014, 4, 1092-1103.
8	butadiene	1	**$Pd(TFA)_2$**	**HeMaRaphos**	**PTSA•H_2O**	nBuOH	toluene	40	120	24	85	**7.1**	300.0	0.4	**0.15**	Science, 2019, 366, 1514-1517.
9	butadiene	1	**$Pd(TFA)_2$**	**HeMaRaphos**	**PTSA•H_2O**	nBuOH	toluene	40	120	120	64	**533.3**	300.0	0.4	**0.07**	Science, 2019, 366, 1514-1517.
10	deca-1,3-diyn-1-ylbenzene	0.25	**$Pd(TFA)_3$**	**ferrocenediyl-pyridyl phosphine**	**PTSA•H_2O**	MeOH	toluene	40	23	20	95	**4.8**	300.0	0.1	**0.05**	Angew. Chem. Int. Ed. , 2019, 58, 10683-10687.
11	isoprene	1.2	**$[Pd(cod)Cl_2]$**	**Xantphos**	-	benzyl alcohol	toluene	50	100	20	94	**4.7**	300.0	0.2	**0.09**	Angew. Chem. Int. Ed. , 2014, 53, 9030-9034.
12	1-phenylallene	0.25	**$Pd(OAc)_2$, $Cu(OAc)_2$**	**(S,S,S)-SKP**	**Et_3N, $PhNH_2$**	MeOH	MeOH	1	25	24	89	**0.4**	2000.0	0.3	**0.1**	J. Am. Chem. Soc. , 2015, 137, 15346-15349.
13	tetramethylethylene	4	**$Pd(acac)_2$**	**pytbpx**	**PTSA•H_2O**	MeOH		40	120	20	98	**49.0**	300.0	0.8	**0.4**	Nat. Commun., 2017, 8, 14117.
14	styrene	1	**$Pd(OAc)_2$**	**PPh_3**	**$FeCl_3$**	H_2O	1,4-dioxane	50	80	10	91	**9.1**	3.0	0.2	**0.18**	Chem. Commun., 2018, 54, 3967--3970
15	styrene	0.5	**$PdCl_2$**	**pyridylcarbazoylphosphines**	**$MnBr(CO)_5$**	MeOH	toluene	60	120	20	85	**4.3**	4.0	0.1	**0.04**	J. Catal. 2022, 409, 98-104.

Supplementary Note 1: CO utilization efficiency and TOF calculations in Supplementary Table 1.

CO utilization (rate) is defined as the ratio of the amount of ester produced to the total amount of CO and calculated by the following equation. p, V, R and T represent the actual CO pressure (Pa), volume (14×10^{-6} m^3), molar gas constant (8.314 $J\cdot K^{-1}\cdot mol^{-1}$) and temperature (K). The p (Pa) equals the sum of gauge pressure (p_g, Pa) and atmospheric pressure (p_0, 10^5 Pa).

$$CO\ \ utilization\ \ (\%)\ \ =\ \ \frac{n_{ester}}{n_{CO}}\times 100\% = \frac{n_{ester}}{pV/RT}\times 100\%$$

CO utilization efficiency (h^{-1}) is defined as the CO utilization rate per unit time (h) and calculated by CO utilization/t (h).

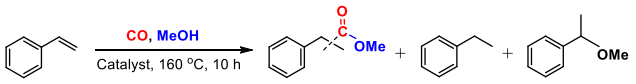
The TOF (h^{-1}) is defined as the molar amount of carbonylation produced per molar Ru metal per hour and calculated by equation.

$$TOF\ \ (h^{-1}) = \frac{n_{coo}}{m_{cat}\times wt.\%_{Ru}/M_{Ru}\times t}\ \times 100\%$$

The n_{coo} is the molar amount of carbonylation (mol), which is equal to the molar amount of monocarbonylated esters or twice the molar amount of bicarbonylated esters. M_{Ru} is the atomic weight of ruthenium (101.1 g/mol), m_{cat} is the mass weight of the catalysts (g), $wt.\%_{Ru}$ is the actual Ru weight percentage of the catalysts, and t is the reaction time (h).

In bicarbonylation reactions, the TOF (h^{-1}), CO utilization (%) and efficiency (h^{-1}), have been doubled according to the above equation, which have shown in Entry 8–10.

Supplementary Table 2 Screening of effective heterogeneous catalysts for styrene methoxylcarbonylation.



Entry	Catalyst	Atmosphere (MPa)	Conversion (%)	Selectivity (%)			C. B. (%)
				carbonylation	hydrogenation	methoxylation	
1	Pd/C	1CO	22	0	8	92	92±4
2	Pt/C	1CO	18	0	9	91	98±2
3	Ir/C	1CO	28	3	17	81	90±3
4	Ru/C	1CO	100	6	74	5	101±2
5	Ru/Hβ	1CO	59	1	3	93	83±5
6	$Ru/WZrO_x$	1CO	10	0	5	95	81±3
7	Ru/Al_2O_3	1CO	7	23	77	0	82±3
8	Ru/CeO_2	1CO	3	80	15	3	95±4
9	Ru/CeO_x	1CO	5	90	10	0	96±4
10	Ru/Nb_2O_5	1CO	7	87	6	7	98±2
11	Ru/NbO_x	1CO	13	90	8	2	91±4
12	Ru/NbO_x	0.1CO	55	90	10	0	101±2

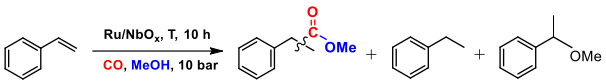
Reaction conditions: 20 mg catalysts with 5 wt.% metal loading in Entry 1-4, 30 mg catalysts with 2 wt.% metal loading in Entry 5-12, styrene (0.2 mmol), MeOH (2 mL), CO, 160 °C, 10 h. The C.B. denotes carbon balance calculated based on benzene rings before and after reactions.

Supplementary Table 3. The best-fitted EXAFS results of Ru/NbO_x[a].

Sample	Shell	CN	R (Å)	σ^2 (10^{-2} Å^2)	ΔE_0 (eV)	r-factor (%)
Ru foil	Ru-Ru	12	2.67	-	-	-
Ru/NbO_x	Ru-O	3.6±0.4	1.94±0.02	0.3±0.1	-7.0±1.8	0.9
	Ru-Ru	5.1±0.9	2.67±0.01	0.3±0.1	-7.0±1.8	
	Ru-O-Nb/Ru	1.3±0.4	3.08±0.05	0.3±0.1	-7.0±1.8	

[a]CN is the coordination number for the absorber-backscattered pair, R is the average absorber-backscattered distance, σ^2 is the Debye-Waller factor, and ΔE_0 is the inner potential correction. * S_0^2 was fixed to 0.72 as determined from Ru foil fitting. The data range used for data fitting in k-space (Δk) and R-space (ΔR) are 3.0-12.7 $Å^{-1}$ and 1.0-3.3 Å, respectively.

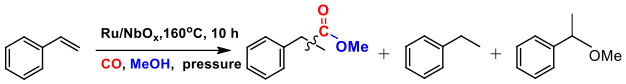
Supplementary Table 4 Optimization of temperature for styrene carbonylation.



Entry	Temperature(℃)	Conv. (%)	Sele.(%)			L/(L+B) (%)	C. B. (%)
			carbonylation	hydrogenation	methoxylation		
1	140	2	56	34	9	61	98
2	160	7	65	31	4	73	83
3	170	22	71	25	4	79	104
4	180	39	63	36	2	79	86
5	200	92	40	56	1	79	107

Reaction conditions: 2 wt.% Ru/NbO_x (30 mg, 5.6 umol Ru), styrene (0.2 mmol), H_3BO_3 (4.0 mmol, 5 mol%), MeOH (2.0 mL), CO (10 bar), 10 h. The L/(L+B) denotes the ratio of linear esters to branched esters.

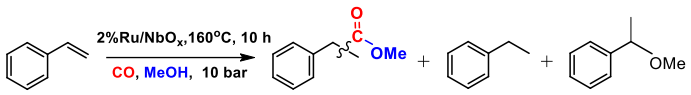
Supplementary Table 5 Pressure-dependent evolutions of styrene carbonylation.



Entry	pressure (bar)	Conv. (%)	Sele.(%)			L/(L+B) (%)	C. B. (%)
			carbonylation	hydrogenation	methoxylation		
1	0.6	24	84	16	0	74	92
2	1.0	15	88	12	0	73	102
3	3.5	5	80	20	0	71	86
4	5.0	4	77	23	0	66	83

Reaction conditions: 1 wt.% Ru/NbO$_x$ (30 mg, 5.6 umol Ru), styrene (0.2 mmol), MeOH (2.0 mL), CO, 160 °C, 10 h.

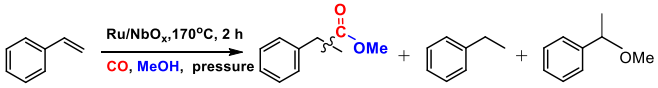
Supplementary Table 6 Effects of catalyst weight loadings on styrene carbonylation.



Entry	catalyst mass (mg)	Conv. (%)	Sele.(%)		
			carbonylation	hydrogenation	methoxylation
1	20	4	87	7	6
2	30	5	87	9	4
3	100	19	83	11	1

Reaction conditions: 2 wt.% Ru/NbO$_x$, styrene (0.2 mmol), MeOH (2.0 mL), CO (10 bar), 160 °C, 10 h.

Supplementary Table 7 Effects of styrene concentration on styrene carbonylation.



Entry	styrene	Conv. (%)	Yield (%)			L/(L+B) (%)
			carbonylation	hydrogenation	methoxylation	
1	1 eq.	26	22	4	0	75
2	3.5 eq.	24	21	2	0	75
3	10 eq.	21	19	2	0	75
4*	10 eq.	24	20	3	0	76

Reaction conditions: 2 wt.% Ru/NbO$_x$ (30 mg), styrene (1 eq, 0.188 mmol), MeOH (2.0 mL), CO (1 bar), 170 °C, 2 h. *(0.6 bar).

Supplementary Table 8 Effects of solvent for styrene carbonylation.

Entry	Solvent	Conv. (%)	Yield (%)			L/(L+B) (%)
			carbonylation	hydrogenation	methoxylation	
1	2-MTHF	16	1	15	0	68
2	cyclohexane	15	4	9	1	83
3	toluene	22	7	13	1	85
4	methanol	95	71	24	0	75

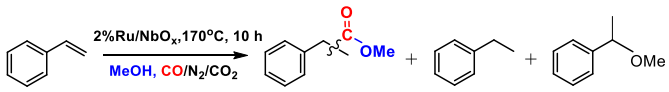
Reaction conditions: 2 wt.% Ru/NbO$_x$, styrene (0.2 mmol), solvent (2.0 mL), CO (1 bar), 170 °C, 16 h.

Supplementary Table 9 Effects of water for styrene carbonylation.

Entry	amount of H_2O	Conv. (%)	Yield (%)			L/(L+B)(%)	C. B. (%)
			carbonylation	hydrogenation	methoxylation		
1	0	68	56	12	0	75	94
2	3 eq.	71	48	22	0	75	89
3	7 eq.	75	56	19	0	76	93
4	21 eq.	3	0	3	0	-	91

Reaction conditions: 2 wt.% Ru/NbO_x (30 mg), styrene (0.2 mmol, 1 eq.), MeOH (2.0 mL), CO (1 bar), 170 °C, 10 h.

Supplementary Table 10 Effects of reaction atmosphere for styrene carbonylation.



Entry	Atmosphere (bar)	Conv. (%)	Yield (%)			L/(L+B) (%)	C. B. (%)
			carbonylation	hydrogenation	methoxylation		
1	1CO	68	56	12	0	75	94
2	$1CO/10N_2$	14	9	5	0	73	90
3	$1CO/2CO_2$	37	28	9	0	75	93
4	$1CO/2CO_2/H_2O$	9	5	4	0	74	85

Reaction conditions: 2 wt.% Ru/NbO_x (30 mg), styrene (0.2 mmol), MeOH (2.0 mL), $CO/N_2/CO_2$/0.4 mmol H_2O, 170 °C, 10 h.

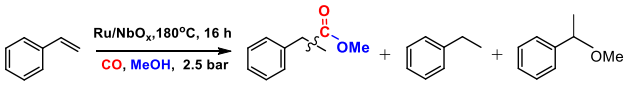
Supplementary Table 11 Ru dispersion, CO pulse chemisorption data and ICP-OES data of Ru_1/NbO_x and 2 wt.% Ru/NbO_x catalysts.

Sample	Ru wt.% from ICP-OES[a]	CO accumulative sorption quantity (mmol/g)[b]	Ru dispersion[b]	Ru active diameter (nm)[b]
Ru_1/NbO_x	0.098%	0.00969	99.8%	1.1
2 wt.% Ru/NbO_x	1.891%	0.08172	44.4%	2.2
4 wt.% Ru/NbO_x	3.331%	0.14432	43.8%	3.1

[a]The ruthenium loading was determined by ICP-OES.

[b]CO pulse chemisorption.

Supplementary Table 12 Effects of fully dispersed Ru and size-dependent Ru clusters on styrene carbonylation.



Entry	catalysts	Conv. (%)	Yield (%)			L/(L+B) (%)	C. B. (%)
			carbonylation	hydrogenation	methoxylation		
1	Ru_1/NbO_x	0.8	0	0.8	0	-	90
2	Ru/NbO_x-2.2 nm	80	62	17	0	75	97
3	Ru/NbO_x-3.1 nm	42	14	27	0	74	95

Reaction conditions: catalyst (30 mg), styrene (0.2 mmol), MeOH (2.0 mL), CO (2.5 bar), 180 °C, 16 h.

Supplementary Table 13 The deconvolution of CO-adsorption FTIR spectra on 2 wt.% Ru/NbO_x catalysts (Figure 2h).

No.	Peak(cm^{-1})	Species	Factor of n_{Ru}/n_{CO}	Ratio of peak area(%)
1	2140	$Ru(CO)_3$	1/3	3.4
2	2081	$Ru(CO)_3$	1/3	13.8
3	2128	$Ru(CO)_2$	1/2	1.1
4	2063	$Ru(CO)_2$	1/2	11.6
5	2015	Ru(CO)	1	52.1
6	1969	Ru(CO)	1	18.0

Supplementary Note 2 Calculation of the average factor of n_{Ru}/n_{CO}.

$$AF_{Ru/CO} = \frac{\sum_1^3 A_{Ru(CO)_n} \times \varepsilon \times 1/n}{\sum_1^3 A_{Ru(CO)_n}} = \quad 1/n \sum_1^3 R_{Ru(CO)_n} = 1/3R_{Ru(CO)_3} + 1/2R_{Ru(CO)_2} + R_{Ru-CO}$$

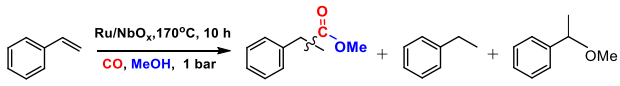
The $A_{Ru(CO)n}$ and ε represent peak areas and extinct coefficients ($\varepsilon_{linear} \approx 0.1\varepsilon_{bridge}$), and $R_{Ru(CO)n}$ are the proportions of the peak area of the $Ru(CO)_n$ (n = 1, 2, 3) species, and evaluated from the peak deconvolution of the CO-adsorption FTIR spectra (Supplementary Table 13). No bridge-bonded CO peak (<1900 cm^{-1}) was observed on Ru/NbO_x. Based on the results of Supplementary Table 13, the $AF_{Ru/CO}$ is 0.822 and the calibrated Ru dispersion of 2 wt.%Ru/NbO_x catalysts is 36.4%.

Supplementary Table 14 The reported band assignment of various Ru carbonyl species absorbed on oxide in CO-probed infrared spectra.

Adsorbed species	Ru adsorption sites	Frequency (cm^{-1})	Samples	Ref.
tricarbonyl species $Ru^{n+}(CO)_3$	Ru^{n+} (n=1-3)	2142-2028, 2082-2067	Ru/Nb_2O_5, Ru/TiO_2, Ru/SiO_2, Ru/Al_2O_3	1-5
	$(SiO)_xRu^{n+}$ (n=1-3) $(RuO)_xRu^{n+}$ (n=1-3)	2140, 2080 2130, 2070	Ru/SiO_2	2-3
dicarbonyl species $Ru(CO)_2$	Ru^{2+}	2132, 2070	Ru/SiO_2	2
	Ru^0	2080, 2015	Ru/SiO_2	2
linear Ru-CO	Ru^{n+} (n=1-3)	2110-2080	Ru/SiO_2	2, 3
	Ru^0	2050-2010	Ru/SiO_2, Ru/Nb_2O_5, Ru/TiO_2	1-5
	$Ru^{\delta+}$	1995	Ru/TiO_2	2,4
	interfacial $(TiO_2)Ru$	1975	Ru/TiO_2	4
		1950	Ru/TiO_2	5
bridged Ru_2-CO	Ru^0	1990-1750	Ru/SiO_2	3
	Ru^0	1810	Ru/TiO_2	4

[1] Komanoya, T.; Kinemura, T.; Kita, Y.; Kamata, K.; Hara, M. ***J. Am. Chem. Soc.*** 139 (2017) 11493-11499.
[2] S.Y. Chin, C.T. Williams, M.D. Amiridis, ***J. Phys. Chem. B*** 110 (2006) 871-882.
[3] G.H. Yokomizo, C. Louis, T. Bell, ***J. Catal.*** 120 (1989) 1-14.
[4] Panagiotopoulou, P.; Kondarides, D. I.; Verykios, X. E. ***J. Phys. Chem. C*** 115 (2011) 1220-1230.
[5] Zhou, J.; Gao, Z.; Xiang, G.; Zhai, T.; Liu, Z.; Zhao, W.; Liang, X.; Wang, L ***Nat. Commun.*** 13 (2022) 327.

Supplementary Table 15 Effects of active Ru components on styrene carbonylation.

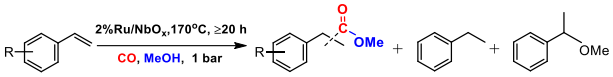


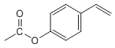
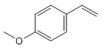
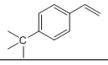
Catalyst	Mass (g)	Time (h)	Conv. (%)	Yield (%)			L/(L+B) (%)	C. B. (%)
				carbonylation	hydrogenation	methoxylation		
Ru/NbO_x	20	10	54	38	15	0	75	90
Ru^0/NbO_x	20	10	28	18	10	0	67	84
Ru^{3+}/NbO_x	20	10	78	47	30	1	78	95

Reaction conditions: styrene (0.2 mmol), MeOH (2.0 mL), CO (1 bar), 170 ºC. The Ru loading of each catalysts is 2 wt.%.

In contrast, $RuCl_3/NbO_x$ catalysts showed a similar carbonylation yield in comparison to 2 wt.% Ru/NbO_x, due to in-situ reduction by active H or H_2 produced during the reaction (Supplementary Fig. 17).

Supplementary Table 16 Substrate scopes of substituted vinyl arenes.



substrate	time/h	Conv.(%)	Yield (%)			L/(L+B) (%)
			carbonylation	hydrogenation	methoxylation	
	20	100	40	45	15	72
	20	100	52	48	0	74
	20	96	46	30	20	72
	23	95	34	47	14	70
	20	72	50	20	2	74

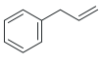
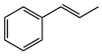
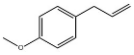
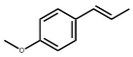
Reaction conditions: 2 wt.% Ru/NbO_x (30 mg), substrate (0.2 mmol), MeOH (2.0 mL), CO (1 bar), 170 ºC.

Supplementary Table 17 Dependence of side chains of aryl olefins on their carbonylation performance.

substrate	p/MPa	T/℃	t/h	Conv.(%)	Yield (%)				L/(L+B) (%)
					carbonylation	isomerisation	hydrogenation	methoxylation	
	0.1	170	16	96	71	0	24	0	75
	0.1	170	23	100	21	69	9	0	53
	0.1	170	21	99	25	68	8	0	48

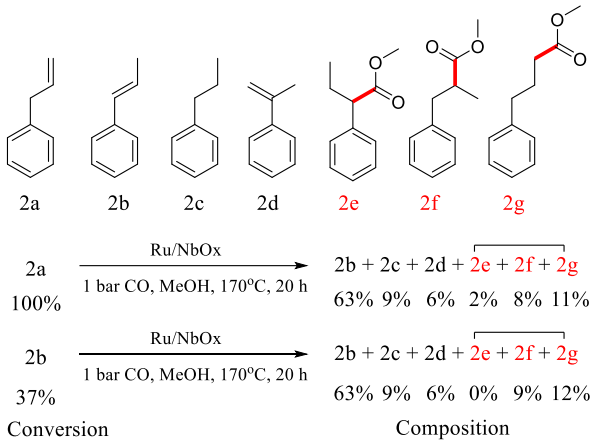
Reaction conditions: 2 wt.% Ru/NbO_x (30 mg), substrate (0.2 mmol), MeOH (2.0 mL).

Supplementary Table 18 Dependence between terminal/internal olefins and carbonylation acitivity in aryl olefins.

substrate	p/MPa	T/℃	t/h	Conv.(%)	Yield (%)				Linear ratio (%)
					carbonylation	isomerisation	hydrogenation	methoxylation	
	0.1	170	23	100	21	69	9	0	53
	0.1	170	23	37	20	6	9	0	57
	0.1	170	20	100	17	77	6	0	35
	0.1	170	20	42	20	5	17	0	39

Reaction conditions: 2 wt.% Ru/NbO_x (30 mg), substrate (0.2 mmol), MeOH (2.0 mL).

Supplementary Table 19 Comparison of product compositions of terminal/internal olefins carbonylation reactions.



Supplementary Table 20 Substrate scope of alcohols for alkoxycarbonylation.

substrate	p/MPa	T/℃	t/h	Conv.(%)	Selectivity (%)			L/(L+B) (%)
					carbonylation	hydrogenation	methoxylation	
MeOH	0.1	170	18	98	81	19	0	75
EtOH	0.1	170	16	86	52	48	0	73
PrOH	0.1	170	18	79	32	32	36	74
i-PrOH	0.1	170	16	78	21	73	6	73

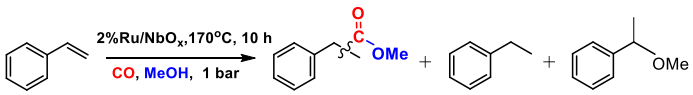
Reaction conditions: 2 wt.%Ru/NbO_x (30 mg), substrate (0.2 mmol), solvent (2.0 mL).

Supplementary Table 21 Cycle performance.

Entry	Substrate	Cylce	Conversion (%)	Yield of carbonylation (%)
1	ethylene	1	32	29
2		2	3	3
3		3	4	4
4	styrene	1	70	52
5		2	7	2

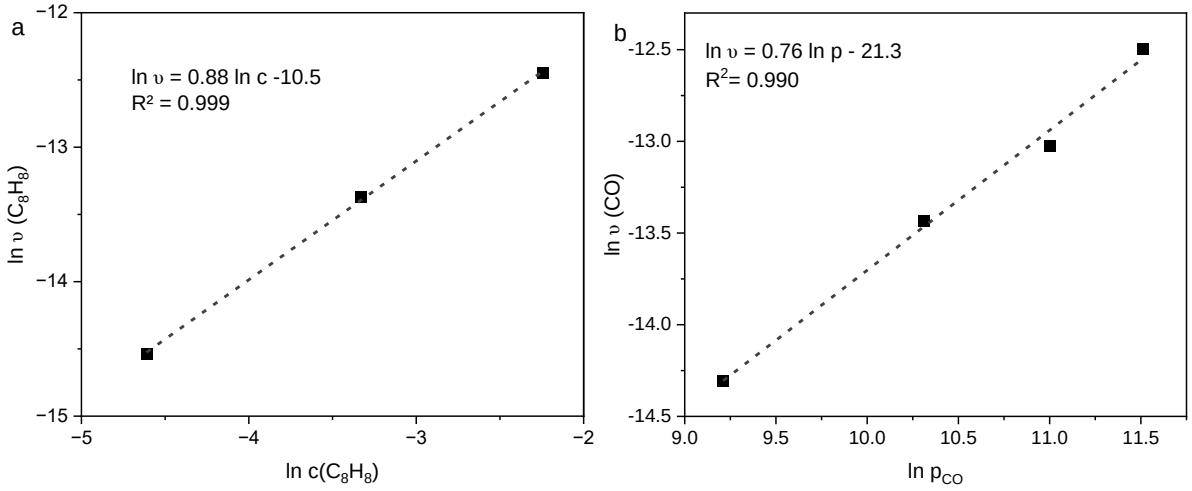
Reaction conditions: [a]2 wt.%Ru/NbO_x (30 mg), ethylene (0.57 mmol), MeOH (2.0 mL), CO (1 bar), 170 ℃, 2 h. [b]2 wt.%Ru/NbO_x (30 mg), styrene (0.2 mmol), MeOH (2.0 mL), CO (1 bar), 170 ℃, 10 h.

Supplementary Table 22 Effects of pyridine poison on styrene carbonylation.



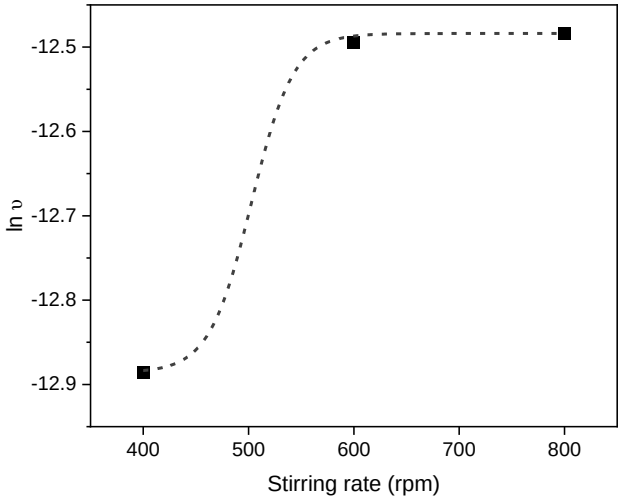
Entry	Poison	Conv. (%)	Yield.(%)		
			carbonylation	hydrogenation	methoxylation
1	pyridine	74	49	16	0
2	no	73	50	14	0

Reaction conditions: 2 wt.%Ru/NbO_x (30 mg), styrene (0.2 mmol), pyridine (6.3 μmol), MeOH (2.0 mL), CO (1 bar), 170 ℃,10 h.



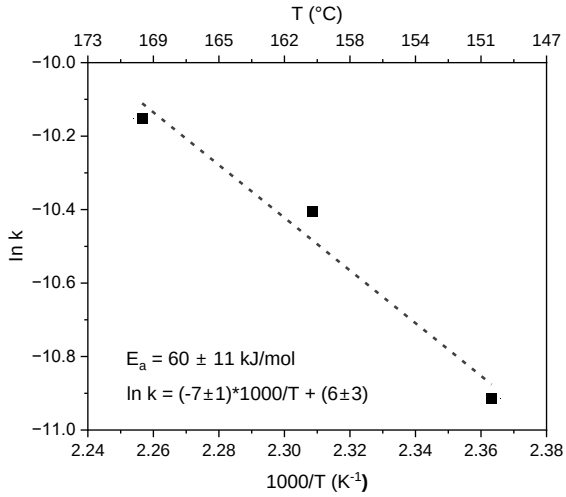
Supplementary Figure 1 Reaction kinetics of methoxycarbonylation.

(a) Reaction orders for styrene (a) and CO (b). Reaction conditions: (a) 20 mg Ru/NbO_x, styrene (0.01~0.1 mol/L), 2 mL MeOH, CO 0.1 MPa, 600 rpm, 170 °C for 2 h. (b) 20 mg Ru/NbO_x, styrene (0.1 mol/L), 2 mL MeOH, CO (10^4 Pa ~10^5 Pa), 600 rpm, 170 °C for 2 h.



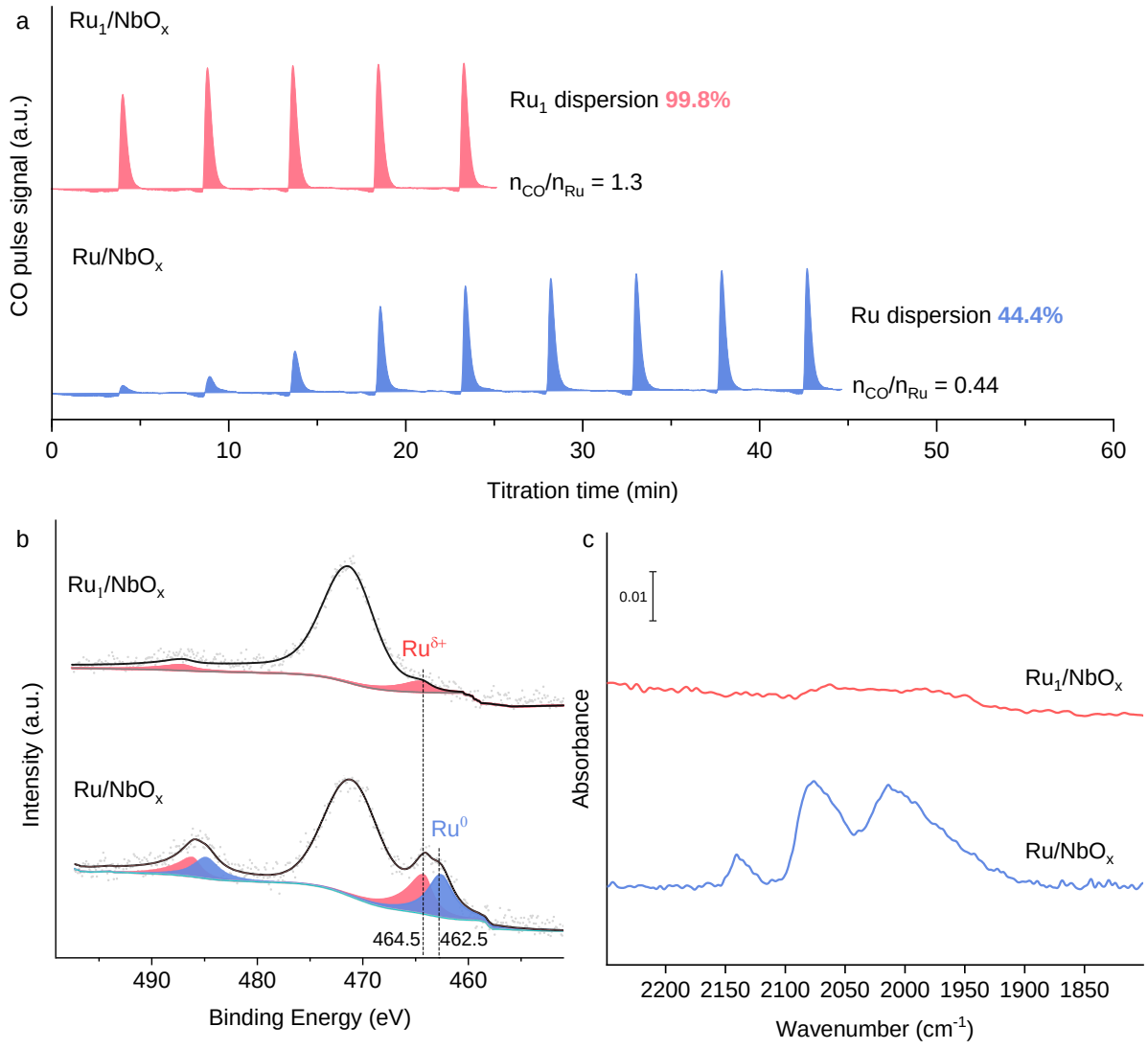
Supplementary Figure 2 The effects of the stirring speed on reaction rate of methoxycarbonylation.

Reaction conditions: 20 mg Ru/NbO_x, 0.2 mmol styrene, 2 mL MeOH, CO 0.1 MPa, 170℃ for 2 h, stirring rate (400, 600, 800 rpm).



Supplementary Figure 3 The determination of apparent activation energy of methoxycarbonylation reactions.

Reaction conditions: 20 mg cat, 0.2 mmol styrene, 2 mL MeOH, CO 0.1 MPa, 600 rpm, 150~180 ℃ for 2 h.

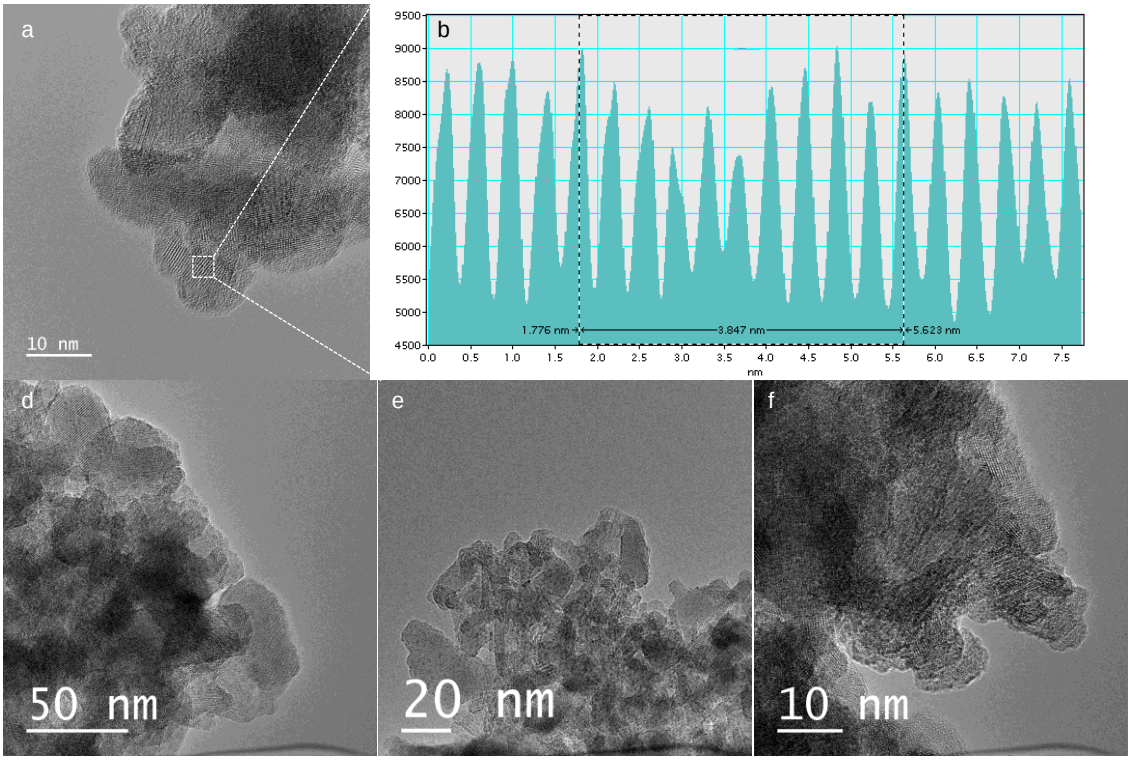


Supplementary Figure 4 Characterizations of Ru_1/NbO_x and 2 wt.% Ru/NbO_x catalyst.

CO pulse chemisorption, Ru3p XPS data and CO-probe FTIR spectra of Ru1/NbO_x and 2 wt.% Ru/NbO_x catalyst.

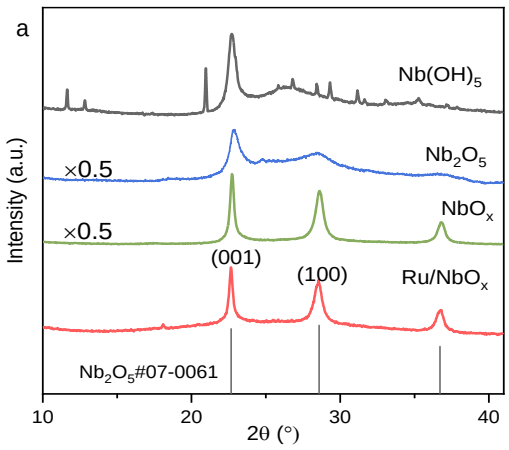
Supplementary Note 3 Characterizations of single-atom Ru_1/NbO_x and nanoparticulate Ru/NbO_x.

The CO adsorption volume on the catalysts was meticulously measured via CO pulse chemisorption (Supplementary Figure 4), while the average factor of n_{Ru}/n_{CO} was derived from CO-probe FTIR spectra (Supplementary Table 13). These measurements were utilized to calculate Ru dispersion, as detailed in the Materials and Methods section of the main text.



Supplementary Figure 5 HRTEM and lattice fringe of main exposed niobium pentoxide (001) facets in 2 wt.%Ru/NbO_x.

The units for the values in Figure (b) is arbitrary unit.

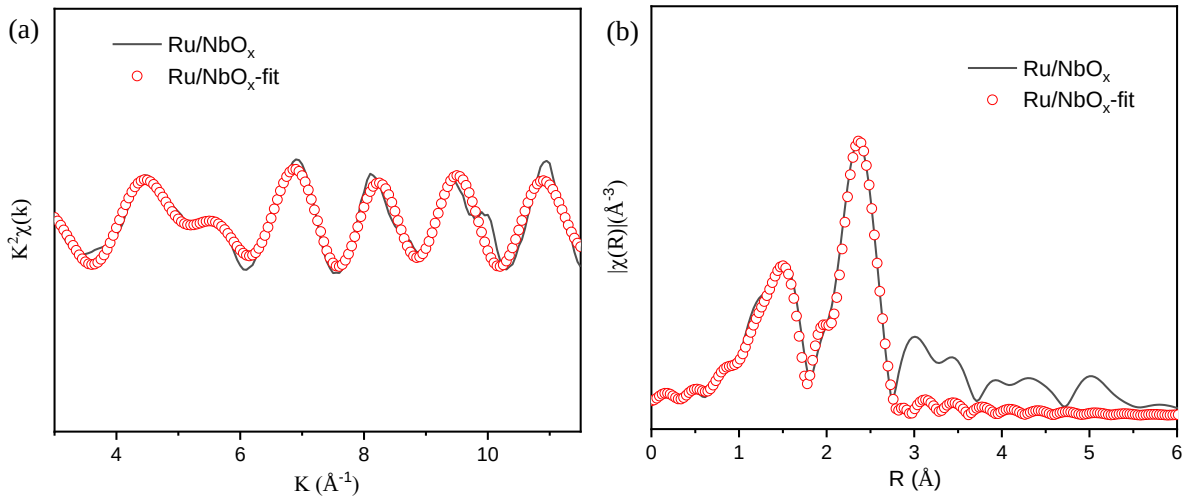


b

samples	O_V site concentration (spins/g)
$Nb(OH)_5$	$5.679*10^{14}$
Nb_2O_5	$6.420*10^{14}$
Ru/Nb_2O_5	$8.090*10^{14}$
NbO_x	$1.208*10^{15}$
Ru/NbO_x	$1.739*10^{15}$

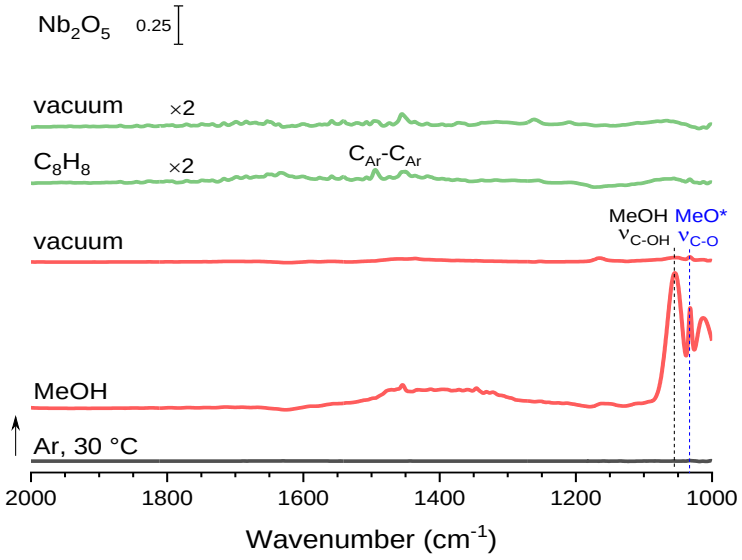
Supplementary Figure 6 Physcial characterizations of Nb-based materials.

(a) XRD patterns and (b) quantitative EPR data on oxygen vacancy concentrations.



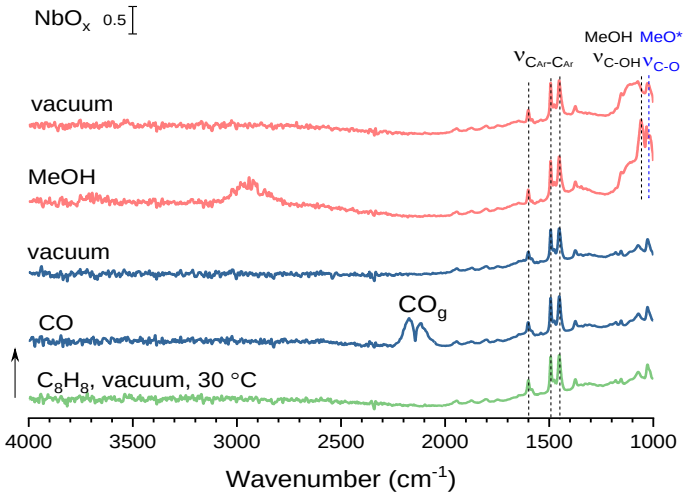
Supplementary Figure 7 EXAFS fitting of Ru/NbO$_x$ catalyst.

(a) Ru K-edge EXAFS fitting curve, shown in k^2 weighted *k*-space. (b) EXAFS fitting curve in the region of 1.0-3.3 Å, shown in k^2 weighted *R*-space.



Supplementary Figure 8 In situ FTIR on Nb$_2$O$_5$ material at room temperature.

The preparation method of Nb$_2$O$_5$ with fewer oxygen defects was detailed in Methods and infrared experiments are given in Methods as well.

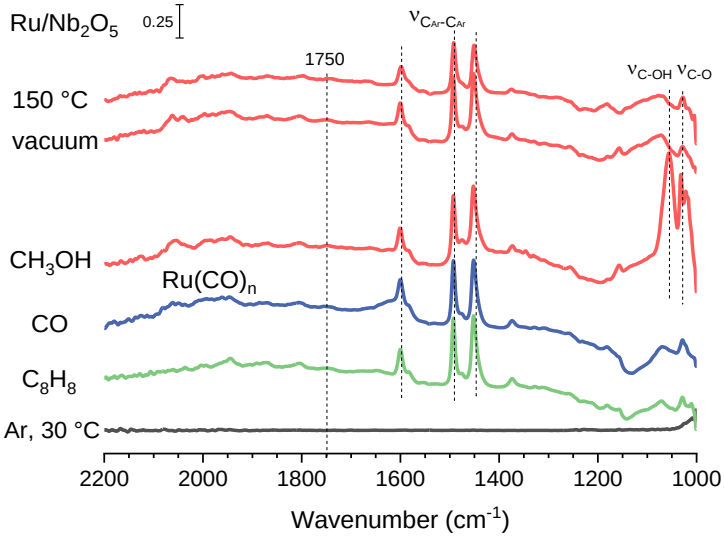


Supplementary Figure 9 In situ FTIR on NbO_x material at room temperature.

The preparation method of NbO_x with abundant oxygen defects was detailed in Methods and infrared experiments are given in Methods as well.

Supplementary Note 4 In situ FTIR analysis of Supplementary Figure 9.

As shown in Supplementary Figure 9, styrene can be adsorbed on NbO_x support, because the characteristic vibrations of aromatic ring were presented in 1600, 1490 and 1450 cm^{-1} after the adsorption of styrene in an infrared cell. Then pure CO gas (40 mL/min) passed through the cell for a while until the signal kept unchanged, and vacuumed until the gaseous CO peak was removed thoroughly. Following that, methanol was bubbled by Ar (40 mL/min) into the cell. Then MeOH adsorbed and CH_3O* generated from methanol dissociation in support can be observed, as suggested from the stretching vibrations of C-OH and C-O bonds. Through vacuum, the adsorbed methanol molecules were taken away and leaving CH_3O* species on the surface of catalysts.

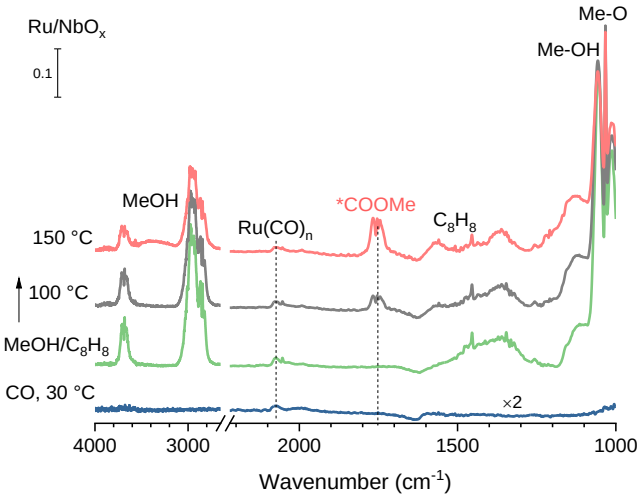


Supplementary Figure 10 In situ FTIR surface reaction on 0.5 wt.%Ru/Nb_2O_5 through sequent adsorption.

Supplementary Note 5 In situ FTIR analysis of Supplementary Figure 10.

In a typical FTIR, a self-supported catalyst wafer with 13 mm diameter was treated in 10% H_2/Ar at 350 °C for 30 min with a heating rate of 10 °C/min. Once cooling, the atmosphere was switched to Ar (40 mL/min). The background spectrum was recorded at 30 °C when the signal kept unchanged. The spectrum was shown here (the bottom).Subsequently, styrene was bubbled by Ar (40 mL/min) until unchanged. Pure Ar (40 mL/min) was introduced untill unchanged. The steady state spectra was shown here (green spectrum).Then the pure CO gas was introduced into the reaction cell until the spectra were unchanged and then pure Ar (40

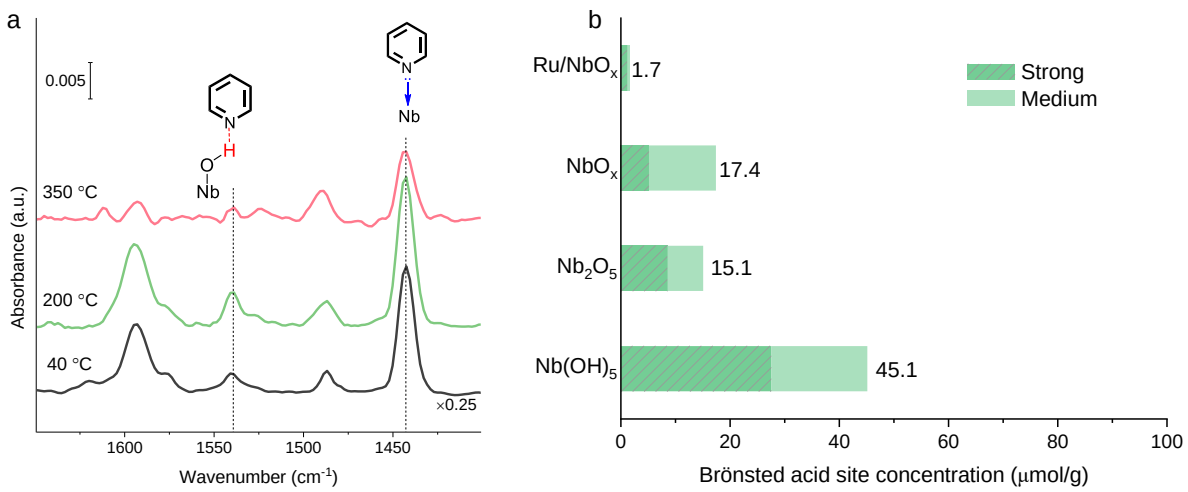
mL/min) was introduced untill unchanged. The steady state spectra were shown here.
The cell was vacuumized and methanol vapour was introduced by saturation adsorption tube until unchanged. The steady state spectra were shown here. Then it was vacuumized for 5 minutes and record the spectra. Finally, the temperature was programmed to the desired temperature and collected the spectra.



Supplementary Figure 11 In situ FTIR surface reaction on 0.5 wt.%Ru/NbO$_x$ through sequent adsorption.

Supplementary Note 6 In situ FTIR analysis of Supplementary Figure 11.

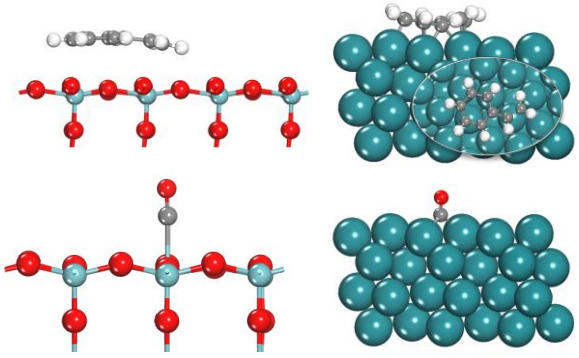
In a typical FTIR, a self-supported catalyst wafer with 13 mm diameter was treated in 10% H_2/Ar at 350 °C for 30 min with a heating rate of 10 °C/min. Once cooling, the atmosphere was switched to Ar (40 mL/min). The background spectrum was recorded at 30 °C when the signal kept unchanged. The pure CO gas (40 mL/min) was introduced into the reaction cell until the spectrum were unchanged. Pure Ar (40 mL/min) was introduced untill unchanged. The steady state spectrum was shown here (the bottom spectra). The methanol/styrene (1/10 V/V) mixture was bubbled by Ar (40 mL/min) until unchanged. Pure Ar (40 mL/min) was introduced the spectrum untill unchanged. The steady state spectrum were shown here. The temperature was programmed to the desired temperature and collected the spectra.



Supplementary Figure 12 Acidity quantification via pyridine-probe FTIR spectra.

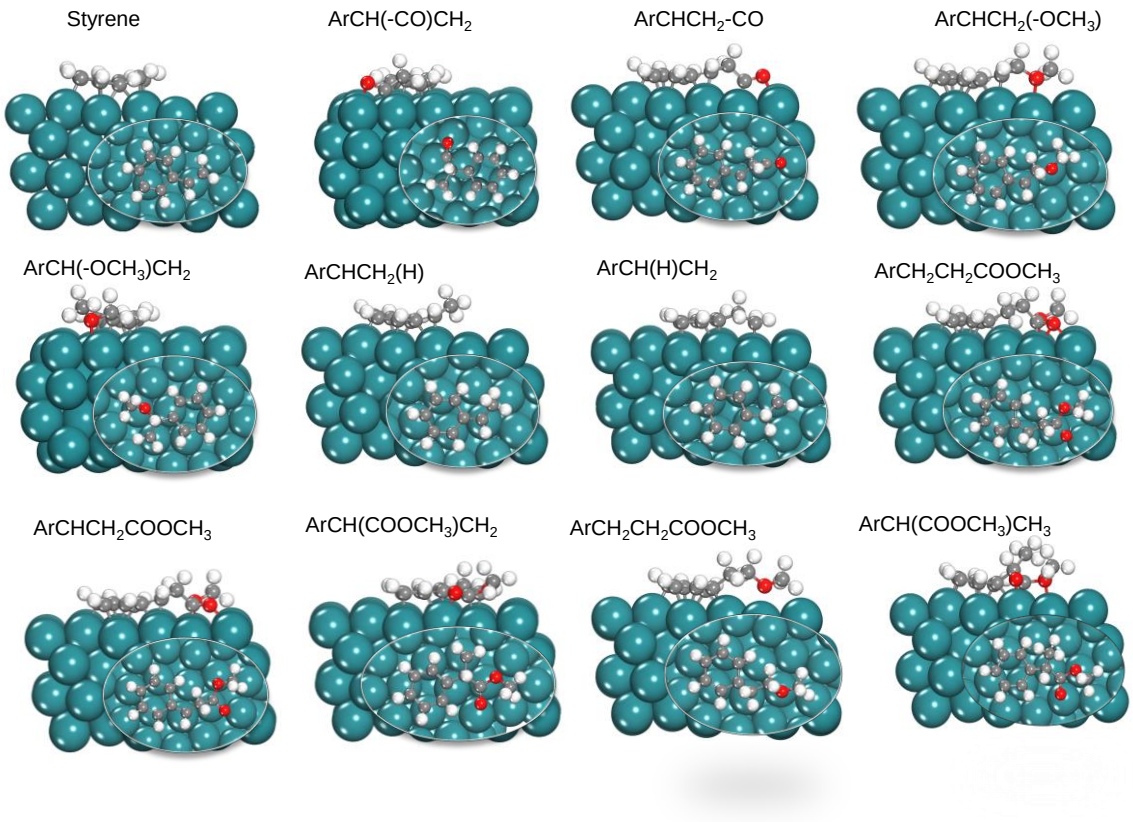
(a) Pyridine-probe FTIR spectra of Ru/NbO_x catalyst at 40 °C, 200 °C and 350 °C, respectively. (b) The concentrations of Brönsted acid sites of Ru/NbO_x equivalents at 200 °C.

Substrate / Adsorbate	NbO_x	Ru
methanol	-0.96	-0.61
styrene	-0.98	-3.46
CO*	-0.23	-1.65



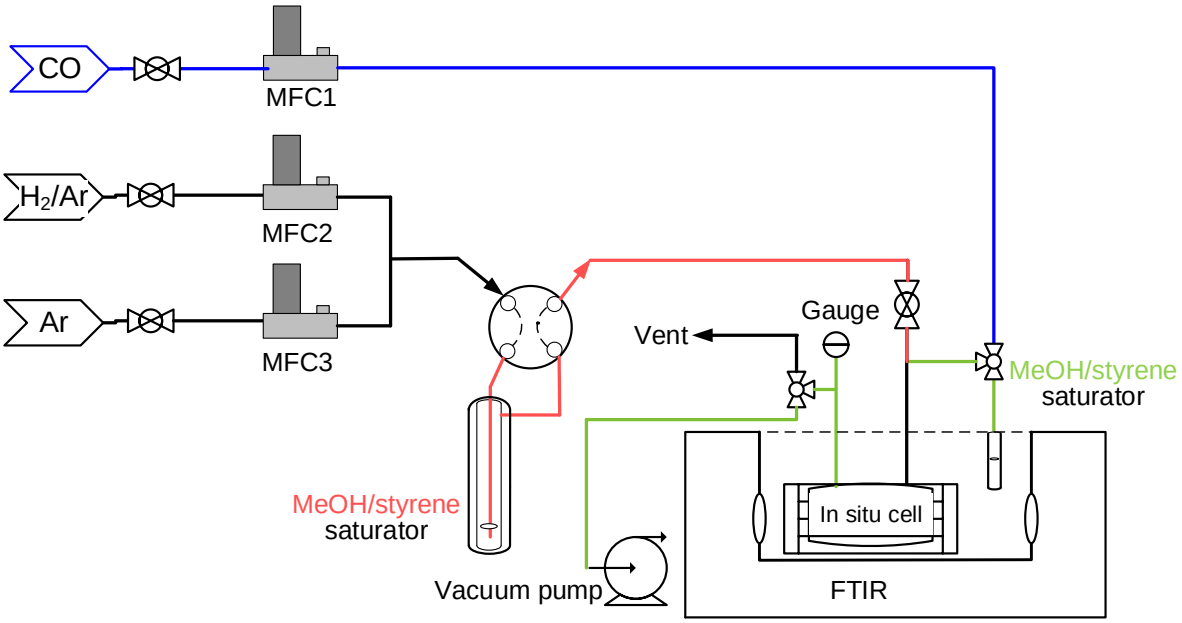
Supplementary Figure 13 Adsorption energy (eV) of styrene and CO on Ru surface.

The corresponding adsorption models are also attached.



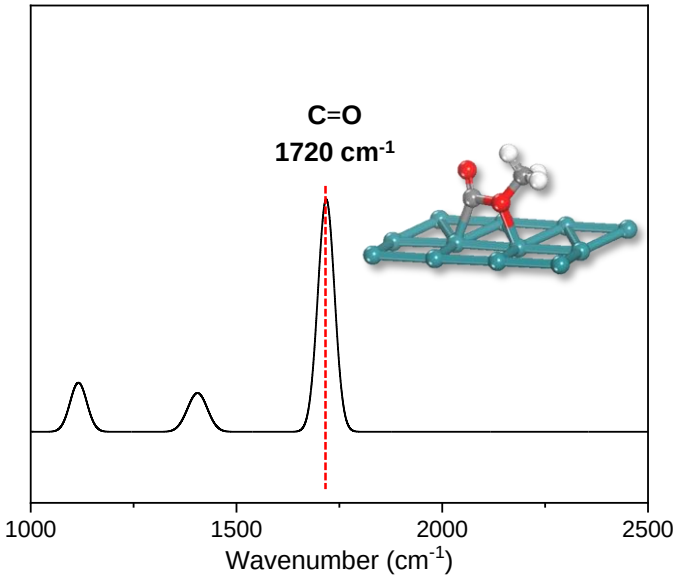
Supplementary Figure 14 Structures of the key intermediates in Figure 5.

Nb, O, C and H atoms are shown in green, red, grey and white, respectively. More details see Methods and Supplementary note 7.



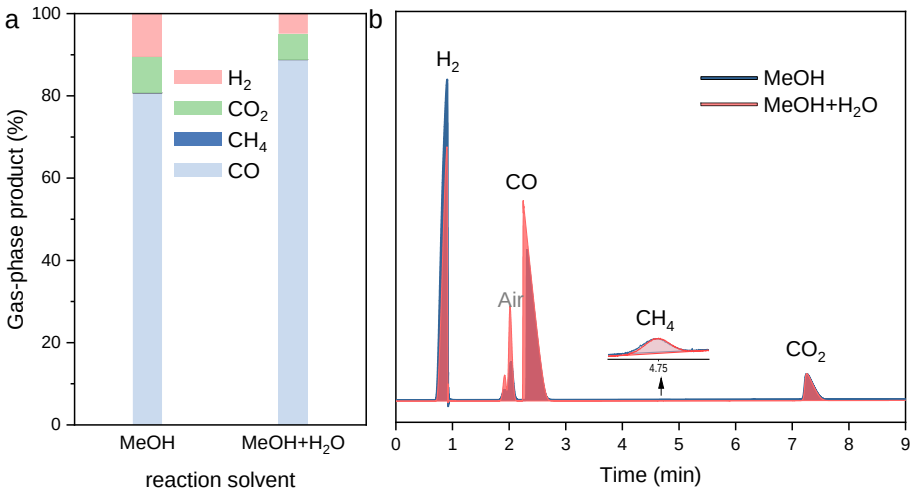
Supplementary Figure 15 The illustration scheme of in situ infrared spectroscopic system applied in this work.

The in situ infrared experiments are detailed in Methods.



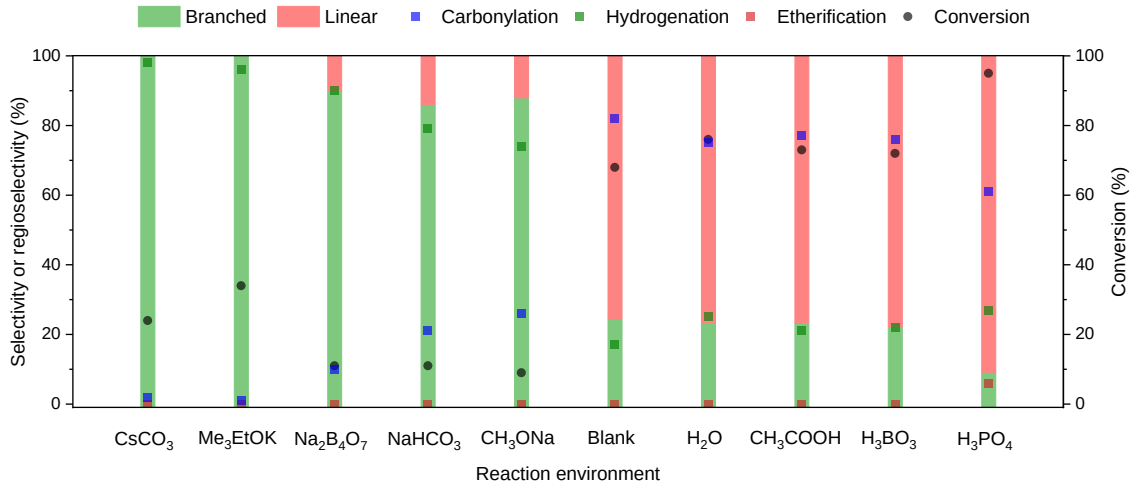
Supplementary Figure 16 The simulated infrared vibration frequency of *COOMe using Vienna Ab initio Simulation Package (VASP).

The stretching vibration frequency of C=O of *COOMe with strong oscillator strength is located at 1720 cm^{-1}.



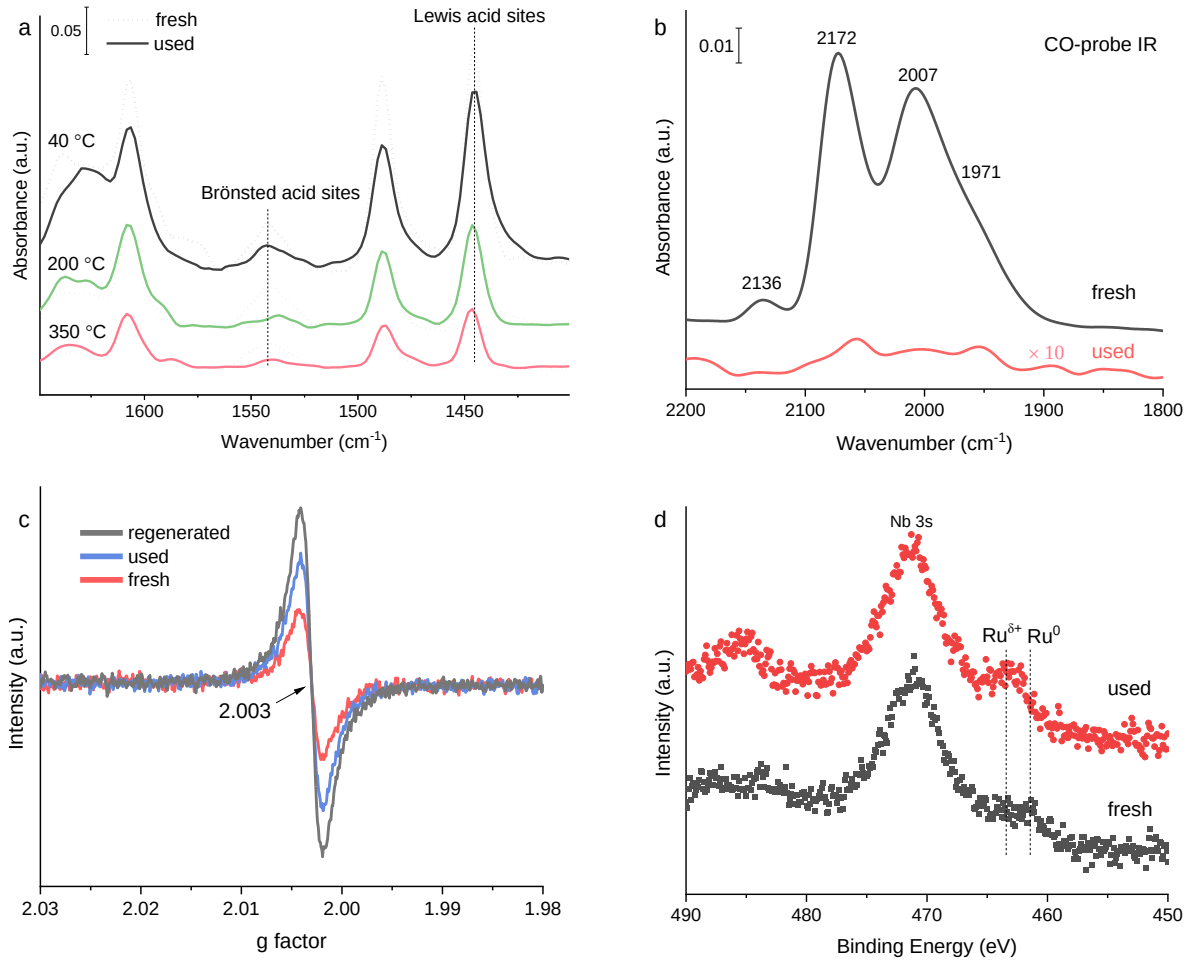
Supplementary Figure 17 Identification and test of gas in carbonylation reaction.

(a) Gas-phase composition. (b) Gas chromatogram. Reaction conditions: 30 mg 2 wt.% Ru/NbO_x, 0.2 mmol styrene, 2 mL MeOH (20 ul H2O), CO (1 bar), 160 ℃, 10 h.

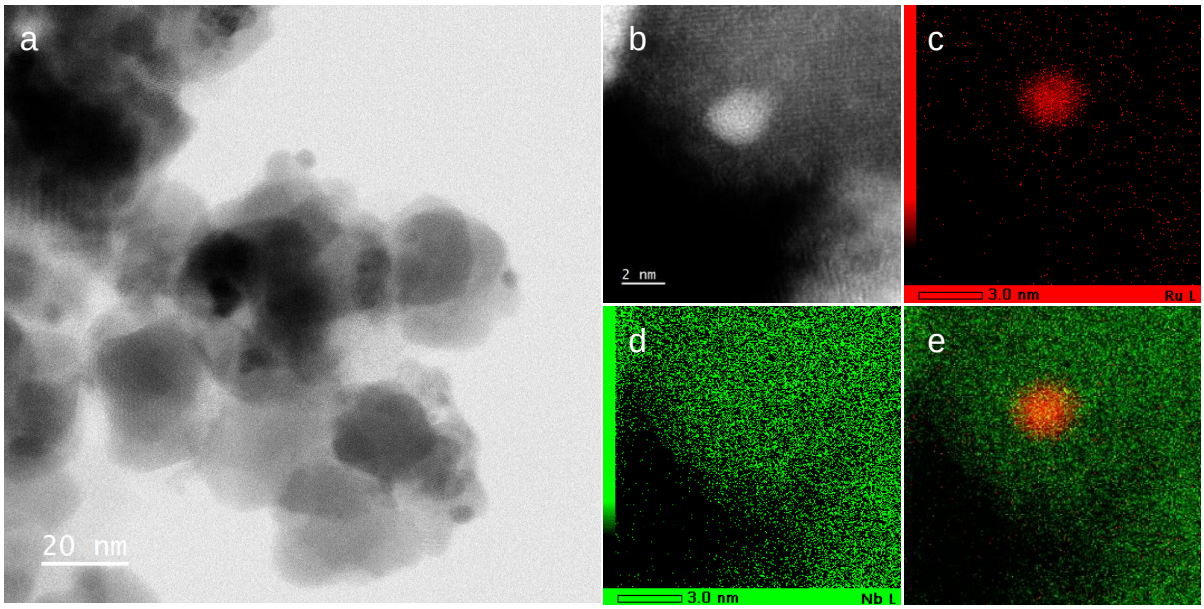


Supplementary Figure 18 Regioselectivity regulation of methoxycarbonylation reactions on Ru/NbO$_x$.

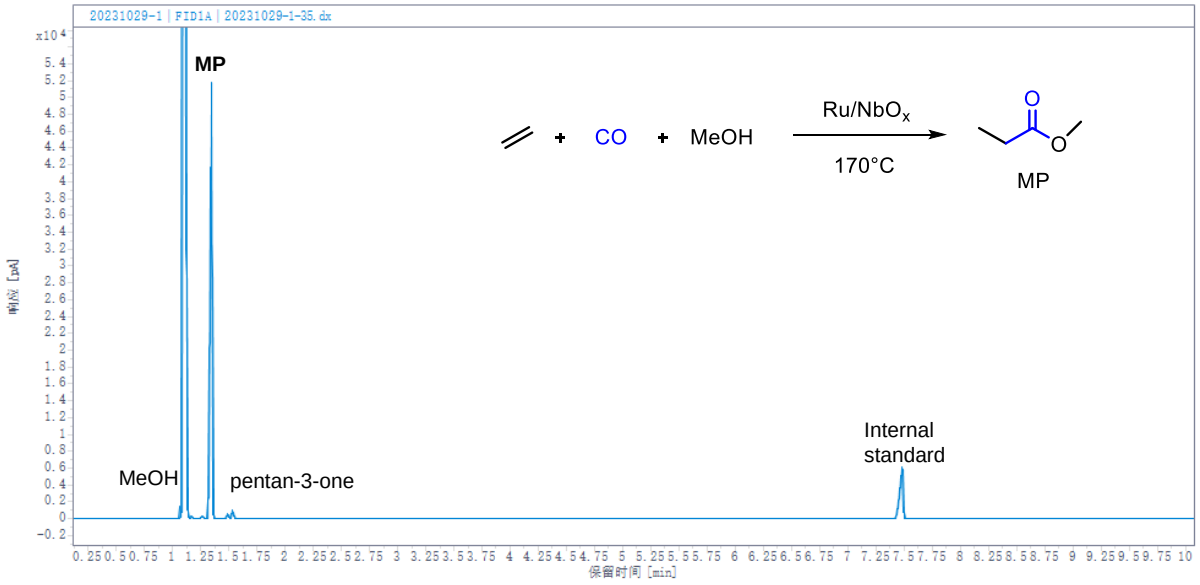
Reaction conditions: 2 wt.% Ru/NbO$_x$ (30 mg), styrene (2 mmol), 4 mmol MeOH (2 mL), additives (4 mmol), CO (1 bar), 170 °C, 10 h.



Supplementary Figure 19 Characterizations of Ru/NbO$_x$ catalysts before and after carbonylation reaction. (a) Pyridine-probe FTIR. (b) CO-probe FTIR. (c) EPR. (d) Ru 3*d* XPS.



Supplementary Figure 20 AC-HAADF STEM images and the corresponding Ru and Nb element map of the used 2 wt.% Ru/NbO_x.



Supplementary Figure 21 GC spectra of MP production from ethylene methoxycarbonylation in a scale-up run.

Reaction conditions: 150 mg Ru/NbO_x, 4 umol C_2H_4 (6 bar), 8.5 umol CO (14 bar), 20 ul dodecane, 2 mL MeOH, 170℃, 10 h.

Supplementary Note 7 The structural data of Nb_2O_5, NbO_x and Ru/NbO_x support, the dissociative adsorption process of methanol, and the hydromethoxycarbonylation process of styrene were attached. The details include the optimized xyz coordinates, the corresponding total energy, thermodynamic zero point energy (*ZPE*) correction, and the entropy contribution ($T\Delta S$).

Nb_2O_5: CH_3OH adsorption
(*E* = -1140.9262 eV)
AutoCreatByScript: O Nb
1.00000000000000
7.9332688600000001 0.0000006300000000 0.0000000000000000
0.0000000000000000 11.4522889699999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.7181709299999994
O Nb
90 36
Selective dynamics
Direct
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0.9534627765720097 0.0949785566820012 0.0000000000000000
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0.9534627765720097 0.7616452233489994 0.0000000000000000
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0.9484906587390037 0.5949783090590083 0.0728553503239983
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0.9435183522889974 0.7616444741430041 0.1457107178800001

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0.9392793396900032	0.2616444789110020	0.1979144111660034
0.4392793396900064	0.5949778122439966	0.1979144111660034
0.9392793396900032	0.5949778122439966	0.1979144111660034
0.4392793396900064	0.9283111455780046	0.1979144111660034
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0.6931363662749562	0.4287124761239600	0.3303821382639223
0.1931280850034064	0.4289018522699089	0.3303894198117502
0.1931258870212754	0.7621454062644015	0.3303793669014862
0.6931329809726962	0.7621702948367827	0.3303702844526099
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0.4352619040095059	0.9286843835455802	0.3451987960368796
0.9351494531570844	0.9286684266480182	0.3451915860542960
0.4320110407142365	0.0953357917086065	0.3968797735297834
0.9318765477955336	0.0953208941341097	0.3968721600619210
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0.1734216550874398	0.2617711666759022	0.4115368922019293
0.6734110886716794	0.2618284946979861	0.4114937089505133
0.1734120740477011	0.5951130227874503	0.4115114220948593
0.6734058185867633	0.5951421696804881	0.4115485140269376
0.6734027379797095	0.9284286430941552	0.4115317247951497
0.1734187425136890	0.9285219663849881	0.4115282581651662
0.4256362781767872	0.2621208587633009	0.4715336185915799
0.9254798951832817	0.2620673587251856	0.4715310797903773

0.4254844588619043	0.5954222782076862	0.4715356570948228
0.9256327314511008	0.5954796004674099	0.4715383393947027
0.9255252105953309	0.9287714296794908	0.4715419059129604
0.4255880249235065	0.9287793897277911	0.4715361908139508
0.9053295108040091	0.4287544791524617	0.5436354423839752
0.4053150954948626	0.0954267771506894	0.5436467381170766
0.9053518012716576	0.0954201444380374	0.5436574821820398
0.4053503939583061	0.4287518460836294	0.5436514955965771
0.4053441654788096	0.7620886601590460	0.5436396697873105
0.9053420873497257	0.7620930752315738	0.5436630708254500
0.6603859641051265	0.2620738306256559	0.5398235223838069
0.1603827204000494	0.2620906829102407	0.5397974685086144
0.6603900340759071	0.5954218117390122	0.5398071501078068
0.1603913502470372	0.5954152926091943	0.5398262849869044
0.1603888191402443	0.9287455730356814	0.5398082999929622
0.6603795679269031	0.9287582744050202	0.5398288023119390
0.4212494542350058	0.2616454108449986	0.0151065289700014
0.9212494542350093	0.2616454108449986	0.0151065289700014
0.4212494542350058	0.5949787441780003	0.0151065289700014
0.9212494542350093	0.5949787441780003	0.0151065289700014
0.4212494542350058	0.9283120775110072	0.0151065289700014
0.9212494542350093	0.9283120775110089	0.0151065289700014
0.4757319089200000	0.2616445689349973	0.1306041949610020
0.9757319089200033	0.2616445689349974	0.1306041949610020
0.4757319089200000	0.5949779022690094	0.1306041949610020
0.9757319089200033	0.5949779022690009	0.1306041949610020
0.4757319089200000	0.9283112356020069	0.1306041949610020
0.9757319089200033	0.9283112356020092	0.1306041949610020
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0.9070655843150029	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150029	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150098	0.2130205561419984
0.9070655843150029	0.7616445948150102	0.2130205561419984
0.9653223725684019	0.0953108215970485	0.3289725032015784
0.4653017838618465	0.0953381073037183	0.3289719692821170
0.4652996178734511	0.4286525643562009	0.3289721640923026
0.9653177900059943	0.4286713698467616	0.3289733406095800
0.4653027102944991	0.7620011378160395	0.3289723829004780
0.9653042045391568	0.7619921808051743	0.3289724723356092
0.4015044008330633	0.2620355010886776	0.4130542076792449
0.9015216967312509	0.2620323300451974	0.4130462778076836
0.4014924917231171	0.5953657707169493	0.4130500680660887
0.9015205926786316	0.5953739788703358	0.4130589915360232

0.4015069503070589	0.9287112724966186	0.4130529212448273
0.9015133721560311	0.9286973606846664	0.4130590901896004
0.4312374794780725	0.2621845288550268	0.5297478852221488
0.9312145188887533	0.2621777833322589	0.5297433031987099
0.4312273824122727	0.5955123902469770	0.5297471145425419
0.9312395985052325	0.5955277535810783	0.5297512638973978
0.4312335149133767	0.9288538264692252	0.5297481415459849
0.9312206316086598	0.9288505033809509	0.5297544037119349

NbO_x

(*E* = -1131.9928 eV)

AutoCreatByScript: O Nb

1.00000000000000

7.9332688600000001 0.0000006300000000 0.0000000000000000

0.0000000000000000 11.4522889699999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.7181709299999994

O Nb

89 36

Selective dynamics

Direct

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0.9534627765720126 0.0949785566820012 0.0000000000000000

0.4534627765720146 0.4283118900150100 0.0000000000000000

0.9534627765720126 0.4283118900150030 0.0000000000000000

0.4534627765720146 0.7616452233490305 0.0000000000000000

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0.6955712230439985 0.2616453474380017 0.0135137049989993

0.1955712230439985 0.5949786807720315 0.0135137049989993

0.6955712230439985 0.5949786807720017 0.0135137049989993

0.1955712230439985 0.9283120141050357 0.0135137049989993

0.6955712230439985 0.9283120141050035 0.0135137049989993

0.4484906587389972 0.2616449757260111 0.0728553503239982

0.9484906587390199 0.2616449757260000 0.0728553503239982

0.4484906587389972 0.5949783090590017 0.0728553503239982

0.9484906587390199 0.5949783090590316 0.0728553503239982

0.4484906587389972 0.9283116423920035 0.0728553503239982

0.9484906587390199 0.9283116423920035 0.0728553503239982

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0.7014097329350051 0.2616445452180088 0.1321970365760023

0.2014097329349997 0.5949778785510290 0.1321970365760023

0.7014097329350051 0.5949778785509992 0.1321970365760023

0.2014097329349997 0.9283112118840395 0.1321970365760023

0.7014097329350051 0.9283112118840009 0.1321970365760023

0.4435183522890077 0.0949778074770009 0.1457107178800001

0.9435183522889974 0.0949778074770021 0.1457107178800001

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0.9435183522889974 0.4283111408100143 0.1457107178800001

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0.9435183522889974 0.7616444741430216 0.1457107178800001

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0.9392793396900032 0.2616444789110020 0.1979144111660034

0.4392793396900138 0.5949778122439966 0.1979144111660034

0.9392793396900032	0.5949778122439966	0.1979144111660034
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0.9392793396900032	0.9283111455780004	0.1979144111660034
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0.6813874112409977	0.0949778936079979	0.2114279908170005
0.1813874112409989	0.4283112269410178	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
0.1813874112409989	0.7616445602750019	0.2114279908170005
0.6813874112409977	0.7616445602750019	0.2114279908170005
0.4343069956900116	0.0949774386079991	0.2707694632339977
0.9343069956900010	0.0949774386079989	0.2707694632339977
0.4343069956900116	0.4283107719410190	0.2707694632339977
0.9343069956900010	0.4283107719409998	0.2707694632339977
0.4343069956900116	0.7616441052750166	0.2707694632339977
0.9343069956900010	0.7616441052750106	0.2707694632339977
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0.6894421780900338	0.0957992537234093	0.3303318393395864
0.6898051389759928	0.4287264140704642	0.3302676763825102
0.1900384239136696	0.4250565989805027	0.3299886232331342
0.1899720056047489	0.7665242133364906	0.3300662451397820
0.6897400767381620	0.7628557763841951	0.3303148242497137
0.9312418849605459	0.2612387839255291	0.3469123822348867
0.4335768039700260	0.2613752195327312	0.3469777156698370
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0.9375547429349573	0.5956281363570769	0.3449195188442701
0.4334788141277865	0.9298610360794058	0.3469525892019441
0.9312527902808784	0.9300157416551481	0.3469013012855460
0.4286955113798663	0.0955817459953139	0.3983525315848318
0.9264952672047663	0.0956135649846032	0.3983029610964342
0.4249873956799820	0.4279778654442572	0.3968555806246147
0.9277335017991238	0.4279678813179956	0.3967342421538036
0.9278018613523110	0.7631986681313967	0.3967934331699053
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0.1710573905191125	0.2605838151810764	0.4161843119070851
0.6710954018322172	0.2619650913800050	0.4167698123736688
0.1687284213020165	0.5954777713482334	0.4155880196341638
0.6678469544908702	0.5955132345587373	0.4097656226649477
0.6710562680644198	0.9287771739149585	0.4166320940444032
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0.4218740773930665	0.2700700178017124	0.4744423530491425
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0.4366989019606384	0.5953496572031917	0.4713013734957621
0.8985800471159362	0.5952821059458480	0.4713683018460023
0.9252008012816223	0.9209051086022026	0.4742794491802828

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0.8846522092169541	0.4434881186041135	0.5469940300425259
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0.9349853124637389	0.0958049354465301	0.5405764178929383
0.4531000093307607	0.4444113349414109	0.5474778331252633
0.4528820968336695	0.7469948351771076	0.5473484161566184
0.8852785841223466	0.7479164001654476	0.5468796273029100
0.6690585483179422	0.2589048385168563	0.5406695161155872
0.1684759085747442	0.2845601193657021	0.5417494819127808
0.1681558226233475	0.5951913750113967	0.5319478134192680
0.1685627168723375	0.9071332048885054	0.5416577944838608
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0.9212494542350100	0.2616454108449986	0.0151065289700014
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0.9212494542350100	0.5949787441780003	0.0151065289700014
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0.9757319089200038	0.2616445689349974	0.1306041949610020
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0.4757319089200072	0.9283112356020100	0.1306041949610020
0.9757319089200038	0.9283112356020100	0.1306041949610020
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0.9070655843150148	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150148	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150270	0.2130205561419984
0.9070655843150148	0.7616445948150344	0.2130205561419984
0.9597839956166531	0.0956041539306551	0.3290718641724757
0.4600014180981259	0.0955721836022683	0.3290706806614705
0.4605335384564537	0.4283998527061810	0.3289464210643628
0.9610028512639304	0.4279323337410601	0.3288912379892048
0.4604522793206943	0.7627018150146050	0.3289512950378570
0.9609694380012411	0.7632378957565441	0.3288899594338667
0.4010674391902848	0.2623856145117418	0.4137061824993613
0.9010786989763758	0.2626088737758430	0.4136691268615971
0.4014057953767195	0.5955600995456845	0.4119733698673949
0.8995212004525246	0.5956026125477817	0.4114044868449255
0.4010247033504691	0.9288089519411082	0.4136851744308769
0.9010400763957985	0.9286598297297435	0.4136423919094541
0.4276805098448102	0.2643331295356329	0.5310324371441653
0.9263134491576186	0.2651156700556734	0.5308898649407960

0.4036562053951772	0.5956327263424581	0.5278451831871329
0.9327114606314686	0.5956020517383172	0.5277171624294643
0.4278198259772953	0.9274516355106657	0.5310321988792994
0.9264149404943691	0.9266362120445693	0.5308778892784752

Nb_2O_5: CH_3OH adsorption
(*E* = -1172.0421 eV, ZPE = 1.427442046 eV, *S***T* = 0.38777092 eV)
AutoCreatByScript: H C O Nb
1.00000000000000
7.9332688600000001 0.0000006300000000 0.0000000000000000
0.0000000000000000 11.4522889699999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.7181709299999994
H C O Nb
4 1 91 36
Selective dynamics
Direct
0.6683632886861002 0.6541850176669897 0.6126922712979506
0.3547546289342547 0.5315775403293933 0.6092050456562147
0.6437372989706355 0.4990883582963614 0.6156644290541418
0.5704098475698549 0.5914038770250771 0.6570670484314570
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0.1955712230439985 0.5949786807720169 0.0135137049989993
0.6955712230439985 0.5949786807720017 0.0135137049989993
0.1955712230439985 0.9283120141050208 0.0135137049989993
0.6955712230439985 0.9283120141050035 0.0135137049989993
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0.9484906587390119 0.2616449757260000 0.0728553503239982
0.4484906587389972 0.5949783090590017 0.0728553503239982
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0.9435183522889974 0.0949778074770039 0.1457107178800001
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0.9435183522889974 0.4283111408100120 0.1457107178800001

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0.9392793396900032	0.5949778122439966	0.1979144111660034
0.4392793396900079	0.9283111455780004	0.1979144111660034
0.9392793396900032	0.9283111455780004	0.1979144111660034
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0.6813874112409977	0.0949778936079988	0.2114279908170005
0.1813874112409991	0.4283112269410086	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
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0.9343069956900010	0.0949774386079998	0.2707694632339976
0.4343069956900057	0.4283107719410092	0.2707694632339976
0.9343069956900010	0.4283107719409998	0.2707694632339976
0.4343069956900057	0.7616441052750190	0.2707694632339976
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0.1898549264728025	0.7616912737452681	0.3303151254840756
0.6900642709343842	0.7657038404042532	0.3300322264184726
0.9343618279069543	0.2618057331438108	0.3459349968957766
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0.9276785218636713	0.5953716894837372	0.3454057370200821
0.4310956273263812	0.9290145880672327	0.3460263850447153
0.9344449493209489	0.9288456967757293	0.3460091967307391
0.4275937777560369	0.0961300565228757	0.3967746894184958
0.9312253321071069	0.0952177392476657	0.3975844370824233
0.4304617798973011	0.4289727985592993	0.3972980246214299
0.9275541860658861	0.4286934030785230	0.3971613229764273
0.9277561770799280	0.7619687136210436	0.3971549191815975
0.4305778339153211	0.7622065459408165	0.3979597370422716
0.1715315092028192	0.2628954048518085	0.4135375168809575
0.6718011772123867	0.2604732160904543	0.4127610929157456
0.1705457665655830	0.5955451051576799	0.4098055472476345
0.6712471803806840	0.5955661163916550	0.4144777993573808
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0.1718630162086195	0.9268833005130442	0.4139690223535388

0.4268014381203725	0.2615435233573730	0.4722834271127427
0.9233767366681170	0.2639697753029762	0.4724348391071887
0.4087576078361747	0.5912549532763874	0.4727821951874550
0.9358196106453515	0.5951252406100865	0.4719441782392381
0.9227187330778728	0.9266947996253241	0.4726636406275163
0.4293184999080540	0.9426633419983017	0.4719404382645068
0.9056481873159843	0.4300321241265932	0.5455633650764826
0.4047503193137125	0.0980077268566682	0.5470425779275234
0.9102189423879089	0.0954530217672217	0.5442610660028374
0.4083861188519219	0.4261020847848022	0.5449657503820067
0.4095850893526228	0.7663823837922052	0.5396911482479791
0.9061885008144211	0.7612442894539397	0.5455153350413244
0.6636255794934641	0.2610526615574305	0.5409387339803838
0.1612522673418514	0.2636932341005487	0.5402557678155272
0.6633378071654843	0.5958965329063364	0.5362997440134681
0.1614617124657457	0.5947992409683392	0.5428535218408127
0.1628581989915573	0.9283030352868852	0.5400730567207693
0.6624575459055326	0.9317948334369468	0.5413952013476314
0.4264289120985675	0.5989641620106841	0.6035870727470072
0.4212494542350074	0.2616454108449986	0.0151065289700014
0.9212494542350144	0.2616454108449986	0.0151065289700014
0.4212494542350074	0.5949787441780003	0.0151065289700014
0.9212494542350144	0.5949787441780003	0.0151065289700014
0.4212494542350074	0.9283120775110023	0.0151065289700014
0.9212494542350144	0.9283120775110212	0.0151065289700014
0.4757319089200030	0.2616445689349973	0.1306041949610020
0.9757319089200063	0.2616445689349974	0.1306041949610020
0.4757319089200030	0.5949779022690176	0.1306041949610020
0.9757319089200063	0.5949779022690009	0.1306041949610020
0.4757319089200030	0.9283112356020153	0.1306041949610020
0.9757319089200063	0.9283112356020206	0.1306041949610020
0.4070655843149993	0.0949779281480000	0.2130205561419984
0.9070655843150041	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150041	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150223	0.2130205561419984
0.9070655843150041	0.7616445948150239	0.2130205561419984
0.9622593748702578	0.0951805634258557	0.3291662582067964
0.4620457379875957	0.0957649128981415	0.3292256900988436
0.4622416466196588	0.4292194641413382	0.3292189345034044
0.9617722221021139	0.4286946784886038	0.3291634534170082
0.4620155979192443	0.7618290280591540	0.3292788655400225
0.9616636497596621	0.7618419816874420	0.3291853097689449
0.3998631460659697	0.2628564483289935	0.4137786365857635

0.8999119017137147	0.2620672103604114	0.4137513982548521
0.3981185756734907	0.5954195513579796	0.4148577456291584
0.8998671749000459	0.5954405447952436	0.4136815494240702
0.4002165566459555	0.9296871255422474	0.4135337449390051
0.9002551305425769	0.9286749441463480	0.4138791681051558
0.4336807226136358	0.2637762924644826	0.5304715837789026
0.9318936386437282	0.2625224565094419	0.5304979443444415
0.4311781425414496	0.5991181750707976	0.5321259237175366
0.9343620617517251	0.5951937150783401	0.5300860571281568
0.4339822725848162	0.9358118547517500	0.5298746590436116
0.9329418192044455	0.9281936318870887	0.5307060256311408

Nb_2O_5: Transition state for CH_3OH dissociation
(*E* = -1171.7298 eV, ZPE = 1.278640088 eV, *S***T* = 0.417567218 eV)
AutoCreatByScript: H C O Nb
1.00000000000000
7.9332688600000001 0.0000006300000000 0.0000000000000000
0.0000000000000000 11.4522889699999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.7181709299999994
H C O Nb
4 1 91 36
Selective dynamics
Direct
0.2357514577214416 0.6029354398690020 0.5848406268421695
0.5917400719386553 0.6115255726669862 0.6330364393783637
0.4906402770118340 0.4738542857850604 0.6246002701502898
0.3981244914722071 0.5793070997487680 0.6587529065470580
0.4688175469813988 0.5675585475689855 0.6301481697618150
0.4534627765720079 0.0949785566820325 1.0000000000000000
-0.0465372234279875 0.0949785566820012 1.0000000000000000
0.4534627765720079 0.4283118900150047 1.0000000000000000
-0.0465372234279744 0.4283118900150032 1.0000000000000000
0.4534627765720079 0.7616452233492312 1.0000000000000000
-0.0465372234279744 0.7616452233491414 1.0000000000000000
0.1955712230439985 0.2616453474379983 1.0135137049990011
0.6955712230439985 0.2616453474379983 1.0135137049990011
0.1955712230439985 0.5949786807721748 1.0135137049990011
0.6955712230439985 0.5949786807720017 1.0135137049990011
0.1955712230439985 0.9283120141052881 1.0135137049990011
0.6955712230439985 0.9283120141050035 1.0135137049990011
0.4484906587389972 0.2616449757260013 1.0728553503239988
-0.0515093412609511 0.2616449757260002 1.0728553503239988
0.4484906587389972 0.5949783090590017 1.0728553503239988
-0.0515093412609524 0.5949783090591024 1.0728553503239988
0.4484906587389972 0.9283116423920035 1.0728553503239988
-0.0515093412609524 0.9283116423920038 1.0728553503239988
0.2014097329349994 0.2616445452179974 0.1321970365760023
0.7014097329350044 0.2616445452180839 0.1321970365760023
0.2014097329349994 0.5949778785511722 0.1321970365760023
0.7014097329350044 0.5949778785509992 0.1321970365760023
0.2014097329349994 0.9283112118842010 0.1321970365760023
0.7014097329350044 0.9283112118840009 0.1321970365760023
0.4435183522890007 0.0949778074770009 0.1457107178800001
-0.0564816477110023 0.0949778074770174 0.1457107178800001
0.4435183522890007 0.4283111408100028 0.1457107178800001
-0.0564816477110023 0.4283111408100028 0.1457107178800001

0.4435183522890007	0.7616444741432578	0.1457107178800001
-0.0564816477110023	0.7616444741431428	0.1457107178800001
0.4392793396900061	0.2616444789110020	0.1979144111660034
-0.0607206603099968	0.2616444789110020	0.1979144111660034
0.4392793396900061	0.5949778122439966	0.1979144111660034
-0.0607206603099968	0.5949778122441510	0.1979144111660034
0.4392793396900061	0.9283111455780004	0.1979144111660034
-0.0607206603099968	0.9283111455780004	0.1979144111660034
0.1813874112409984	0.0949778936079966	0.2114279908170005
0.6813874112409977	0.0949778936080203	0.2114279908170005
0.1813874112409984	0.4283112269411141	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
0.1813874112409984	0.7616445602750019	0.2114279908170005
0.6813874112409977	0.7616445602750019	0.2114279908170005
0.4343069956900041	0.0949774386079981	0.2707694632339970
-0.0656930043099990	0.0949774386079981	0.2707694632339970
0.4343069956900041	0.4283107719411249	0.2707694632339970
-0.0656930043099990	0.4283107719409998	0.2707694632339970
0.4343069956900041	0.7616441052750063	0.2707694632339970
-0.0656930043099990	0.7616441052751846	0.2707694632339970
0.1897567780879993	0.0966683991521332	0.3296150738215803
0.6898838359537163	0.0963879454491281	0.3304908206703812
0.6900004425116620	0.4281478238518736	0.3301120959235525
0.1891634192483040	0.4336849395131672	0.3305900139464495
0.1891544482747437	0.7605246504683182	0.3306079650199117
0.6896586290703336	0.7664551708883417	0.3302316668410925
0.4384599705660133	0.5966984833321745	0.3458840059108206
-0.0734955222389754	0.5963806479959091	0.3465936439524668
0.4299829564583151	0.2638305327832416	0.3453531694141185
-0.0655615371277047	0.2633816732375147	0.3456260572479631
-0.0646608555399512	0.9291153867939315	0.3457731334904228
0.4293164281316915	0.9292438533485721	0.3457491073198386
0.4249965446610594	0.0972043475608557	0.3959415974008405
-0.0716163172025631	0.7625129706531965	0.3976858561036512
-0.0727250956368505	0.4300492580386397	0.3976570696203217
-0.0674274150846849	0.0961278571122493	0.3969637670129839
0.4329825004798569	0.4303278234580351	0.3976797772175428
0.4320787583036544	0.7622855503932493	0.3985757066753665
0.1741491461748879	0.5956856578206935	0.4118216625096686
0.6715845452117838	0.2605783244356622	0.4119270032875927
0.6723810474656032	0.9298471926589559	0.4117321766872661
0.1711920977185090	0.2656109706532601	0.4130902822584998
0.1714866836474511	0.9261318093885206	0.4140068801682304
0.6763027802927200	0.5963407664301668	0.4176052266564164

0.4330372272918441	0.9516100960616927	0.4707394590481896
0.4277464658967318	0.2584726437676197	0.4716622921800290
-0.0528484414304320	0.5981482166779049	0.4738422214924774
-0.0772823391085438	0.2593811568915336	0.4719107154757495
-0.0790068844968257	0.9349078364452831	0.4723072971510907
0.4139144058730588	0.5903788292123633	0.4744020773067254
0.6740924342054923	0.6015085331939989	0.5430857854409360
0.4052618976395745	0.7690442098594310	0.5324800169627535
0.4115967399125808	0.4309613749042785	0.5419092526196853
0.1631133324636367	0.9331878051477185	0.5397604068981899
0.1614351963203590	0.2679440588883198	0.5397305201250877
0.6626585580756633	0.2636925215882875	0.5405644803282136
0.6605405857601320	0.9340890963648377	0.5413107699621721
-0.0920788865876865	0.7671238358970410	0.5429280302988848
-0.0915373527051535	0.0988998666129179	0.5457943856150453
-0.0966301811303740	0.4310544293117669	0.5422710197021948
0.4028764192587966	0.1014446578812473	0.5464123432508667
0.1481378262327516	0.5972012343847685	0.5547490731821663
0.3798187775572191	0.6208200386410425	0.5973145598822123
0.4212494542350055	0.2616454108449986	1.0151065289700014
-0.0787505457649912	0.2616454108450635	1.0151065289700014
-0.0787505457649912	0.5949787441780003	1.0151065289700014
0.4212494542350055	0.5949787441780003	1.0151065289700014
0.4212494542350055	0.9283120775110023	1.0151065289700014
-0.0787505457649912	0.9283120775112003	1.0151065289700014
0.4757319089200003	0.2616445689349973	0.1306041949610020
-0.0242680910799963	0.2616445689349974	0.1306041949610020
0.4757319089200003	0.5949779022691092	0.1306041949610020
-0.0242680910799963	0.5949779022690010	0.1306041949610020
0.4757319089200003	0.9283112356020030	0.1306041949610020
-0.0242680910799963	0.9283112356020033	0.1306041949610020
0.4070655843149993	0.0949779281480307	0.2130205561419984
-0.0929344156849991	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
-0.0929344156849991	0.4283112614820945	0.2130205561419984
0.4070655843149993	0.7616445948152319	0.2130205561419984
-0.0929344156849991	0.7616445948151462	0.2130205561419984
-0.0379858937525760	0.0959445897751670	0.3290803156944559
-0.0390368692715989	0.4301174330930202	0.3292250884788574
-0.0391740885105694	0.7621454419189981	0.3292444048747328
0.4615578929881132	0.0966314615231657	0.3291923213714812
0.4617580323177460	0.4308614412095156	0.3292780089932731
0.4613783425921480	0.7617332767655398	0.3293501007584864
-0.0950361770474384	0.5965696794141305	0.4147130768070018

0.3998016438880335	0.9305029528098433	0.4129506567773879
0.3994486584030449	0.2638282046456047	0.4133106280892211
-0.1004533008512764	0.2626175790832346	0.4133637633161651
-0.0998973475324027	0.9301435796058458	0.4136200359145682
0.4024567608834510	0.5959586201379451	0.4167265051738515
-0.0697618676060640	0.5979420569664824	0.5314759741280933
0.4338482883063595	0.9375875892908353	0.5284239804992540
0.4337507237997196	0.2634536117609269	0.5297108160217925
-0.0677610150155126	0.2630021891372387	0.5299417969574616
-0.0665970168929433	0.9331378601627751	0.5303257007494466
0.4452626130239641	0.5998572764867299	0.5347736173461051

Nb_2O_5: Final state for CH_3OH dissociation
(*E* = -1172.3475 eV, ZPE = 1.411184356 eV, *S***T* = 0.375869317 eV)
AutoCreatByScript: H C O Nb
1.00000000000000
7.9332688600000001 0.0000006300000000 0.0000000000000000
0.0000000000000000 11.4522889699999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.7181709299999994
H C O Nb
4 1 91 36
Selective dynamics
Direct
0.1498762027505622 0.4931476594002956 0.5571926471509011
0.7095990660996188 0.6467748933438060 0.6129531222673711
0.6564005261221197 0.4947103487054332 0.6180954391441064
0.5726820973889472 0.6005916027812511 0.6533281244220126
0.6086139169114440 0.5846902061465241 0.6213220366466812
0.4534627765720093 0.0949785566820042 0.0000000000000000
0.9534627765720113 0.0949785566820012 0.0000000000000000
0.4534627765720093 0.4283118900150115 0.0000000000000000
0.9534627765720113 0.4283118900150059 0.0000000000000000
0.4534627765720093 0.7616452233490222 0.0000000000000000
0.9534627765720113 0.7616452233489994 0.0000000000000000
0.1955712230439985 0.2616453474380004 0.0135137049989993
0.6955712230439985 0.2616453474380082 0.0135137049989993
0.1955712230439985 0.5949786807720187 0.0135137049989993
0.6955712230439985 0.5949786807720017 0.0135137049989993
0.1955712230439985 0.9283120141050263 0.0135137049989993
0.6955712230439985 0.9283120141050035 0.0135137049989993
0.4484906587389972 0.2616449757260066 0.0728553503239981
0.9484906587390095 0.2616449757260000 0.0728553503239981
0.4484906587389972 0.5949783090590017 0.0728553503239981
0.9484906587390095 0.5949783090590187 0.0728553503239981
0.4484906587389972 0.9283116423920035 0.0728553503239981
0.9484906587390095 0.9283116423920035 0.0728553503239981
0.2014097329349997 0.2616445452179974 0.1321970365760023
0.7014097329350055 0.2616445452180059 0.1321970365760023
0.2014097329349997 0.5949778785510161 0.1321970365760023
0.7014097329350055 0.5949778785509992 0.1321970365760023
0.2014097329349997 0.9283112118840239 0.1321970365760023
0.7014097329350055 0.9283112118840009 0.1321970365760023
0.4435183522890011 0.0949778074770009 0.1457107178800001
0.9435183522889976 0.0949778074770036 0.1457107178800001
0.4435183522890011 0.4283111408100096 0.1457107178800001
0.9435183522889976 0.4283111408100099 0.1457107178800001

0.4435183522890011	0.7616444741430204	0.1457107178800001
0.9435183522889976	0.7616444741430212	0.1457107178800001
0.4392793396900067	0.2616444789110020	0.1979144111660034
0.9392793396900032	0.2616444789110020	0.1979144111660034
0.4392793396900067	0.5949778122439966	0.1979144111660034
0.9392793396900032	0.5949778122439966	0.1979144111660034
0.4392793396900067	0.9283111455780129	0.1979144111660034
0.9392793396900032	0.9283111455780051	0.1979144111660034
0.1813874112409991	0.0949778936079966	0.2114279908170005
0.6813874112409977	0.0949778936079997	0.2114279908170005
0.1813874112409991	0.4283112269410131	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
0.1813874112409991	0.7616445602750019	0.2114279908170005
0.6813874112409977	0.7616445602750019	0.2114279908170005
0.4343069956900045	0.0949774386079989	0.2707694632339972
0.9343069956900010	0.0949774386079989	0.2707694632339972
0.4343069956900045	0.4283107719410115	0.2707694632339972
0.9343069956900010	0.4283107719409998	0.2707694632339972
0.4343069956900045	0.7616441052750205	0.2707694632339972
0.9343069956900010	0.7616441052750189	0.2707694632339972
0.1912715103119501	0.0954271447487794	0.3296739984249494
0.6916796742039949	0.0953080621000533	0.3301461696924261
0.6912939238216923	0.4269006851127968	0.3302351413574559
0.1905530347069233	0.4288732771626473	0.3303569167322007
0.1904249373535915	0.7628997102195463	0.3304046653120576
0.6909131016721638	0.7650790015247912	0.3302896239033012
0.9341249556202755	0.2619322323784683	0.3456252735871644
0.4325128906337067	0.2626756769340949	0.3455823775094977
0.4362629849753926	0.5956786153943101	0.3445363117420641
0.9293648271669774	0.5956859434754037	0.3452159181945160
0.4321029883087437	0.9283984104382451	0.3459380309350358
0.9343909893000261	0.9293432953223620	0.3457487057011362
0.4277910457744480	0.0957271423450463	0.3958273030529970
0.9316041139255455	0.0955964970552833	0.3970604441606844
0.4312697121402703	0.4295440585334169	0.3979799221448573
0.9281149953101875	0.4286704376980658	0.3968207382307693
0.9285096222062664	0.7627162004235538	0.3967559248461605
0.4311057172964867	0.7614086093450916	0.3985173647432369
0.1711136183404821	0.2626791858076529	0.4132924799974296
0.6724258117106101	0.2600760368920386	0.4124020306751391
0.1709469056146306	0.5947886369363322	0.4102893046113407
0.6733486208058161	0.5950522016312927	0.4150065317611736
0.6728442211189454	0.9287103439126417	0.4126382739973684
0.1716300806760996	0.9268738283819151	0.4140154745520005

0.4285326988422842	0.2537277403831892	0.4712024097137553
0.9232277691424021	0.2643395739993712	0.4720396952042776
0.4028138981414485	0.5943063609625711	0.4747676352100310
0.9389885502581585	0.5991695205983115	0.4714425386858876
0.9225218582900104	0.9321708612010021	0.4722108230536437
0.4309907511750724	0.9477472310572049	0.4710856263106420
0.9070381307236195	0.4310336314756548	0.5438236440228957
0.4083520757533811	0.0964610926568919	0.5467162532070783
0.8978164954298916	0.0961195099385656	0.5436546350604445
0.3980157188193421	0.4249218434504238	0.5388235380383367
0.3838575053232249	0.7678490387976202	0.5357887085805466
0.9193756129361219	0.7594355394214108	0.5436497566321786
0.6613553937234378	0.2655344710422577	0.5406989135854408
0.1579085669567752	0.2602731855755756	0.5404002537490693
0.6620803529023382	0.5982527703290381	0.5304821202476494
0.1513864230482370	0.5773003781089745	0.5512879307257275
0.1591366503440395	0.9357200767300914	0.5397976708988925
0.6596643084378446	0.9211135487742893	0.5407955647159216
0.4686436127425475	0.6022518518071786	0.5959549547214233
0.4212494542350064	0.2616454108449986	0.0151065289700014
0.9212494542350096	0.2616454108449986	0.0151065289700014
0.4212494542350064	0.5949787441780003	0.0151065289700014
0.9212494542350096	0.5949787441780003	0.0151065289700014
0.4212494542350064	0.9283120775110097	0.0151065289700014
0.9212494542350096	0.9283120775110224	0.0151065289700014
0.4757319089200007	0.2616445689349973	0.1306041949610020
0.9757319089200046	0.2616445689349974	0.1306041949610020
0.4757319089200007	0.5949779022690180	0.1306041949610020
0.9757319089200046	0.5949779022690009	0.1306041949610020
0.4757319089200007	0.9283112356020061	0.1306041949610020
0.9757319089200046	0.9283112356020203	0.1306041949610020
0.4070655843149993	0.0949779281480007	0.2130205561419984
0.9070655843150023	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150023	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150249	0.2130205561419984
0.9070655843150023	0.7616445948150198	0.2130205561419984
0.9635209255221079	0.0956259813098936	0.3289004484002077
0.4635437660751225	0.0956423954144601	0.3291911986480502
0.4631224043898766	0.4308556630680253	0.3293094849879287
0.9627122796207189	0.4286889389820003	0.3289295769722274
0.4626965962741896	0.7601407383541637	0.3293544806840422
0.9625068327713814	0.7625463542560368	0.3289353514890965
0.3995378781839602	0.2629454207619015	0.4127080543839047

0.9000372068927456	0.2623728079036383	0.4130356729407468
0.3989139456214123	0.5953646681995639	0.4183240230845175
0.9022746888358348	0.5960315770127987	0.4124179395398365
0.3999909146061236	0.9289212342448132	0.4126177340981960
0.9004682075679845	0.9295697440568761	0.4130643296355976
0.4326124112200189	0.2626939963889478	0.5289391053178989
0.9288389152864429	0.2640984006716858	0.5297574158783770
0.4151566757290731	0.6026451167892403	0.5389384619564166
0.8989954745560773	0.5996041961476124	0.5279045364836283
0.4321453712214446	0.9371428804058317	0.5285717804631246
0.9310403449965978	0.9332246884936812	0.5298330141347413

NbO_x: CH_3OH adsorption on O_{vac}

(*E* = -1163.5018 eV, *ZPE* = 1.445002558 eV, *S***T* = 0.389615451 eV)

AutoCreatByScript: H C O Nb

1.00000000000000

7.9332688600000001 0.0000006300000000 0.0000000000000000

0.0000000000000000 11.4522889699999997 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.7181709299999994

H C O Nb

4 1 90 36

Selective dynamics

Direct

0.6704747490214820 0.5096411778830169 0.5712547674208370

0.6654198685167917 0.7556343779740589 0.5929274953259149

0.7793494894395001 0.6444916154067206 0.6205778090667811

0.5515193917888288 0.6439489820585211 0.6203763705931693

0.6656155723225136 0.6646688272791907 0.6028911705546524

0.4534627765720096 0.0949785566820060 0.0000000000000000

0.9534627765720401 0.0949785566820012 0.0000000000000000

0.4534627765720096 0.4283118900150237 0.0000000000000000

0.9534627765720401 0.4283118900150030 0.0000000000000000

0.4534627765720096 0.7616452233490510 0.0000000000000000

0.9534627765720401 0.7616452233489994 0.0000000000000000

0.1955712230439985 0.2616453474379983 0.0135137049989993

0.6955712230439985 0.2616453474379983 0.0135137049989993

0.1955712230439985 0.5949786807720306 0.0135137049989993

0.6955712230439985 0.5949786807720017 0.0135137049989993

0.1955712230439985 0.9283120141050479 0.0135137049989993

0.6955712230439985 0.9283120141050035 0.0135137049989993

0.4484906587389972 0.2616449757260132 0.0728553503239981

0.9484906587390211 0.2616449757260000 0.0728553503239981

0.4484906587389972 0.5949783090590017 0.0728553503239981

0.9484906587390211 0.5949783090590307 0.0728553503239981

0.4484906587389972 0.9283116423920035 0.0728553503239981

0.9484906587390211 0.9283116423920035 0.0728553503239981

0.2014097329350001 0.2616445452179974 0.1321970365760023

0.7014097329350060 0.2616445452180119 0.1321970365760023

0.2014097329350001 0.5949778785510281 0.1321970365760023

0.7014097329350060 0.5949778785509992 0.1321970365760023

0.2014097329350001 0.9283112118840465 0.1321970365760023

0.7014097329350060 0.9283112118840009 0.1321970365760023

0.4435183522890012 0.0949778074770009 0.1457107178800001

0.9435183522889974 0.0949778074770081 0.1457107178800001

0.4435183522890012 0.4283111408100180 0.1457107178800001

0.9435183522889974 0.4283111408100090 0.1457107178800001

0.4435183522890012	0.7616444741430454	0.1457107178800001
0.9435183522889974	0.7616444741430477	0.1457107178800001
0.4392793396900074	0.2616444789110020	0.1979144111660034
0.9392793396900032	0.2616444789110020	0.1979144111660034
0.4392793396900074	0.5949778122439966	0.1979144111660034
0.9392793396900032	0.5949778122439966	0.1979144111660034
0.4392793396900074	0.9283111455780004	0.1979144111660034
0.9392793396900032	0.9283111455780004	0.1979144111660034
0.1813874112409989	0.0949778936079966	0.2114279908170005
0.6813874112409977	0.0949778936080025	0.2114279908170005
0.1813874112409989	0.4283112269410266	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
0.1813874112409989	0.7616445602750019	0.2114279908170005
0.6813874112409977	0.7616445602750019	0.2114279908170005
0.4343069956900041	0.0949774386080001	0.2707694632339971
0.9343069956900010	0.0949774386079996	0.2707694632339971
0.4343069956900041	0.4283107719410379	0.2707694632339971
0.9343069956900010	0.4283107719409998	0.2707694632339971
0.4343069956900041	0.7616441052750449	0.2707694632339971
0.9343069956900010	0.7616441052750121	0.2707694632339971
0.1878523446077165	0.0964464001524932	0.3306715868720819
0.6879598303504793	0.0961411762981955	0.3305124654258595
0.6877407190451780	0.4317378457958396	0.3306830444435504
0.1879967515465128	0.4282602494676797	0.3303360084424437
0.1878718894428447	0.7646974403774681	0.3303185939977127
0.6876032788223235	0.7615165118574926	0.3307748439043772
0.9294631376903799	0.2625326102640718	0.3468795215165664
0.4314791354711328	0.2626294888228239	0.3468214446669456
0.4246940252114849	0.5962573227802032	0.3465207957056131
0.9351891105113322	0.5962936043170052	0.3463272233396509
0.4306271891197642	0.9297409333103979	0.3469337399301764
0.9297656526999026	0.9299693394594880	0.3469594733347089
0.4269846449997077	0.0963845763967067	0.3980160644834737
0.9252349896342590	0.0964599492948276	0.3981718677565808
0.4228544456956386	0.4289940876197156	0.3974104762100971
0.9274461779341246	0.4291834462800094	0.3974213987910376
0.9279465636731069	0.7633619904601802	0.3976628299187557
0.4222738017765061	0.7633718254108439	0.3976363641429237
0.1698919631454780	0.2612494488037749	0.4165111135995559
0.6698881088273373	0.2633956271070140	0.4168557297169735
0.1679642431845640	0.5960836925281439	0.4197407750607827
0.6670064924959315	0.5963260157848114	0.4115062795867832
0.6693897038519800	0.9281421029893286	0.4164789371274619
0.1694856416164483	0.9305872806924113	0.4170386296048350

0.4211308123964114	0.2688446712073130	0.4745315080029218
0.9233677435808063	0.2702234899891313	0.4745465220408877
0.4462494320922250	0.5954300344421727	0.4726049269344270
0.8891405290184136	0.5956975096703940	0.4730959364754865
0.9206091133050799	0.9305705199266476	0.4744735241321525
0.4235296935447990	0.9309578402754615	0.4744422031874376
0.8966880054947227	0.4410654749891812	0.5487192403823665
0.4114025300961144	0.0995344873327527	0.5439056206560050
0.9227694145585028	0.1000455882288207	0.5436139699722073
0.4343742977877341	0.4407310308517223	0.5483892988289343
0.4235263945829021	0.7561667605405958	0.5455799495447726
0.9100243871570595	0.7564847196123106	0.5458679963086920
0.6667097062275774	0.2665909320609564	0.5413831147422251
0.1663937858924043	0.2796412687396003	0.5417402015717208
0.6666130240811121	0.5946966874005551	0.5653265038741024
0.1675604575340358	0.5911304273549610	0.5294641203435267
0.1670015812067254	0.9228451598062765	0.5415314963174572
0.6667986737222242	0.9291406024951177	0.5427415813701585
0.4212494542350059	0.2616454108449986	0.0151065289700014
0.9212494542350090	0.2616454108449986	0.0151065289700014
0.4212494542350059	0.5949787441780003	0.0151065289700014
0.9212494542350090	0.5949787441780003	0.0151065289700014
0.4212494542350059	0.9283120775110023	0.0151065289700014
0.9212494542350090	0.9283120775110477	0.0151065289700014
0.4757319089200007	0.2616445689349973	0.1306041949610020
0.9757319089200047	0.2616445689349974	0.1306041949610020
0.4757319089200007	0.5949779022690319	0.1306041949610020
0.9757319089200047	0.5949779022690009	0.1306041949610020
0.4757319089200007	0.9283112356020035	0.1306041949610020
0.9757319089200047	0.9283112356020393	0.1306041949610020
0.4070655843149993	0.0949779281480025	0.2130205561419984
0.9070655843150027	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150027	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150534	0.2130205561419984
0.9070655843150027	0.7616445948150538	0.2130205561419984
0.9575666471834866	0.0963252771334696	0.3291317773699245
0.4578084599042360	0.0962126616187169	0.3291090540904684
0.4577558806679204	0.4288032549022136	0.3290591415175230
0.9581797748369048	0.4284751002437429	0.3290137441452359
0.4575040415292295	0.7633259678620758	0.3290717811171807
0.9580339260848738	0.7637102739641051	0.3290063953287823
0.4005107746434239	0.2627901699757454	0.4139299120533652
0.9006309611079508	0.2631508415926573	0.4139621421033218

0.3983736180686995	0.5960849124720313	0.4122349430923953
0.8973887643195853	0.5962384978321071	0.4117848456850597
0.3997370765268748	0.9300086788610650	0.4137108291093666
0.8997748643109895	0.9298549747594531	0.4136592740184594
0.4265572108204158	0.2659024108209990	0.5312326949647200
0.9265395760261956	0.2670038874729438	0.5312534159313451
0.4049478289358026	0.5976417753891037	0.5280720474409663
0.9306027395397163	0.5981873025959938	0.5284054755757828
0.4238909729110156	0.9324305920009611	0.5310139790266732
0.9244522626435092	0.9325842877902695	0.5310210000735636

NbO_x: Transition state for CH_3OH dissociation on O_{vac}

(*E* = -1163.4727 eV, *ZPE* = 1.323233956 eV, *S***T* = 0.342454862 eV)

AutoCreatByScript: H C O Nb

1.000000000

7.93326886	0.00000063	0.00000000
0.00000000	11.45228897	0.00000000
0.00000000	0.00000000	32.71817093

H	C	O	Nb
4	1	90	36

Selective Dynamics

Direct

0.5996599641273221	0.5017076164656207	0.5643906243875106
0.6743729192105058	0.7381858384197806	0.6011053069585512
0.7664265748835344	0.6105238424796099	0.6245582756969843
0.5421238994791866	0.6230139090231095	0.6202133573852564
0.6630116655343005	0.6438054559762516	0.6054621907924606
0.4534627759987453	0.0949785564412324	0.0000000000000000
0.9534627759987454	0.0949785568778262	0.0000000000000000
0.4534627759987453	0.4283118900656284	0.0000000000000000
0.9534627759987454	0.4283118896290343	0.0000000000000000
0.4534627759987453	0.7616452236900243	0.0000000000000000
0.9534627759987454	0.7616452232534301	0.0000000000000000
0.1955712225792383	0.2616453474619344	0.0135137049973227
0.6955712225792385	0.2616453470253403	0.0135137049973227
0.1955712225792383	0.5949786810863302	0.0135137049973227
0.6955712225792385	0.5949786806497360	0.0135137049973227
0.1955712225792383	0.9283120138375383	0.0135137049973227
0.6955712225792385	0.9283120142741320	0.0135137049973227
0.4484906591203063	0.2616449755415910	0.0728553504748134
0.9484906591203064	0.2616449759781847	0.0728553504748134
0.4484906591203063	0.5949783091659868	0.0728553504748134
0.9484906591203064	0.5949783087293927	0.0728553504748134
0.4484906591203063	0.9283116427903827	0.0728553504748134
0.9484906591203064	0.9283116423537886	0.0728553504748134
0.2014097326332138	0.2616445455542733	0.1321970366024981
0.7014097326332139	0.2616445451176792	0.1321970366024981
0.2014097326332138	0.5949778783054813	0.1321970366024981
0.7014097326332139	0.5949778787420751	0.1321970366024981
0.2014097326332138	0.9283112119298773	0.1321970366024981
0.7014097326332139	0.9283112114932831	0.1321970366024981
0.4435183519041861	0.0949778077930770	0.1457107177598574
0.9435183519041862	0.0949778073564829	0.1457107177598574
0.4435183519041861	0.4283111405442850	0.1457107177598574
0.9435183519041862	0.4283111409808788	0.1457107177598574

0.4435183519041861	0.7616444741686811	0.1457107177598574
0.9435183519041862	0.7616444737320867	0.1457107177598574
0.4392793401432762	0.2616444792044060	0.1979144110425368
0.9392793401432764	0.2616444787678119	0.1979144110425368
0.4392793401432762	0.5949778119556141	0.1979144110425368
0.9392793401432764	0.5949778123922078	0.1979144110425368
0.4392793401432762	0.9283111455800099	0.1979144110425368
0.9392793401432764	0.9283111451434157	0.1979144110425368
0.1813874110904645	0.0949778938145262	0.2114279907272310
0.6813874110904646	0.0949778933779321	0.2114279907272310
0.1813874110904645	0.4283112265657342	0.2114279907272310
0.6813874110904646	0.4283112270023280	0.2114279907272310
0.1813874110904645	0.7616445601901303	0.2114279907272310
0.6813874110904646	0.7616445606267240	0.2114279907272310
0.4343069951117225	0.0949774389413255	0.2707694632121662
0.9343069951117228	0.0949774385047314	0.2707694632121662
0.4343069951117225	0.4283107716925336	0.2707694632121662
0.9343069951117228	0.4283107721291273	0.2707694632121662
0.4343069951117225	0.7616441053169295	0.2707694632121662
0.9343069951117228	0.7616441048803353	0.2707694632121662
0.1861015120064897	0.0969449946350809	0.3309363012121167
0.6863396748663831	0.0962466228797929	0.3305286292787272
0.6860326627074633	0.4331950050156147	0.3307918472323966
0.1862113179408873	0.4286317884176536	0.3304570516222313
0.1854689896391587	0.7649825014112035	0.3305374213350012
0.6853054000743902	0.7611691008751758	0.3311744548062363
0.9279633578433900	0.2628058891342383	0.3471367618409835
0.4313704653645132	0.2634641953360180	0.3470633170263225
0.4219795369446235	0.5969407969062878	0.3470287151531792
0.9332886380961507	0.5963722719466231	0.3474341565217808
0.4285084105923017	0.9302637130400402	0.3470391332172186
0.9272822476862334	0.9294580920631605	0.3472842352437701
0.4269951541765851	0.0970937315593295	0.3982855938945973
0.9233069065555408	0.0960033624017649	0.3983900248546076
0.4219558443151012	0.4301451742155800	0.3978071967362266
0.9266722645777068	0.4295505055000781	0.3981382326618953
0.9260599583410567	0.7627499061073919	0.3985608929025788
0.4193316902157783	0.7639600274442806	0.3978728993699281
0.1713402323793171	0.2611928759299943	0.4166152423117743
0.6711129389354896	0.2637485445146643	0.4173408843426444
0.1659541890276993	0.5955868563320804	0.4213378238500449
0.6653620119462335	0.5961709933016062	0.4131434024511956
0.6665327021325737	0.9277516327012829	0.4169531034967301
0.1666545774927891	0.9312270789659977	0.4174141191822424

0.4255386032637246	0.2742643134607070	0.4749814072201254
0.9294308033826049	0.2673625728864741	0.4748533160132861
0.4409829178536124	0.6041807214528188	0.4734514463886627
0.8849319156945857	0.5958534010422274	0.4754605256902116
0.9164895767820986	0.9304838194815094	0.4751879954800395
0.4192766196001582	0.9333817199214216	0.4746234785930926
0.9143129393449048	0.4373104623103868	0.5484609970524412
0.4195367141508930	0.1039400174768615	0.5437182248989492
0.9336073642158148	0.1005877134994574	0.5452148553219872
0.4573985067234947	0.4494039807518879	0.5512457761953504
0.4305868879880621	0.7615128706213792	0.5466786813440001
0.9122777228049224	0.7589037753092104	0.5474981217111698
0.6768706361478339	0.2688282998827871	0.5410185400605462
0.1804720759205431	0.2832784096525108	0.5417923883314096
0.6692383863062472	0.5884526723027503	0.5654814537030112
0.1658973650364852	0.5946396256088059	0.5325495137634211
0.1745673825555939	0.9253513605693225	0.5420311370076946
0.6725491161533635	0.9339672596729849	0.5428205674454553
0.4212494545407353	0.2616454110145320	0.0151065290617088
0.9212494545407355	0.2616454105779379	0.0151065290617088
0.4212494545407353	0.5949787437657400	0.0151065290617088
0.9212494545407355	0.5949787442023338	0.0151065290617088
0.4212494545407353	0.9283120773901359	0.0151065290617088
0.9212494545407355	0.9283120778267295	0.0151065290617088
0.4757319090783974	0.2616445688838477	0.1306041948109597
0.9757319090783976	0.2616445693204415	0.1306041948109597
0.4757319090783974	0.5949779025082436	0.1306041948109597
0.9757319090783976	0.5949779020716495	0.1306041948109597
0.4757319090783974	0.9283112352594517	0.1306041948109597
0.9757319090783976	0.9283112356960453	0.1306041948109597
0.4070655838077825	0.0949779285519269	0.2130205562197055
0.9070655838077826	0.0949779281153327	0.2130205562197055
0.4070655838077825	0.4283112613031349	0.2130205562197055
0.9070655838077826	0.4283112617397287	0.2130205562197055
0.4070655838077825	0.7616445949275308	0.2130205562197055
0.9070655838077826	0.7616445944909367	0.2130205562197055
0.9555675338601851	0.0960842728361970	0.3293360329663148
0.4560314951937732	0.0969158711946260	0.3291926536187944
0.4557185863482762	0.4296212535141163	0.3291766707571266
0.9560329599115595	0.4288276693475042	0.3292713426141392
0.4549536532409921	0.7637930745803732	0.3291772627828862
0.9553628553060285	0.7632422567242813	0.3292530735611020
0.4022016720103951	0.2638144858663084	0.4143093533254550
0.9022060283483198	0.2627651152964399	0.4144790110368189

0.3960106931255575	0.5971105678896662	0.4127843744350778	T	T	T
0.8959511136497651	0.5959307317016462	0.4133639731553295	T	T	T
0.3967057723038018	0.9308875202155644	0.4138181241539226	T	T	T
0.8968436272056463	0.9294359619174463	0.4143506490324458	T	T	T
0.4366670739556910	0.2691880184804436	0.5315829481180597	T	T	T
0.9379982755305235	0.2664829002355397	0.5316546431405296	T	T	T
0.3992748671321346	0.6070524832780945	0.5288425950527302	T	T	T
0.9220234646125434	0.5974214078118230	0.5309662110136790	T	T	T
0.4113650334548224	0.9369086729253239	0.5311566177455630	T	T	T
0.9108939149202114	0.9329171997077915	0.5319257527333909	T	T	T

NbO_x: : Final state for CH_3OH dissociation on O_{vac}
(*E* = -1164.0909 eV, *ZPE* = 1.35506866 eV, *S***T* = 0.235162441 eV)
AutoCreatByScript: H C O Nb
1.00000000000000
7.9332688600000001 0.0000006300000000 0.0000000000000000
0.0000000000000000 11.4522889699999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 32.7181709299999994
H C O Nb
4 1 90 36
Selective dynamics
Direct
0.5707676889698230 0.4262492293923589 0.5584497411264676
0.6648643882850948 0.7617069665585002 0.5890753154870447
0.7748336758293862 0.6403902278962105 0.6116121744232494
0.5510321817491916 0.6408597029427269 0.6109190524384979
0.6641222911118119 0.6667037718208170 0.5934836631943503
0.4534627765720083 0.0949785566820056 0.0000000000000000
0.9534627765720117 0.0949785566820012 0.0000000000000000
0.4534627765720083 0.4283118900150149 0.0000000000000000
0.9534627765720117 0.4283118900150030 0.0000000000000000
0.4534627765720083 0.7616452233490336 0.0000000000000000
0.9534627765720117 0.7616452233489994 0.0000000000000000
0.1955712230439985 0.2616453474379991 0.0135137049989993
0.6955712230439985 0.2616453474379991 0.0135137049989993
0.1955712230439985 0.5949786807720229 0.0135137049989993
0.6955712230439985 0.5949786807720017 0.0135137049989993
0.1955712230439985 0.9283120141050401 0.0135137049989993
0.6955712230439985 0.9283120141050035 0.0135137049989993
0.4484906587389972 0.2616449757260097 0.0728553503239981
0.9484906587390074 0.2616449757260000 0.0728553503239981
0.4484906587389972 0.5949783090590017 0.0728553503239981
0.9484906587390074 0.5949783090590229 0.0728553503239981
0.4484906587389972 0.9283116423920035 0.0728553503239981
0.9484906587390074 0.9283116423920035 0.0728553503239981
0.2014097329349997 0.2616445452179974 0.1321970365760023
0.7014097329350059 0.2616445452180080 0.1321970365760023
0.2014097329349997 0.5949778785510204 0.1321970365760023
0.7014097329350059 0.5949778785509992 0.1321970365760023
0.2014097329349997 0.9283112118840375 0.1321970365760023
0.7014097329350059 0.9283112118840009 0.1321970365760023
0.4435183522890053 0.0949778074770009 0.1457107178800001
0.9435183522889974 0.0949778074770053 0.1457107178800001
0.4435183522890053 0.4283111408100069 0.1457107178800001
0.9435183522889974 0.4283111408100160 0.1457107178800001

0.4435183522890053	0.7616444741430343	0.1457107178800001
0.9435183522889974	0.7616444741430317	0.1457107178800001
0.4392793396900066	0.2616444789110020	0.1979144111660034
0.9392793396900032	0.2616444789110020	0.1979144111660034
0.4392793396900066	0.5949778122439966	0.1979144111660034
0.9392793396900032	0.5949778122439966	0.1979144111660034
0.4392793396900066	0.9283111455780004	0.1979144111660034
0.9392793396900032	0.9283111455780004	0.1979144111660034
0.1813874112409990	0.0949778936079966	0.2114279908170005
0.6813874112409977	0.0949778936080010	0.2114279908170005
0.1813874112409990	0.4283112269410163	0.2114279908170005
0.6813874112409977	0.4283112269409983	0.2114279908170005
0.1813874112409990	0.7616445602750019	0.2114279908170005
0.6813874112409977	0.7616445602750019	0.2114279908170005
0.4343069956900049	0.0949774386079985	0.2707694632339972
0.9343069956900010	0.0949774386079985	0.2707694632339972
0.4343069956900049	0.4283107719410176	0.2707694632339972
0.9343069956900010	0.4283107719409998	0.2707694632339972
0.4343069956900049	0.7616441052750272	0.2707694632339972
0.9343069956900010	0.7616441052750070	0.2707694632339972
0.1870106637857920	0.0956331153259324	0.3306623247577736
0.6872247749906727	0.0952046009214761	0.3304115532363789
0.6867258054410040	0.4322606335043969	0.3307397833988036
0.1870673758107446	0.4288173519390228	0.3304404029279737
0.1872416059400475	0.7631205557491739	0.3305784768092490
0.6868878394938944	0.7603555302589183	0.3309137889732903
0.9276438112416531	0.2624397094357645	0.3461604629164108
0.4298130372026233	0.2627632606333152	0.3459239621571362
0.4245333820810452	0.5958578782432372	0.3472283718501593
0.9331755180652065	0.5958727716309361	0.3473060593518429
0.4297480950639195	0.9286489284485495	0.3464156857380292
0.9290185404728957	0.9287201076892369	0.3467833494658192
0.4245654886259300	0.0960529493200240	0.3969249959832616
0.9224689489413074	0.0958137877553795	0.3977818824377166
0.4213200463205403	0.4288238484052612	0.3976994547259335
0.9256146488365163	0.4291869826738094	0.3976578258811470
0.9268508887968635	0.7619857853692128	0.3981665773980778
0.4225639639125020	0.7624861003037651	0.3979835510349660
0.1655407772320576	0.2613223879982706	0.4148222717413111
0.6654810003129279	0.2634147755115617	0.4149963756132743
0.1687738108400082	0.5957607734742849	0.4208333583434323
0.6679062023616352	0.5957385082155134	0.4147686163455542
0.6676242348681132	0.9272281793655394	0.4156724380116816
0.1679567289302743	0.9294180748891440	0.4162608180723620

0.4143001092062635	0.2583651188651236	0.4735679192747937
0.9146150348136087	0.2662011870543958	0.4739821836241951
0.4409307798231564	0.5939816315123594	0.4740293888169713
0.9011412225444688	0.5917531010081536	0.4749802326895812
0.9198006301098886	0.9319266280206853	0.4738745831409450
0.4241614389683416	0.9402921041645571	0.4730977377112073
0.9082490045187610	0.4358066689256554	0.5491089099750972
0.4184037980275161	0.1002076202026663	0.5477247002691472
0.9215339806469338	0.1019406502961527	0.5452568708794165
0.4484884483435653	0.4329602417101605	0.5533816169211786
0.4121504157780896	0.7643081330734025	0.5423180975693959
0.9302541429673541	0.7603871133005422	0.5449647707748658
0.6654005972661965	0.2711315139305124	0.5396727031220442
0.1713007248807353	0.2795662099448942	0.5396039477642001
0.6656852450024423	0.6090067503891092	0.5542322623630532
0.1760303305608636	0.5838322025432727	0.5366897316402638
0.1716640688941274	0.9332040967609929	0.5394743864267831
0.6696382408645625	0.9288859032197532	0.5408567348869471
0.4212494542350062	0.2616454108449986	0.0151065289700014
0.9212494542350097	0.2616454108449986	0.0151065289700014
0.4212494542350062	0.5949787441780003	0.0151065289700014
0.9212494542350097	0.5949787441780003	0.0151065289700014
0.4212494542350062	0.9283120775110023	0.0151065289700014
0.9212494542350097	0.9283120775110356	0.0151065289700014
0.4757319089200071	0.2616445689349973	0.1306041949610020
0.9757319089200166	0.2616445689349974	0.1306041949610020
0.4757319089200071	0.5949779022690229	0.1306041949610020
0.9757319089200166	0.5949779022690009	0.1306041949610020
0.4757319089200071	0.9283112356020046	0.1306041949610020
0.9757319089200166	0.9283112356020061	0.1306041949610020
0.4070655843149993	0.0949779281480010	0.2130205561419984
0.9070655843150012	0.0949779281479977	0.2130205561419984
0.4070655843149993	0.4283112614820013	0.2130205561419984
0.9070655843150012	0.4283112614820013	0.2130205561419984
0.4070655843149993	0.7616445948150374	0.2130205561419984
0.9070655843150012	0.7616445948150370	0.2130205561419984
0.9571103259744370	0.0959765060454654	0.3291614686335091
0.4575464499735860	0.0961939155216943	0.3289460714600520
0.4569211248652958	0.4284600672671196	0.3290029606383038
0.9572457162911848	0.4282115601163178	0.3291382983440340
0.4568850973345159	0.7624990601041043	0.3290002786142475
0.9572610551780194	0.7626535935406733	0.3291378619872052
0.3971829476059979	0.2618988846451641	0.4133866331600952
0.8973386924051765	0.2625067631489987	0.4139736298281214

0.3977055870570871	0.5955155112989824	0.4125332131708405
0.8980359636199056	0.5953598379882038	0.4131012804254771
0.3976180849522414	0.9300271087335609	0.4126838858116144
0.8976362069271119	0.9292648332710836	0.4135207366282006
0.4039742587242403	0.2573210883318198	0.5304841723507654
0.9050896588076482	0.2655232020944366	0.5310753731587631
0.4117840903214741	0.6050393964893229	0.5293853732388648
0.9300335466539306	0.5957687051695147	0.5307251861081794
0.4236894717838843	0.9355256816513624	0.5295095230594171
0.9251737443712078	0.9322442343364961	0.5306101711295279

Ru: Initial state for CH_3O and CO coupling

(*E* = -1129.4938 eV, *ZPE* = 1.279792158 eV, *S***T* = 0.660446654 eV)

AutoCreatByScript: H C O Ru

1.00000000000000

15.1228015700000000 0.0000000000000000 0.0000000000000000

-3.6418149199999998 13.0568463000000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.5088567099999999

H C O Ru

3 2 2 120

Selective dynamics

Direct

0.7215403344373915	0.6564317110359889	0.3991758079813897
0.8452227829354348	0.6951454593967140	0.4012303287209217
0.7829167443339710	0.6074485070576909	0.4583515823915915
0.7742869869881482	0.0887647909884902	0.3636555369869706
0.7832739293021957	0.6299489671133875	0.4090979379918673
0.7855266642805724	0.5442542926261271	0.3709412144644978
0.7859101304036599	0.0725175344585698	0.4169463820872999
0.8073722568249989	0.1380862835040006	0.0000000000000000
0.1407055901600032	0.1380862835040006	0.0000000000000000
0.4740389234929985	0.1380862835040006	0.0000000000000000
0.1407055901590016	0.3380862835039939	0.0000000000000000
0.4740389234929993	0.3380862835039939	0.0000000000000000
0.8073722568260019	0.3380862835039939	0.0000000000000000
0.1407055901600022	0.5380862835049970	0.0000000000000000
0.4740389234929971	0.5380862835049970	0.0000000000000000
0.8073722568280033	0.5380862835049970	0.0000000000000000
0.1407055901600020	0.7380862835039910	0.0000000000000000
0.4740389234929972	0.7380862835039910	0.0000000000000000
0.8073722568259989	0.7380862835039910	0.0000000000000000
0.1407055901600021	0.9380862835039873	0.0000000000000000
0.4740389234929976	0.9380862835039873	0.0000000000000000
0.8073722568259986	0.9380862835039873	0.0000000000000000
0.3201838529240036	0.1920708306439960	0.0159535054489979
0.6535171862569991	0.1920708306439960	0.0159535054489979
0.9868505195880036	0.1920708306439960	0.0159535054489979
0.3201838529240035	0.3920708306439969	0.0159535054489979
0.6535171862569992	0.3920708306439969	0.0159535054489979
0.9868505195889982	0.3920708306439969	0.0159535054489979
0.3201838529240030	0.5920708306439909	0.0159535054489979
0.6535171862569982	0.5920708306439909	0.0159535054489979
0.9868505195900006	0.5920708306439909	0.0159535054489979
0.3201838529240035	0.7920708306449944	0.0159535054489979
0.6535171862569982	0.7920708306439925	0.0159535054489979

0.9868505195910036	0.7920708306419870	0.0159535054489979
0.3201838529240036	0.9920708306439923	0.0159535054489979
0.6535171862569982	0.9920708306439923	0.0159535054489979
0.9868505195889979	0.9920708306439923	0.0159535054489979
0.2186901232590019	0.0615218340180015	0.0955531191689971
0.5520234565920038	0.0615218340180015	0.0955531191689971
0.8853567899250010	0.0615218340180015	0.0955531191689971
0.2186901232590018	0.2615218340179952	0.0955531191689971
0.5520234565920035	0.2615218340179952	0.0955531191689971
0.8853567899249987	0.2615218340179952	0.0955531191689971
0.2186901232590018	0.4615218340179955	0.0955531191689971
0.5520234565920035	0.4615218340179955	0.0955531191689971
0.8853567899249988	0.4615218340179955	0.0955531191689971
0.2186901232590003	0.6615218340179920	0.0955531191689971
0.5520234565920035	0.6615218340179920	0.0955531191689971
0.8853567899249971	0.6615218340179920	0.0955531191689971
0.2186901232599952	0.8615218340179887	0.0955531191689971
0.5520234565920035	0.8615218340179887	0.0955531191689971
0.8853567899249980	0.8615218340179887	0.0955531191689971
0.0648350526889985	0.1155063811579980	0.1115066246180014
0.3981683860230025	0.1155063811579980	0.1115066246180014
0.7315017193540015	0.1155063811579980	0.1115066246180014
0.0648350526889982	0.3155063811579973	0.1115066246180014
0.3981683860230022	0.3155063811579973	0.1115066246180014
0.7315017193559971	0.3155063811579973	0.1115066246180014
0.0648350526889978	0.5155063811589943	0.1115066246180014
0.3981683860230018	0.5155063811589943	0.1115066246180014
0.7315017193559975	0.5155063811589943	0.1115066246180014
0.0648350526889983	0.7155063811579934	0.1115066246180014
0.3981683860230020	0.7155063811579934	0.1115066246180014
0.7315017193559973	0.7155063811579934	0.1115066246180014
0.0648350526889974	0.9155063811579867	0.1115066246180014
0.3981683860230021	0.9155063811579867	0.1115066246180014
0.7315017193559967	0.9155063811579867	0.1115066246180014
0.9637798961069813	0.5854621906901840	0.1912891592045443
0.9630713576864377	0.3854308175112247	0.1927005816469426
0.9632251835354658	0.7844504419652680	0.1926269652157457
0.9644916987664396	0.1850693101837787	0.1918154678718250
0.6295591901239790	0.9852772952929431	0.1928271018101061
0.9639400136976222	0.9859846742206354	0.1926696343645328
0.2962927108209871	0.7846904549180361	0.1928954287454559
0.2968438536463731	0.9850684983300507	0.1929213947149394
0.2969508280410585	0.1852887857880574	0.1931048764120430
0.2967705479395595	0.3850447030413112	0.1929745125489012

0.6304644603172632	0.5845350473349235	0.1931628480878853
0.2964627235908192	0.5852567614371265	0.1930738456983380
0.6308626239251187	0.7854493342376574	0.1933245831327886
0.6296982938145831	0.1854647497507263	0.1918391413980598
0.6309652315000405	0.3860434258603624	0.1929769166569256
0.4767470741260992	0.0389174844496779	0.2079847441560808
0.4768866142502680	0.4385027818337778	0.2080905689698682
0.1437002563218255	0.8388872837948178	0.2080387928961453
0.8096770369640922	0.2370217478102162	0.2088017847461524
0.4764200776759045	0.8387835957711925	0.2082521254241861
0.1436879092240546	0.4389325980807163	0.2082080809244968
0.8099230597330533	0.0390531206267683	0.2081924378563266
0.1438366568114903	0.0387097258899113	0.2082589648029388
0.8102089156511623	0.6385007424664886	0.2084326911581074
0.4765715487762007	0.6386487818198424	0.2082308312177099
0.8103877048995992	0.8393279856260654	0.2081978425991635
0.1434376788338836	0.2385518384369962	0.2082686565765438
0.1427682304798185	0.6381812714460362	0.2083502231325900
0.4770443631299207	0.2391596025087486	0.2085784751744860
0.8100029444454476	0.4393619696598717	0.2088013726560235
0.7039583213511200	0.7087944313206561	0.2847458403642354
0.3721714008509304	0.1075211191910149	0.2858629739751993
0.3716649551571449	0.5076491714276889	0.2856824471621059
0.3714515566542432	0.9072742723777025	0.2856522140658733
0.3720048672942288	0.3075132919974287	0.2860406929076541
0.0394926719965032	0.3081026301899246	0.2856209326814979
0.0365733422488626	0.5074205654762101	0.2854984162745965
0.0378957070985532	0.7071092969063572	0.2854307533248929
0.0391060132610361	0.9079610669619220	0.2853327425397758
0.7059350790372005	0.1071568784259941	0.2886936870966016
0.3715346822474128	0.7075445432121898	0.2858522429943048
0.7039733645509461	0.9062840433277819	0.2858865787319188
0.0393013668917775	0.1079362529876400	0.2858274381384770
0.7050016311907872	0.3072444404936501	0.2853458050303541
0.7058654852024768	0.5084576979430681	0.2894402433034594
0.8877666569157032	0.3611271669004314	0.2989179272764468
0.8880416531657448	0.7646319098948539	0.2986172474367431
0.8895258339868463	0.1632351127595838	0.3012669418444066
0.5520750969741655	0.7617918335352702	0.2991867354463877
0.8879927095458519	0.9621093564591702	0.2988299369486300
0.5516721663707147	0.5618883074226948	0.2991225122826647
0.5508642669790712	0.9604076354228788	0.2995516352332907
0.2204840781323700	0.1621803026598542	0.2994609001146462
0.2193917767282562	0.5618522918392208	0.2992477861166408

0.2195634171072448	0.7619930679388337	0.2993276808255297
0.2200281699468064	0.9622001042941752	0.2992173549748584
0.2202312394658587	0.3622075557221783	0.2992368510264763
0.5528460532222405	0.1621028861066191	0.2989924357079397
0.5533056864628946	0.3623189159196010	0.2988977165316080
0.8886164962284457	0.5618949290832728	0.3040103462619126

Ru: Transition state for CH_3O and CO coupling
(E = -1128.3366 eV, ZPE = 1.23736119 eV, S*T = 0.525245129 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
3 2 2 120
Selective dynamics
Direct
0.6260784738043597 0.5321345695153813 0.4200700146629057
0.7412045548547221 0.6101751629305385 0.4322680695954081
0.6993533527606433 0.4911967857840776 0.4745903757130893
0.6832282034194477 0.3549230907318531 0.3766758480538424
0.6974245886685532 0.5313304095089307 0.4305044389638595
0.7330049399183796 0.4798547013245758 0.3814975309550824
0.6459584215689150 0.3194440330116243 0.4240540843769676
0.1407055901600032 0.1380862835039403 0.0000000000000000
0.4740389234930254 0.1380862835039403 0.0000000000000000
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0.4740389234930072 0.3380862835038232 0.0000000000000000
0.8073722568260429 0.3380862835038232 0.0000000000000000
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0.4740389234929944 0.5380862835047558 0.0000000000000000
0.8073722568280335 0.5380862835047558 0.0000000000000000
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0.4740389234929903 0.7380862835036190 0.0000000000000000
0.8073722568260038 0.7380862835036190 0.0000000000000000
0.1407055901599787 -0.0619137164962383 0.0000000000000000
0.4740389234930017 -0.0619137164962250 0.0000000000000000
0.8073722568260133 -0.0619137164962383 0.0000000000000000
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0.6535171862570576 0.1920708306438992 0.0159535054489979
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0.3201838529240034 0.3920708306437910 0.0159535054489979
0.6535171862570239 0.3920708306437910 0.0159535054489979
0.9868505195890583 0.3920708306437910 0.0159535054489979
0.3201838529239984 0.5920708306437140 0.0159535054489979
0.6535171862569981 0.5920708306437140 0.0159535054489979
0.9868505195900260 0.5920708306437140 0.0159535054489979
0.3201838529240152 -0.2079291693551473 0.0159535054489979
0.6535171862569974 0.7920708306435739 0.0159535054489979

0.9868505195910328 0.7920708306415821 0.0159535054489979
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0.6535171862570184 -0.0079291693562731 0.0159535054489979
0.9868505195890415 -0.0079291693562827 0.0159535054489979
0.2186901232590162 0.0615218340179675 0.0955531191689971
0.5520234565921429 0.0615218340179675 0.0955531191689971
0.8853567899251421 0.0615218340179675 0.0955531191689971
0.2186901232590000 0.2615218340178746 0.0955531191689971
0.5520234565920035 0.2615218340178746 0.0955531191689971
0.8853567899250724 0.2615218340178746 0.0955531191689971
0.2186901232589941 0.4615218340177490 0.0955531191689971
0.5520234565920035 0.4615218340177490 0.0955531191689971
0.8853567899250371 0.4615218340177490 0.0955531191689971
1.2186901232590404 0.6615218340176605 0.0955531191689971
0.5520234565920034 0.6615218340176605 0.0955531191689971
0.8853567899250187 0.6615218340176605 0.0955531191689971
0.2186901232599966 -0.1384781659821979 0.0955531191689971
0.5520234565920362 -0.1384781659821979 0.0955531191689971
0.8853567899250195 0.8615218340175480 0.0955531191689971
1.0648350526889985 0.1155063811579354 0.1115066246180021
0.3981683860230350 0.1155063811579354 0.1115066246180021
0.7315017193541794 0.1155063811579354 0.1115066246180021
1.0648350526889983 0.3155063811578409 0.1115066246180021
0.3981683860230106 0.3155063811578409 0.1115066246180021
0.7315017193560484 0.3155063811578409 0.1115066246180021
1.0648350526889976 0.5155063811587531 0.1115066246180021
0.3981683860229997 0.5155063811587531 0.1115066246180021
0.7315017193560198 0.5155063811587531 0.1115066246180021
1.0648350526889974 0.7155063811576179 0.1115066246180021
0.3981683860229910 0.7155063811576179 0.1115066246180021
0.7315017193560153 0.7155063811576179 0.1115066246180021
1.0648350526889967 0.9155063811574945 0.1115066246180021
0.3981683860230087 -0.0844936188422338 0.1115066246180021
0.7315017193560174 -0.0844936188422357 0.1115066246180021
0.6304084736507563 0.5857379554536319 0.1927393063896570
0.9636407171082978 0.3847475050089888 0.1925581040365705
0.6301528171157934 0.3853902859552412 0.1936114508164705
0.6299664886794580 0.7849852036888845 0.1928336524150752
0.9636618374409234 0.7850182433317834 0.1927874349438946
0.6304164720753073 -0.0147018799422408 0.1929555372104677
0.9632363821141557 0.5849997456277949 0.1929798243877321
0.9638275253570283 0.1851302199772448 0.1927449360368020
0.9635396101552917 -0.0151287064945853 0.1929068257067405
0.2967908548044615 0.5851582222224950 0.1927857687518814

0.2966473175895319 -0.2150815368878819 0.1928725048539640
0.2967058134048821 -0.0150559467319497 0.1928303648845178
0.6299788916313072 0.1847721191087778 0.1923362171480774
0.2964940789345508 0.1850923136870772 0.1928433192397213
0.2966336835006465 0.3848221568800858 0.1928822805910106
0.8091198332631980 0.2389015074667922 0.2082835037121988
1.1434540208169708 0.8384705790538409 0.2080372856723930
0.4766163680861934 -0.1612553422559228 0.2079771967098759
0.8099900513632897 0.8386158911145039 0.2081685971672499
0.8102404657486370 0.0387057100856688 0.2084281292798948
0.1434021559992255 0.0384059198567651 0.2082854261273203
1.1433376420100552 0.6383958364547405 0.2083415737083080
1.1434634806079020 0.4385626327916113 0.2080610682072468
0.8097913651676885 0.4380796160717032 0.2087982533062967
0.4769965398244478 0.0393369824594099 0.2085586704758794
0.4767427866662864 0.6382971773978089 0.2080785338433908
0.1427447550905517 0.2380928047674210 0.2084573852280727
0.4771787286031654 0.2387767937571151 0.2081907391871118
0.8089478174389756 0.6374582528600172 0.2086332260218242
0.4771980726196628 0.4383830325896686 0.2082819690370244
0.3718242854364556 0.7076283051582655 0.2856176080375666
0.7055723518148846 0.1073397752982830 0.2858588211926913
0.7054007887199953 0.3097209030076912 0.2887234830874907
0.3714474992680664 0.1075374210450047 0.2857737854073520
1.0396054638341710 0.3071389532998199 0.2857979933289453
0.7051981364840095 -0.0922239189995881 0.2857888499716245
1.0390423042821193 0.9072219619275317 0.2857448784018380
1.0383382706820996 0.7074447538239915 0.2857679402647829
1.0390897004533575 0.5070701903057361 0.2857626174377179
0.3719694287140339 -0.0925767864612620 0.2857168864639016
1.0384264204365647 0.1070726193900800 0.2858454036627179
0.7056489374443260 0.7089239620394304 0.2856276886038714
0.7058299001284039 0.5096447934805204 0.2861312497671983
0.3703336372468960 0.3068812747002752 0.2853252333098870
0.3715423975944840 0.5073315376254613 0.2857764574025222
0.8887254019447531 0.3616637193874629 0.2986371651063892
0.5533872040569132 0.7624738101469044 0.2991971971599379
0.8876058259620476 0.5617746591713944 0.2993726428770911
0.5535448793691992 -0.0382518063779137 0.2990204177014523
0.2203573415888274 0.5621688851187078 0.2992195785424265
0.2196612240245009 0.1614457834452352 0.2994887270961154
0.8870465319703394 0.1620026857485666 0.2990567095619088
0.8872369271413351 0.7626755579099532 0.2992707264202833
0.2199876732719797 -0.2379375847909744 0.2993243440967101

0.2205210384903220 -0.0380249194251775 0.2992828403125964
0.2200864758766914 0.3621013113929121 0.2995081136640092
0.8871079884409051 -0.0384340623149632 0.2993536813872186
0.5519786625201589 0.5638425355265927 0.2988951500159894
0.5518830067613022 0.1589161966346404 0.2989434471805200
0.5483207197267426 0.3625887389519763 0.2998457134188383

Ru: Final state for CH_3O and CO coupling

(*E* = -1129.177 eV, *ZPE* = 1.25463467 eV, *S***T* = 0.668489 eV)

%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics

Direct

H	0.7859517546959999	0.3430194796070000	0.4446242190879998
H	0.6850391697539999	0.3858915917069999	0.4618291475749999
H	0.6893493391219998	0.2596540007950000	0.4846255141279998
C	0.5767946624469997	0.2462747162779999	0.3820069673429999
C	0.7112393689099998	0.3203705111299999	0.4497067678839999
O	0.6753541298219999	0.2781086112200000	0.3897989861609999
O	0.5279564679659999	0.2613069709170000	0.4241850729359999
Ru	0.1407055901600000	0.1380862835040000	0.0000000000000000
Ru	0.4740389234929999	0.1380862835040000	0.0000000000000000
Ru	0.8073722568249998	0.1380862835040000	0.0000000000000000
Ru	0.1407055901590000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568260010	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835049999	0.0000000000000000
Ru	0.4740389234929998	0.5380862835049999	0.0000000000000000
Ru	0.8073722568279997	0.5380862835049999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.9380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.9380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.9380862835039999	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.1920708306440000	0.0159535054490000
Ru	0.9868505195879999	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.3920708306440000	0.0159535054490000
Ru	0.9868505195889999	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306449998	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195909998	0.7920708306419999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.9920708306439999	0.0159535054490000

Ru	0.9868505195889999	0.9920708306439999	0.0159535054490000
Ru	0.2186901232590000	0.0615218340179999	0.0955531191690000
Ru	0.5520234565919998	0.0615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.0615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.4615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.6615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340179999	0.0955531191690000
Ru	0.8853567899249999	0.6615218340179999	0.0955531191690000
Ru	0.2186901232599999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899249999	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890003	0.1155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.1155063811580000	0.1115066246180000
Ru	0.7315017193540009	0.1155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193559997	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811589999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811589999	0.1115066246180000
Ru	0.7315017193559997	0.5155063811589999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.7155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.7155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.9155063811569998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559997	0.9155063811579998	0.1115066246180000
Ru	0.2964675081359999	0.1847051192070000	0.1927997771510000
Ru	0.9633327335179998	0.1852154134539999	0.1927200849069999
Ru	0.9636890881299998	0.5851539320559999	0.1927980265580000
Ru	0.9639541430309998	0.3851446849819999	0.1925034601739999
Ru	0.6304016511879999	0.5851570974459999	0.1929919310060000
Ru	0.2967585528219999	0.5849936160249999	0.1928403392820000
Ru	0.6300473315159999	0.7850729630269998	0.1929523052029999
Ru	0.9632451393969996	0.9850633143499999	0.1928461022069999
Ru	0.2962069616110000	0.9851463950099999	0.1928046674549999
Ru	0.6301350017600000	0.9853368894139999	0.1931047237250000
Ru	0.2969371784300000	0.3850392607900000	0.1930096639049999
Ru	0.2967747222320000	0.7848699476799999	0.1929328055439999
Ru	0.9633634259739998	0.7850801612279998	0.1928828545559999

Ru	0.6299918592809998	0.1849082702970000	0.1936440368560000
Ru	0.6302771117160000	0.3848642812520000	0.1937453483709999
Ru	0.8083809416109998	0.2390415317470000	0.2088090620080000
Ru	0.4771557148049999	0.2388915930949999	0.2082462798030000
Ru	0.8088340346659989	0.4373733414859999	0.2087636984289999
Ru	0.1434416959190000	0.4383576433340000	0.2082400003740000
Ru	0.4767291392079999	0.6383632186639999	0.2080337432340000
Ru	0.4768193692020000	0.8385156108629998	0.2082164611539999
Ru	0.8097640347689998	0.8384516740389999	0.2083480660210000
Ru	0.1433077529010000	0.8382063936269999	0.2082663765539999
Ru	0.1430582585640000	0.0385775369360000	0.2082398709330000
Ru	0.8102607665709999	0.0385112994229999	0.2080702620550000
Ru	0.8102828805279999	0.6387478564910000	0.2080640175600000
Ru	0.4756455137469999	0.0372729039569999	0.2068174557109999
Ru	0.4771334346739999	0.4383802151679999	0.2081982931019999
Ru	0.1434760271110000	0.6385639619469999	0.2082277197269999
Ru	0.1432668425970000	0.2383699139950000	0.2084333332880000
Ru	0.3704613885370000	0.3067314568490000	0.2852422806000000
Ru	0.3713362788219998	0.1068399745700000	0.2854216515879999
Ru	0.3722572725369999	0.7074329361349999	0.2857147044219999
Ru	0.7051657422819999	0.9075665974419999	0.2858761409630000
Ru	0.0386568307099999	0.9075460826319999	0.2856927668089999
Ru	0.7056061152359999	0.1060778127720000	0.2857949033450000
Ru	0.0390829545800000	0.3071596869590000	0.2857630996689999
Ru	0.3720170182199999	0.5075441587619999	0.2857172863160000
Ru	0.7061166992099999	0.5094330712999999	0.2857290100000000
Ru	0.7053052178559998	0.7076419674779999	0.2859882547370000
Ru	0.3722898460660000	0.9078284768099999	0.2854530552949999
Ru	0.0382911289760002	0.1071238293100000	0.2858039003419999
Ru	0.0394583329069999	0.5078649863379999	0.2857871745869999
Ru	0.0388444831949999	0.7075286638779998	0.2859310002920000
Ru	0.7082089906110000	0.3083553338360000	0.2883364022250000
Ru	0.8870397142790009	0.1620740673490000	0.2989640296120000
Ru	0.8891852244539997	0.3628574881869999	0.2985862112799999
Ru	0.8875139006189999	0.5624115513729999	0.2990792526130000
Ru	0.5537854701499998	0.5626864745899999	0.2990614859549999
Ru	0.5533791632510000	0.9621103759849999	0.2991019323090000
Ru	0.2202680446660000	0.3622337875619999	0.2992843474219999
Ru	0.2205855344029999	0.5621955281799999	0.2993334036670000
Ru	0.5534288079619999	0.7625222076560000	0.2992700140640000
Ru	0.2205077391840000	0.7620212072379999	0.2992373042520000
Ru	0.2200367964290000	0.9613403549829998	0.2994354294570000
Ru	0.2197580103529999	0.1614841024960000	0.2992263445239999
Ru	0.8869024008309998	0.7617114134229999	0.2993129789050000

Ru	0.8866550918619996	0.9621376883689999	0.2993380672470000
Ru	0.5510777995850000	0.3640315762460000	0.2998827148209999
Ru	0.5500631914009999	0.1604882951000000	0.3009321175109999

Ru: Initial state for CH_3OCO and styrene coupling ($ArCHCH_2(COOMe)$)

(E = -1233.6925 eV, ZPE = 4.79911640 eV, $S*T$ = 1.2505961376379 eV)

%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics

Direct

H	0.6534894872510000	0.5736236144929998	0.4012925786339999
H	0.5044389581249998	0.5706725308209999	0.4032032457649998
H	0.0794673524639999	0.7823276246839997	0.4208704015199998
H	0.4465560082089999	0.2415413631299999	0.4025093016429999
H	0.2831818524959999	0.2285903175640000	0.4046616421249998
H	0.3438752047299999	0.5563082475379999	0.4087869471609998
H	0.7309723363070001	0.4947061402449999	0.4083871473409999
H	0.2332981377030000	0.3869711425060000	0.4196319600689998
H	0.9950401497629998	0.8438674732489998	0.4474080752459999
H	0.6029880772179999	0.3431059717689999	0.4214291972599998
H	0.0184696840760000	0.7411271625019998	0.4924266026899998
C	0.9635495167779999	0.6337698162369999	0.3708356324429997
C	0.4605371686339999	0.4997182589049998	0.3826194661009998
C	0.3625621626250000	0.4913796522289999	0.3877068608499999
C	0.3283832571660000	0.3008998028650000	0.3873199821729998
C	0.6660148402849999	0.5001203098129999	0.3879144588549999
C	0.4253421719749999	0.3089730979890000	0.3882937755089999
C	0.4939429834369999	0.4072766741320000	0.3889824421219998
C	0.2938751969000000	0.3917393090590000	0.3902700581999999
C	0.5893339572959999	0.4084099768510000	0.3972190430659999
C	0.0141291246790001	0.7714986385469999	0.4456317337799998
O	0.0437445188460000	0.6152544206679999	0.3763980170199998
O	0.9399893574449998	0.7006463347109999	0.4113199711259998
Ru	0.1407055901600000	0.1380862835039999	0.0000000000000000
Ru	0.4740389234930003	0.1380862835039999	0.0000000000000000
Ru	0.8073722568259998	0.1380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568260009	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.5380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.5380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234930000	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901599998	0.9380862835039996	0.0000000000000000

Ru	0.4740389234929998	0.9380862835039996	0.0000000000000000
Ru	0.8073722568259998	0.9380862835039996	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862569995	0.1920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569995	0.3920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195900000	0.7920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439996	0.0159535054490000
Ru	0.6535171862569995	0.9920708306439996	0.0159535054490000
Ru	0.9868505195899999	0.9920708306439996	0.0159535054490000
Ru	0.2186901232589999	0.0615218340179999	0.0955531191690000
Ru	0.5520234565919998	0.0615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.0615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249997	0.4615218340180000	0.0955531191690000
Ru	0.2186901232589999	0.6615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340179999	0.0955531191690000
Ru	0.8853567899249999	0.6615218340179999	0.0955531191690000
Ru	0.2186901232589999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899250000	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890002	0.1155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.1155063811579999	0.1115066246180000
Ru	0.7315017193559996	0.1155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193559996	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811579999	0.1115066246180000
Ru	0.7315017193559995	0.5155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.7155063811579999	0.1115066246180000
Ru	0.7315017193559995	0.7155063811579999	0.1115066246180000

Ru	0.0648350526890000	0.9155063811579998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559996	0.9155063811579998	0.1115066246180000
Ru	0.6309615284999999	0.5842235810920000	0.1917984884509999
Ru	0.6304473129929999	0.1853314624539998	0.1925689265709999
Ru	0.6311904204410002	0.7858928048559999	0.1926227586449999
Ru	0.6298595863260004	0.3850878493720000	0.1925338692729999
Ru	0.9634526574120002	0.1857356186309997	0.1929241372879999
Ru	0.9644323567289999	0.7854237458919998	0.1933883998519999
Ru	0.9638884700549999	0.3859766977099999	0.1932553027530000
Ru	0.9629144248359998	0.5841651778870000	0.1936174983740000
Ru	0.2975072529369999	0.7851422650639999	0.1923768827269999
Ru	0.6305935346350002	0.9852124394929998	0.1927357361359999
Ru	0.2975893674359998	0.5850930212729999	0.1927594891399999
Ru	0.9637861385290000	0.9852924745499998	0.1930392237659999
Ru	0.2975945210249997	0.9853070767479998	0.1928909581140000
Ru	0.2964313298540000	0.1846294008400000	0.1933143875150000
Ru	0.2963909145120000	0.3855228707309998	0.1941729539509999
Ru	0.4772309570639999	0.8387028382459998	0.2078893813149999
Ru	0.8106455898159999	0.0387560941359997	0.2078856102219999
Ru	0.4774091794769999	0.0385116097709999	0.2080559371950000
Ru	0.4753127409769999	0.4378061532069998	0.2081057181829999
Ru	0.1428519072419998	0.8385456485839997	0.2078747890619999
Ru	0.8101979669629997	0.2388247372839999	0.2085595983830000
Ru	0.1437564336840000	0.2397162282920000	0.2084620878839999
Ru	0.4765356344039998	0.2393678763380000	0.2080496774890000
Ru	0.1438213654049998	0.6373828175309999	0.2084950890309999
Ru	0.8112017697249998	0.8380381519629997	0.2091702040050000
Ru	0.1422861382360000	0.4398558529399999	0.2094145603460000
Ru	0.8094267928569998	0.6385910246069999	0.2083537786649999
Ru	0.1436917162110000	0.0392126252279998	0.2086789589459999
Ru	0.4774868219599999	0.6368995034539999	0.2087382058409999
Ru	0.8083448157039999	0.4367866357759999	0.2068999249629998
Ru	0.3731320574720000	0.1051979645870000	0.2847733410880000
Ru	0.3734851930610000	0.7097006194419999	0.2854858074530000
Ru	0.7056000041139999	0.7104091149289998	0.2854934859399999
Ru	0.0384206959910000	0.3068906083740000	0.2857408266099998
Ru	0.7060201637159999	0.1080075262669999	0.2857803186589999
Ru	0.7058445020469998	0.3059053900179999	0.2854918658699999
Ru	0.3723752555039999	0.9073512866589999	0.2856942052909999
Ru	0.0381223583840000	0.1092875246999998	0.2859756577209998
Ru	0.0386230308089999	0.5073534435039999	0.2894095410719999
Ru	0.0413338826239999	0.7087616201119996	0.2855996982410000
Ru	0.7061522376130003	0.9085148612349998	0.2858699172119998

Ru	0.0393851069190001	0.9095645984989996	0.2859555272729998
Ru	0.3735083096660000	0.5096220389439999	0.2877828128000000
Ru	0.3679785213460000	0.3018689180479999	0.2871709872199999
Ru	0.7050215031209999	0.5076551832379997	0.2885287617859999
Ru	0.5551691531289997	0.1599793815499999	0.2983609061009999
Ru	0.5545732492900003	0.7652155591239997	0.2986491331029998
Ru	0.8825264694919996	0.5612703805789999	0.3007314430149999
Ru	0.2204491168409999	0.5666827565349999	0.2980378287659999
Ru	0.8851659574859999	0.3612451231559999	0.2990896412230000
Ru	0.8856255272559999	0.7648862608499998	0.2998076124130000
Ru	0.2226980512110000	0.7637285973129998	0.2978677150279999
Ru	0.2203955572709998	0.9609169355319995	0.2990633137689999
Ru	0.5542573062469998	0.9627505310309995	0.2992860578009999
Ru	0.8878531861309998	0.9637283281019999	0.2994239784459999
Ru	0.8866267905799996	0.1627627544650000	0.2995726708119999
Ru	0.2172221842279999	0.1546158717610000	0.2999837435150000
Ru	0.5557662497849999	0.5694122668049999	0.2998301792629999
Ru	0.5512698240469999	0.3585426761480000	0.3024291264159999
Ru	0.2161853228640000	0.3639145971050000	0.3026405199250000

Ru: Transition state for CH_3OCO and styrene coupling ($ArCHCH_2(COOMe)$)

(*E* = -1232.5635 eV, *ZPE* = 4.75357629249999 eV, *S***T* = 1.37493981256008 eV)

%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics

Direct

H	0.4976854605669999	0.5566786847319999	0.3997197298649999
H	0.4182028031130000	0.2257177761090000	0.4017339132579999
H	0.2567436795570000	0.2247048153470000	0.4038817967119999
H	0.3385956740259999	0.5548154391679999	0.4095281053999999
H	0.7582665057919997	0.8016384366609999	0.4338851136809999
H	0.8545686537859998	0.7506044436459999	0.4180567843690000
H	0.2192685332390000	0.3902937435909999	0.4220970487919999
H	0.5706864160379999	0.3077983401950000	0.4167769409350000
H	0.6222812429280000	0.5341514581799999	0.4436999745429998
H	0.7765919460119999	0.6966239034099999	0.4797902178559999
H	0.6917708126379998	0.4434826430459999	0.4534307156419998
C	0.7472642732019998	0.5704385697899999	0.3750639301439999
C	0.4480122336219999	0.4871769202449999	0.3811219403199999
C	0.3061487460619999	0.2960332876619999	0.3884975174279999
C	0.4008952376700000	0.2957727041889999	0.3880062319279999
C	0.3521050918609999	0.4869085073099999	0.3885737505429999
C	0.4745984360750000	0.3901651532079999	0.3871256095219999
C	0.2787292086870000	0.3906790241940000	0.3929232779259999
C	0.5666455272959999	0.3842010431469999	0.4028172051159999
C	0.7825104867679998	0.7325478480900000	0.4336326234049999
C	0.6410838426709999	0.4674404301949999	0.4252512099069999
O	0.7224532012039999	0.6631979975789999	0.3903800238619999
O	0.8259457985309998	0.5656997499249999	0.3959132838519999
Ru	0.1407055901600000	0.1380862835020000	0.0000000000000000
Ru	0.4740389234929999	0.1380862835040000	0.0000000000000000
Ru	0.8073722568269998	0.1380862835040000	0.0000000000000000
Ru	0.1407055901590000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568250000	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.5380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.5380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234919999	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.9380862835029999	0.0000000000000000

Ru	0.4740389234929999	0.9380862835029999	0.0000000000000000
Ru	0.8073722568249999	0.9380862835029999	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862559999	0.1920708306440000	0.0159535054490000
Ru	0.9868505195909998	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.3920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.7920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.9920708306429998	0.0159535054490000
Ru	0.9868505195889999	0.9920708306429998	0.0159535054490000
Ru	0.2186901232590000	0.0615218340180000	0.0955531191690000
Ru	0.5520234565929999	0.0615218340180000	0.0955531191690000
Ru	0.8853567899239998	0.0615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.4615218340180000	0.0955531191690000
Ru	0.2186901232600000	0.6615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340179999	0.0955531191690000
Ru	0.8853567899249999	0.6615218340179999	0.0955531191690000
Ru	0.2186901232589999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899249999	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890000	0.1155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.1155063811580000	0.1115066246180000
Ru	0.7315017193559998	0.1155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193549998	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811579999	0.1115066246180000
Ru	0.7315017193549999	0.5155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811590000	0.1115066246180000
Ru	0.3981683860229999	0.7155063811590000	0.1115066246180000
Ru	0.7315017193559997	0.7155063811590000	0.1115066246180000

Ru	0.0648350526890000	0.9155063811579998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559997	0.9155063811579998	0.1115066246180000
Ru	0.9629918920629998	0.5843235054819999	0.1918752951150000
Ru	0.9635482541999998	0.7844032472009999	0.1923283223310000
Ru	0.9630166385819999	0.1850844101240000	0.1926674019940000
Ru	0.9626786273089998	0.3854903180770000	0.1928351265590000
Ru	0.6301397740069998	0.3844765382440000	0.1907967363710000
Ru	0.9638047877309998	0.9849372194999999	0.1927148259210000
Ru	0.6304750745539999	0.1853365478869999	0.1924148207030000
Ru	0.6305624858779999	0.5844405159719999	0.1924003703799999
Ru	0.2965735721020000	0.5852126796209999	0.1932434364610000
Ru	0.2968470116109999	0.7844969890529999	0.1929760354600000
Ru	0.2973314038509999	0.9850507627729999	0.1930408811909999
Ru	0.6310222997419999	0.7849724673169999	0.1932259676170000
Ru	0.6303759967279998	0.9845584048159998	0.1930247189169999
Ru	0.2971110192859999	0.1848917991080000	0.1937720733319999
Ru	0.2962662936570000	0.3851296436440000	0.1937260967810000
Ru	0.1433927412650000	0.8386353169029998	0.2078019665209999
Ru	0.4770066724869999	0.0379459827120000	0.2083113278129999
Ru	0.8104700060669998	0.0383495420340000	0.2080310282220000
Ru	0.1437299374690000	0.2386464713989999	0.2079135582340000
Ru	0.4769728375699999	0.8378992784139999	0.2080305101079999
Ru	0.8097624897449999	0.2381812639090000	0.2082966277259999
Ru	0.8087695898049999	0.4396959321519999	0.2097425744320000
Ru	0.1425519945150000	0.6376606604639999	0.2083875171260000
Ru	0.8098957823829998	0.6374579308189999	0.2097340396160000
Ru	0.1442445893809999	0.4386072573769999	0.2080762149079999
Ru	0.4763558352520000	0.6366736010609999	0.2086377734909999
Ru	0.1438892542740000	0.0390467646870000	0.2085005110110000
Ru	0.4767511457490000	0.2389750573510000	0.2085505938470000
Ru	0.8090538571139999	0.8371867911039997	0.2087779562360000
Ru	0.4753680006679999	0.4375167692759999	0.2086645876469999
Ru	0.3733182332139999	0.1054083694180000	0.2850778595930000
Ru	0.0385584708410000	0.3078031655110000	0.2851819716649999
Ru	0.7060496665259998	0.3059580155170000	0.2855527744970000
Ru	0.0348318097950000	0.5063401978390000	0.2855969375460000
Ru	0.3715516493459999	0.7087844605909999	0.2856996442190000
Ru	0.7055786834689999	0.1075669039090000	0.2857907512610000
Ru	0.0379514219430000	0.7065006858229999	0.2854359756650000
Ru	0.3717365180829999	0.9067394485399999	0.2857795711530000
Ru	0.0397927025789999	0.9079452028269998	0.2857032747280000
Ru	0.0381779554290000	0.1081460238060000	0.2857429041180000
Ru	0.7060671350479999	0.9085382111489998	0.2859127490960000

Ru	0.7046368388129998	0.5083742535029999	0.2901076452470000
Ru	0.3704253879289999	0.3026351742939999	0.2875058076859999
Ru	0.7055875697050000	0.7094023836319999	0.2881439385439999
Ru	0.3711094827229999	0.5085530504719998	0.2886494810949999
Ru	0.8900904092669998	0.7659700021299999	0.2979954584299999
Ru	0.5525641019479999	0.7640696751369999	0.2987056300209999
Ru	0.5549621726139999	0.1597803296660000	0.2984615558140000
Ru	0.2162452128039999	0.5653570873200000	0.2988094301870000
Ru	0.8881518281580000	0.9629833277659999	0.2989642535579999
Ru	0.2194770959310000	0.7627206331279999	0.2989976638760000
Ru	0.2203178530139999	0.9615728050099998	0.2989407804709999
Ru	0.8870421399379997	0.1619475934490000	0.2991662198030000
Ru	0.8864835628719999	0.3594974367150000	0.2996461619490000
Ru	0.5520627405699999	0.5668080045209999	0.2995195502660000
Ru	0.5539465101319999	0.9622335074069999	0.2993609023730000
Ru	0.2165662732830000	0.1549871810140000	0.3000366058139999
Ru	0.2147738409690000	0.3623918480059999	0.3019255343039999
Ru	0.8864187692479999	0.5614093607390001	0.3061961995060000
Ru	0.5536421480359999	0.3611207909349999	0.3012220327210000

Ru: Final state for CH_3OCO and styrene coupling ($ArCHCH_2(COOMe)$)

(*E* = -1233.3688 eV, *ZPE* = 4.82974809549999 eV, *S***T* = 1.31179512432938 eV)

%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics

Direct

H	0.8672660413499999	0.7123294936919999	0.3909338863569999
H	0.4920467039129999	0.5607492965249999	0.3997887434890000
H	0.4265832059179999	0.2298413362150000	0.4017344666950000
H	0.8021114965059999	0.8009037073829999	0.4167180828859999
H	0.2633783329420000	0.2202884487719999	0.4026122623299999
H	0.3317886646239999	0.5502533470289999	0.4093188131659999
H	0.2186997211610000	0.3813401790479999	0.4220643937569999
H	0.5768177233920000	0.3242089746569999	0.4238614036119998
H	0.8110882955419999	0.6929190910769999	0.4639446487759999
H	0.6043000295079999	0.5455175750729999	0.4457080277969999
H	0.6777168409739998	0.4691523390959999	0.4663357168059999
C	0.7118086038449999	0.5504122054960000	0.3808322473969999
C	0.4454908798659999	0.4892467248599999	0.3815086623339999
C	0.3104909127880000	0.2934022875269999	0.3873830585939999
C	0.4064393934349999	0.2981228027810000	0.3878629872059999
C	0.3484718085519999	0.4840517065719999	0.3883605975409999
C	0.4768943790410000	0.3953581645390000	0.3885344920799999
C	0.2784286103140000	0.3853706573660000	0.3923302999350000
C	0.8049133583399999	0.7211090267529999	0.4166236299599999
C	0.5704462991329999	0.3956100700790000	0.4030192398290000
C	0.6399126461310000	0.4910409607549999	0.4271811416210000
O	0.7213642587839999	0.6628731484769999	0.3877493152429999
O	0.7910671080109999	0.5254447202639999	0.3790011900510000
Ru	0.1407055901600000	0.1380862835040000	0.0000000000000000
Ru	0.4740389234929999	0.1380862835040000	0.0000000000000000
Ru	0.8073722568259998	0.1380862835040000	0.0000000000000000
Ru	0.1407055901600000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.5380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.5380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.9380862835039999	0.0000000000000000

Ru	0.4740389234929999	0.9380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.9380862835039999	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.1920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.3920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.7920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.9920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.9920708306439999	0.0159535054490000
Ru	0.2186901232590000	0.0615218340180000	0.0955531191690000
Ru	0.5520234565919998	0.0615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.0615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.4615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.6615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340179999	0.0955531191690000
Ru	0.8853567899249999	0.6615218340179999	0.0955531191690000
Ru	0.2186901232589999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899249999	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890000	0.1155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.1155063811580000	0.1115066246180000
Ru	0.7315017193559998	0.1155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193559997	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.5155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.7155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.7155063811579999	0.1115066246180000

Ru	0.0648350526890000	0.9155063811579998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559997	0.9155063811579998	0.1115066246180000
Ru	0.9630914751089997	0.5845889784419999	0.1918129469190000
Ru	0.9633322800709998	0.7848265802049999	0.1921888467229999
Ru	0.9630998845699998	0.1847925152630000	0.1926411118799999
Ru	0.9634638788629999	0.3852260734310000	0.1925938551069999
Ru	0.6303255673879999	0.3849607896550000	0.1924191744390000
Ru	0.9639465498029998	0.9849105143959998	0.1927218652719999
Ru	0.6303935749119998	0.1859241388050000	0.1927931327350000
Ru	0.6308560565859998	0.5847251676710000	0.1928463572159999
Ru	0.2965804649099999	0.5850891664329999	0.1929527068090000
Ru	0.2968231439510000	0.7846764645069999	0.1929246434640000
Ru	0.2969718985479999	0.9847936336779999	0.1929526117990000
Ru	0.6306348885119999	0.7848480562239999	0.1931306314300000
Ru	0.6302586477520000	0.9847128348439999	0.1930215219950000
Ru	0.2966603448430000	0.1846718323040000	0.1936076847260000
Ru	0.2962486670119999	0.3851608712060000	0.1936912134930000
Ru	0.1430387631510000	0.8384221897059999	0.2079220606889999
Ru	0.4769374959259999	0.0380985402230000	0.2080724200630000
Ru	0.8103007205089999	0.0380461255930000	0.2081103269990000
Ru	0.1435473562420000	0.2386814388450000	0.2079671229939999
Ru	0.4769446660239999	0.8381803728069999	0.2081717137510000
Ru	0.8101468544789998	0.2380852026010000	0.2081775787319999
Ru	0.8097814416909999	0.4384621698919999	0.2083645162080000
Ru	0.1429559586840000	0.6377957906739999	0.2083047032680000
Ru	0.8105308613209999	0.6385768155070000	0.2081570598820000
Ru	0.1434215857960000	0.4386328759220000	0.2084843524789999
Ru	0.4761897539840000	0.6367873777979999	0.2085747555610000
Ru	0.1435804617450000	0.0388340109350000	0.2085477918649999
Ru	0.4764590503880000	0.2395709643600000	0.2085510386049999
Ru	0.8086856852759999	0.8374334214319998	0.2088790791010000
Ru	0.4753383332059999	0.4374219572629999	0.2090594367580000
Ru	0.3730834771250000	0.1050856317240000	0.2848862315979999
Ru	0.0382736990510000	0.3071884849029999	0.2853835060550000
Ru	0.7049870411039998	0.3057657561179999	0.2856130916509999
Ru	0.0367641401060000	0.5060169632680001	0.2854924533170000
Ru	0.3715011820119999	0.7088225785069999	0.2856164572600000
Ru	0.7052875623260000	0.1073921206870000	0.2856268335230000
Ru	0.0377788306920000	0.7061550751089999	0.2854990587890000
Ru	0.3716800123580000	0.9064846429729999	0.2857736523850000
Ru	0.0396589883180000	0.9078706512409999	0.2858011121249999
Ru	0.0380484781450000	0.1075503982410000	0.2858001521390000
Ru	0.7053500237399999	0.9083128353739999	0.2861089938990000

Ru	0.7043164606259998	0.5092217851929999	0.2860803095680000
Ru	0.3690399951769999	0.3019143458210000	0.2873665482750000
Ru	0.7056106397219999	0.7079716424709999	0.2876852622500000
Ru	0.3704083552219999	0.5081461629279999	0.2886120310309999
Ru	0.8890454106989999	0.7650461132879999	0.2982544155619999
Ru	0.5523806735159998	0.7639781309020000	0.2986482482660000
Ru	0.5544637777509999	0.1602415109050000	0.2987125239160000
Ru	0.2167436166280000	0.5654819539659999	0.2988102209119999
Ru	0.8877280706119999	0.9632244584149999	0.2987950253680000
Ru	0.2194641091480000	0.7625170030080000	0.2991030048459999
Ru	0.2202463947220000	0.9609616635869999	0.2990565819850000
Ru	0.8867309640489998	0.1614599722230000	0.2991260140840000
Ru	0.8861307873929999	0.3595433576020000	0.2990568395789999
Ru	0.5508552590349999	0.5663785166639999	0.2992955292680000
Ru	0.5536545046910000	0.9626580078919999	0.2994827948400000
Ru	0.2167107642530000	0.1549284210250000	0.2999746400020000
Ru	0.2142982486030000	0.3617221826059999	0.3016841145099999
Ru	0.8887304095879999	0.5628104411759999	0.3034076021900000
Ru	0.5530499474249999	0.3612449547790000	0.3035560225980000

Ru: Transition state for CH_3OCO and styrene coupling ($ArCH(COOMe)CH_2$)
(*E* = -1232.2169 eV, *ZPE* = 4.723855364 eV, *S***T* = 1.20922192450227 eV)
%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics
Direct

H	0.7674982532439999	0.1594109702380000	0.3897159908860000
H	0.7701682778489999	0.4821863344299999	0.4037721012789999
H	0.4204144690720000	0.6143471147760000	0.4040817334119999
H	0.8558992661419999	0.2547668824720000	0.4285492236169999
H	0.2873762704640000	0.4658747205629999	0.4073111996109999
H	0.7007233807460001	0.5704575559100000	0.4066701151959999
H	0.4593148854649999	0.2634029184610000	0.4104763374549999
H	0.3068064923659999	0.2913606575139999	0.4107794111999999
H	0.5714983822229999	0.5864631249519999	0.4230379039869999
H	0.6302732056050000	0.3673513405439999	0.4479470990589999
H	0.7428606198819999	0.2110122131980000	0.4626190831859998
C	0.6405554691649998	0.2807884157139999	0.3700877791769999
C	0.3502537916049999	0.4543290141479999	0.3869720975920000
C	0.7056422338179998	0.4965016626209999	0.3883805562209999
C	0.3612356409499999	0.3497657809190000	0.3879779100499999
C	0.4303527396910000	0.5408073985509999	0.3900353801109999
C	0.4529850366620000	0.3364380636820000	0.3926375725299999
C	0.5326059767379999	0.4247431252719999	0.3958166121610000
C	0.5218399673569999	0.5285467869310000	0.3963604921319999
C	0.6250847316209999	0.4097958806299999	0.4051352448849999
C	0.7817144476549999	0.2299888219450000	0.4190209593719999
O	0.7583785314289999	0.3126408470390000	0.3877257532809999
O	0.5970120500409999	0.2015789598500000	0.3987486005829999
Ru	0.1407055901600000	0.1380862835040000	0.0000000000000000
Ru	0.4740389234929999	0.1380862835040000	0.0000000000000000
Ru	0.8073722568239999	0.1380862835040000	0.0000000000000000
Ru	0.1407055901580000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568250009	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835049999	0.0000000000000000
Ru	0.4740389234929998	0.5380862835049999	0.0000000000000000
Ru	0.8073722568279997	0.5380862835049999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.9380862835039999	0.0000000000000000

Ru	0.4740389234929999	0.9380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.9380862835039999	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.1920708306440000	0.0159535054490000
Ru	0.9868505195869998	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.3920708306440000	0.0159535054490000
Ru	0.9868505195889999	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306449998	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195919998	0.7920708306419999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.9920708306439999	0.0159535054490000
Ru	0.9868505195889999	0.9920708306439999	0.0159535054490000
Ru	0.2186901232590000	0.0615218340179999	0.0955531191690000
Ru	0.5520234565919998	0.0615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.0615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.4615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.6615218340169999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340169999	0.0955531191690000
Ru	0.8853567899240009	0.6615218340169999	0.0955531191690000
Ru	0.2186901232599999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899249999	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890003	0.1155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.1155063811580000	0.1115066246180000
Ru	0.7315017193540009	0.1155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193549998	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811589999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811589999	0.1115066246180000
Ru	0.7315017193559997	0.5155063811589999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.7155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.7155063811579999	0.1115066246180000

Ru	0.0648350526890000	0.9155063811579998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559997	0.9155063811579998	0.1115066246180000
Ru	0.6306717783939999	0.5840246117299999	0.1917546969270000
Ru	0.9626506622139988	0.3847103608310000	0.1924115238030000
Ru	0.6310329452019998	0.3853622020979999	0.1933404874749999
Ru	0.6308194823189999	0.7844848189509998	0.1926012244580000
Ru	0.9636587571209998	0.7849933753809999	0.1926423539100000
Ru	0.6299660691679998	0.9845462998989999	0.1924608833000000
Ru	0.9637745929619999	0.5851846075949999	0.1927770299050000
Ru	0.9638639603469998	0.1849224932690000	0.1927180500440000
Ru	0.9639442848829999	0.9848517717449998	0.1928473952950000
Ru	0.2968020300599999	0.5850268800819999	0.1931041596840000
Ru	0.2967121448680000	0.7850078332839999	0.1931245634490000
Ru	0.2967345444439999	0.9850558970689999	0.1930940013670000
Ru	0.6304341470759998	0.1842617330270000	0.1930572225330000
Ru	0.2975863865669999	0.1858034957449999	0.1932342148329999
Ru	0.2976359273640000	0.3850149555540000	0.1937831071199999
Ru	0.8108442832509998	0.2376283873970000	0.2072574110030000
Ru	0.1429986802459999	0.8386960416349999	0.2079779112580000
Ru	0.4764768615039999	0.8384384787649999	0.2077790311319999
Ru	0.8103505873709997	0.8385154747969998	0.2082284168290000
Ru	0.8104385745959998	0.0373422278110001	0.2078430807500000
Ru	0.1438388349180000	0.0398460529419997	0.2084568778710000
Ru	0.1431848808060000	0.6380300075549998	0.2081091300400000
Ru	0.1437445135670000	0.4379436260530000	0.2083857482020000
Ru	0.8088920124109998	0.4389587518220000	0.2084641573200000
Ru	0.4770712927729999	0.0389430312910000	0.2086462221680000
Ru	0.4760453769169999	0.6371918141819999	0.2084470432680000
Ru	0.1438322038950000	0.2393838935270000	0.2088184176719999
Ru	0.4771479355779999	0.2390105332100000	0.2093840022119999
Ru	0.8086921919669999	0.6369727047049999	0.2086873296610000
Ru	0.4776563407939999	0.4386973951790000	0.2098331523929999
Ru	0.3715957688529999	0.7091847086199999	0.2852014633919999
Ru	0.7055486238609998	0.1034122823850000	0.2839301887590000
Ru	0.7043882770080009	0.3026770104729999	0.2853844053430000
Ru	0.3707056327789999	0.1059983739860000	0.2857244195060000
Ru	0.0370635585279999	0.3065897573099999	0.2855296060529999
Ru	0.7058034815459999	0.9061552255719999	0.2855685009560000
Ru	0.0386192746400000	0.9074173564019998	0.2858099919870000
Ru	0.0391359949240002	0.7080250097180000	0.2858090464129999
Ru	0.0384096762170001	0.5067984018579999	0.2857146115549999
Ru	0.3711147040599999	0.9074231250709998	0.2858041946939999
Ru	0.0383509666530000	0.1073322252510000	0.2861451827159999

Ru	0.7058288481669999	0.7087502887540000	0.2858922551820000
Ru	0.7077877633410000	0.5100449991180001	0.2882448932680000
Ru	0.3717650966229999	0.3078875712069999	0.2890388424270000
Ru	0.3689461458300000	0.5073239362629999	0.2886717058300000
Ru	0.8880240454889998	0.3624541255059999	0.2992388089009999
Ru	0.5545480602499999	0.7638110043039998	0.2981310709029999
Ru	0.8886382633799999	0.5628711163639999	0.2986212737969999
Ru	0.5534207367199999	0.9589291894249999	0.2986869905149999
Ru	0.2169937771000000	0.5656098259839999	0.2990005742649999
Ru	0.2182307485470000	0.1584995855660000	0.2990477300159999
Ru	0.8869698224499998	0.1613169362580000	0.2985417828970000
Ru	0.8872474605679998	0.7621517274170000	0.2989982628310000
Ru	0.2198145751610000	0.7629577008989998	0.2993599357849999
Ru	0.2198437992750000	0.9614532387089998	0.2993485515879999
Ru	0.2148152731540000	0.3600963660009999	0.2996041542960000
Ru	0.8872916949020010	0.9616075576729999	0.2993361504209999
Ru	0.5507906736019999	0.5652853469689999	0.3002188003569999
Ru	0.5503060460759998	0.1534212872510000	0.3009474161160000
Ru	0.5553681210099999	0.3612030094059999	0.3073344234350000

Ru: Final state for CH_3OCO and styrene coupling ($ArCH(COOMe)CH_2$)

(E = -1233.1157 eV, ZPE = 4.837496119 eV, $S*T$ = 1.212619089 eV)

%BLOCK LATTICE_CART

15.122801570000000	0.000000000000000	0.000000000000000
-3.641814920000000	13.056846300000004	0.000000000000000
0.000000000000000	0.000000000000000	21.508856710000003

Selective dynamics

Direct

H	0.7642111501679998	0.1526705153350000	0.3928854871540000
H	0.7884317254579999	0.4847883960470000	0.3987092787670000
H	0.4410738192719999	0.6046189678269999	0.4065400991429999
H	0.4716122900409999	0.2506629967810000	0.4049948840579999
H	0.8542655704909998	0.2387913437610000	0.4362507172189999
H	0.3051121848930000	0.4594174994449999	0.4093616700520000
H	0.7131667818599999	0.5635398255509999	0.4079647392210000
H	0.3219449043879999	0.2841803700339999	0.4108916295969999
H	0.5894318850359999	0.5726058378459999	0.4214981631870000
H	0.7403776206829997	0.1929644914960000	0.4693593908849999
H	0.6512186953279999	0.3915071924819999	0.4618341506409999
C	0.6674027865769999	0.3003024181730000	0.3828946789809999
C	0.3663312177529999	0.4469081056809999	0.3872107552860000
C	0.7196911374299999	0.4923487609230000	0.3866543380469999
C	0.3763991824839999	0.3423618591700000	0.3879569077529999
C	0.4486605779469999	0.5310991807780000	0.3904979654560000
C	0.4677827179899999	0.3265113651770000	0.3910142339409999
C	0.5504833446039998	0.4099324629200000	0.3936262574189999
C	0.5387680539789999	0.5143729603659999	0.3958029153389999
C	0.7802879636929999	0.2171705850639999	0.4267472540779999
C	0.6458972610719999	0.3979346554920000	0.4104300190960000
O	0.7617001191989999	0.3072653255100000	0.4013975911989999
O	0.6081114879440001	0.2083301045190000	0.3913076075060000
Ru	0.1407055901600000	0.1380862835040000	0.0000000000000000
Ru	0.4740389234929999	0.1380862835040000	0.0000000000000000
Ru	0.8073722568259998	0.1380862835040000	0.0000000000000000
Ru	0.1407055901600000	0.3380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.3380862835039999	0.0000000000000000
Ru	0.8073722568260010	0.3380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.5380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.5380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.5380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.7380862835039999	0.0000000000000000
Ru	0.4740389234929999	0.7380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.7380862835039999	0.0000000000000000
Ru	0.1407055901600000	0.9380862835039999	0.0000000000000000

Ru	0.4740389234929999	0.9380862835039999	0.0000000000000000
Ru	0.8073722568259999	0.9380862835039999	0.0000000000000000
Ru	0.3201838529239999	0.1920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.1920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.1920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.3920708306440000	0.0159535054490000
Ru	0.6535171862569997	0.3920708306440000	0.0159535054490000
Ru	0.9868505195899998	0.3920708306440000	0.0159535054490000
Ru	0.3201838529239999	0.5920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.5920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.5920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.7920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.7920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.7920708306439999	0.0159535054490000
Ru	0.3201838529239999	0.9920708306439999	0.0159535054490000
Ru	0.6535171862569997	0.9920708306439999	0.0159535054490000
Ru	0.9868505195899999	0.9920708306439999	0.0159535054490000
Ru	0.2186901232590000	0.0615218340179999	0.0955531191690000
Ru	0.5520234565919998	0.0615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.0615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.2615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.2615218340179999	0.0955531191690000
Ru	0.8853567899249998	0.2615218340179999	0.0955531191690000
Ru	0.2186901232590000	0.4615218340180000	0.0955531191690000
Ru	0.5520234565919999	0.4615218340180000	0.0955531191690000
Ru	0.8853567899249998	0.4615218340180000	0.0955531191690000
Ru	0.2186901232590000	0.6615218340179999	0.0955531191690000
Ru	0.5520234565919999	0.6615218340179999	0.0955531191690000
Ru	0.8853567899249999	0.6615218340179999	0.0955531191690000
Ru	0.2186901232589999	0.8615218340179998	0.0955531191690000
Ru	0.5520234565919999	0.8615218340179998	0.0955531191690000
Ru	0.8853567899249999	0.8615218340179998	0.0955531191690000
Ru	0.0648350526890003	0.1155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.1155063811580000	0.1115066246180000
Ru	0.7315017193559998	0.1155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.3155063811580000	0.1115066246180000
Ru	0.3981683860229999	0.3155063811580000	0.1115066246180000
Ru	0.7315017193559997	0.3155063811580000	0.1115066246180000
Ru	0.0648350526890000	0.5155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.5155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.5155063811579999	0.1115066246180000
Ru	0.0648350526890000	0.7155063811579999	0.1115066246180000
Ru	0.3981683860229999	0.7155063811579999	0.1115066246180000
Ru	0.7315017193559997	0.7155063811579999	0.1115066246180000

Ru	0.0648350526890000	0.9155063811579998	0.1115066246180000
Ru	0.3981683860229999	0.9155063811579998	0.1115066246180000
Ru	0.7315017193559997	0.9155063811579998	0.1115066246180000
Ru	0.6305296428339999	0.5860802886089999	0.1916543026039999
Ru	0.6307293947479999	0.3860504162210000	0.1916151727809999
Ru	0.9626414673119998	0.3850544378490000	0.1927487495209999
Ru	0.9636045703569998	0.1852512512480000	0.1926965429310000
Ru	0.9635928919569998	0.7852078411399999	0.1926987534730000
Ru	0.9636036823200009	0.5853790765619998	0.1929174986780000
Ru	0.6306100216009999	0.7848934754949999	0.1927460794099999
Ru	0.2965566102209999	0.1848769427040000	0.1927171689630000
Ru	0.9633884338269998	0.9848899962179998	0.1927896893590000
Ru	0.6300134310269989	0.9853720291309999	0.1927168608450000
Ru	0.2968537831120000	0.5849123883109999	0.1931245940740000
Ru	0.2968019717100000	0.7849674746599999	0.1930474393319999
Ru	0.2967608907009999	0.9851038114999998	0.1930667271879999
Ru	0.6299034146819998	0.1848730072940000	0.1939366509670000
Ru	0.2970740887350000	0.3852287612399999	0.1939732224260000
Ru	0.8095270200879999	0.2387092395220000	0.2080152043019999
Ru	0.1430427840660000	0.8386469904499998	0.2079134136570000
Ru	0.4769452915419999	0.4397141564699999	0.2082276642160000
Ru	0.8099805158359998	0.8386363836629999	0.2082405100399999
Ru	0.4766249290089999	0.8388648547029999	0.2082126476589999
Ru	0.1434371935760000	0.0393799771009999	0.2082789113279999
Ru	0.8099446117259999	0.0383821917000000	0.2081519593639999
Ru	0.4757626952569999	0.2381925401580000	0.2083842604690000
Ru	0.1435152378320000	0.4381794324789999	0.2083616814900000
Ru	0.1430748394420000	0.6377818803939999	0.2084545193769999
Ru	0.4756419270489999	0.6381638557629999	0.2081944112309999
Ru	0.4774607704449999	0.0396486955440001	0.2087690543080000
Ru	0.1436975059610000	0.2390721437760000	0.2086391411480000
Ru	0.8078091973849999	0.4384699374959999	0.2086370196500000
Ru	0.8084408346640000	0.6375454380469999	0.2089274395809999
Ru	0.0376185521270001	0.3067911432129999	0.2853734475479999
Ru	0.3716536922829999	0.7087273515460000	0.2856876382119999
Ru	0.3716217288190000	0.1052051926120000	0.2854995746469999
Ru	0.0388198453720001	0.9078506290019998	0.2857992129699999
Ru	0.7061074870389998	0.9074957202839998	0.2856636905350000
Ru	0.7045872558929999	0.1051541382070000	0.2853756416420000
Ru	0.0391554773549998	0.7080167358019999	0.2858585996899999
Ru	0.3717998621990000	0.9081241031549998	0.2858112690719999
Ru	0.0381542529460002	0.1074039479850000	0.2858729704910000
Ru	0.0385796855879998	0.5070844232979999	0.2859732954570000
Ru	0.7033220765820007	0.3098848639899999	0.2859436756429999

Ru	0.7058733867789998	0.7093248966039999	0.2862915636969999
Ru	0.3712432859939999	0.3065604639100000	0.2878654876899999
Ru	0.7086059787189999	0.5091326356949999	0.2877675535289999
Ru	0.3706214618199999	0.5063274561569999	0.2891890204659999
Ru	0.8871937415499998	0.3617712774299999	0.2991722854609999
Ru	0.5542417560959999	0.7645177973129999	0.2984271072540000
Ru	0.5536086133739999	0.9601542507119999	0.2989667236409999
Ru	0.2180344991440000	0.1580427703360000	0.2991972768589999
Ru	0.8866982048219999	0.1618682829930000	0.2983718143469999
Ru	0.8885144273849998	0.5622199406899999	0.2991643228699999
Ru	0.2183225105100000	0.5644687630209999	0.2992066243839999
Ru	0.8872659033819997	0.7626805653319999	0.2990975787280000
Ru	0.2202387714169999	0.7629786447789999	0.2991909648900000
Ru	0.2199194050829999	0.9610742156199997	0.2995224554209999
Ru	0.8871637553399998	0.9616196970399998	0.2994100319090000
Ru	0.2148256372030000	0.3598269837790000	0.2997377392719999
Ru	0.5495467777599998	0.3655518402859999	0.2972859994590000
Ru	0.5529461530389999	0.5655083189469999	0.3004718384460000
Ru	0.5519373803959999	0.1613382666690000	0.3038606979330000

Ru: Initial state for $ArCHCH_2(COOMe)$ and H coupling

(*E* =-1237.4959 eV, *ZPE* = 4.9937064535 eV, *S***T* = 1.33609087640458 eV)

AutoCreatByScript: H C O Ru

1.00000000000000

15.1228015700000000 0.0000000000000000 0.0000000000

-3.6418149199999998 13.0568463000000001 0.0000000000

0.0000000000000000 0.0000000000000000 21.5088567099

H C O Ru

12 10 2 120

Selective dynamics

Direct

0.6666138265156273	0.1951151045249037	0.3429124964540304
0.8674100082840033	0.7126795561022290	0.3920684668034318
0.4920844822971226	0.5607785913970814	0.3997483654015048
0.4265048176836859	0.2298154590889580	0.4016690107701538
0.2632277178532448	0.2203145425729222	0.4027263080670028
0.3317815831438304	0.5503449460564598	0.4093529930037179
0.8017536807472015	0.8005812818898945	0.4177844634850186
0.2185721029920077	0.3814440807209499	0.4220764173095368
0.5772912910587640	0.3243974232160673	0.4230107932014514
0.6044824315259725	0.5457085629323349	0.4461103783377282
0.8100140283596654	0.6921514283749175	0.4648274648473900
0.6777751002847776	0.4689472178213874	0.4662197254065907
0.7116213920024690	0.5508579923494671	0.3809504879605313
0.4453868662603959	0.4893014621857896	0.3815504727635518
0.3103857711340058	0.2934453876503130	0.3875918812874669
0.4063053957003127	0.2981293168559744	0.3879125745749268
0.3483979478414682	0.4841153800320493	0.3883968276626970
0.4767512562360353	0.3954029856043291	0.3885131292139260
0.2783654768033740	0.3854240703547488	0.3924252674620434
0.5704324477358310	0.3960078000135012	0.4027365995394079
0.8047592457621701	0.7208428714452465	0.4175148962587667
0.6398543335242431	0.4912469919713737	0.4272520012606923
0.7904384193375502	0.5248740212350794	0.3784798535792607
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0.5527921050890148	0.3626390727644229	0.3031771182805014

Ru: Transition state state for $ArCHCH_2(COOMe)$ and H coupling
(*E* = -1237.004 eV, *ZPE* = 5.0258615655 eV, *S***T* = 1.28862685461328 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
12 10 2 120
Selective dynamics
Direct
0.6393097619770505 0.3455794858785999 0.3600149103892133
0.8578294415668877 0.7390253588494737 0.4026593080875795
0.4117029513341333 0.6121286651524416 0.4040830010171985
0.2736957242100588 0.4695183554524599 0.4049608730943285
0.4348659621339569 0.2552625125845871 0.4073480206111054
0.2854895774824384 0.2908132254533235 0.4083829136999939
0.7668927476365945 0.7932954979057749 0.4273882701509037
0.5601004238813656 0.5760847623370380 0.4221127531334937
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0.7944579537209330 0.6908032181373694 0.4711513507216247
0.7319345674442059 0.4347993085442019 0.4520916839117884
0.7375679581857406 0.5453888213868842 0.3815958170938739
0.3359042140141947 0.4545762379766207 0.3855007787324828
0.3418284644539963 0.3478926019856082 0.3862035200560235
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0.5141378914448027 0.4141047184126441 0.3952845492744582
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0.5475304549512598	0.5639071754924136	0.3010218092293143	
0.5532165885010942	0.3597013665699707	0.3069090388678960	

Ru: Final state state for $ArCHCH_2(COOMe)$ and H coupling
(*E* = -1237.0545 eV, *ZPE* = 5.09127748449999 eV, *S***T* = 1.34305989312597 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
12 10 2 120
Selective dynamics
Direct
0.6081270519746418 0.3505095033746178 0.3849864470378817
0.8661942620550864 0.7121191881081281 0.3935329330269666
0.4927167834949224 0.5645857234333767 0.3994556170134839
0.4280933217860673 0.2335604703478419 0.4018573335739388
0.2656003525501275 0.2228147004809659 0.4025726179533635
0.3319897249026914 0.5523133673596795 0.4090815504183398
0.8001366414043374 0.7993469190134294 0.4192100360385057
0.2198782397701460 0.3831365813696712 0.4221672638429747
0.6064514976180664 0.5536156858908167 0.4514221386289752
0.5555500297710371 0.3457768302019587 0.4562719189515862
0.8061118092275138 0.6893469658836506 0.4655815338349479
0.6830449639484271 0.4807603141006503 0.4716935822223457
0.7076949485851842 0.5508656284809756 0.3822546751943277
0.4466985841064234 0.4926666360142785 0.3812945447688754
0.3119821963815840 0.2959715781526186 0.3868147287030623
0.4083648887171919 0.3017372538913271 0.3872046804767589
0.3491791204476409 0.4863845644845112 0.3880955008916336
0.4790839656749829 0.3993362678410793 0.3866723153991256
0.2794401653356548 0.3875625644533383 0.3921791931516074
0.5699747085427540 0.3978347336803904 0.4159130742115664
0.8030484321513294 0.7195979420590960 0.4184148406276897
0.6409101046959074 0.4978419518995133 0.4334280649823858
0.7853267740689169 0.5219386748268758 0.3775933638288957
0.7205742162328695 0.6631094044901379 0.3872646791926840
0.1407055901600031 0.1380862835040000 0.0000000000000000
0.4740389234929976 0.1380862835040000 0.0000000000000000
0.8073722568259991 0.1380862835040000 0.0000000000000000
0.1407055901600030 0.3380862835039917 0.0000000000000000
0.4740389234929968 0.3380862835039917 0.0000000000000000
0.8073722568259991 0.3380862835039917 0.0000000000000000
0.1407055901600029 0.5380862835039926 0.0000000000000000
0.4740389234929976 0.5380862835039926 0.0000000000000000
0.8073722568259993 0.5380862835039926 0.0000000000000000

0.1407055901600020	0.7380862835039907	0.0000000000000000
0.4740389234929979	0.7380862835039907	0.0000000000000000
0.8073722568259991	0.7380862835039907	0.0000000000000000
0.1407055901600017	0.9380862835039834	0.0000000000000000
0.4740389234929964	0.9380862835039834	0.0000000000000000
0.8073722568259988	0.9380862835039834	0.0000000000000000
0.3201838529240039	0.1920708306439959	0.0159535054489979
0.6535171862569976	0.1920708306439959	0.0159535054489979
0.9868505195899991	0.1920708306439959	0.0159535054489979
0.3201838529240035	0.3920708306439959	0.0159535054489979
0.6535171862569981	0.3920708306439959	0.0159535054489979
0.9868505195900008	0.3920708306439959	0.0159535054489979
0.3201838529240035	0.5920708306439887	0.0159535054489979
0.6535171862569977	0.5920708306439887	0.0159535054489979
0.9868505195899988	0.5920708306439887	0.0159535054489979
0.3201838529240035	0.7920708306439878	0.0159535054489979
0.6535171862569977	0.7920708306439878	0.0159535054489979
0.9868505195900009	0.7920708306439878	0.0159535054489979
0.3201838529240028	0.9920708306439862	0.0159535054489979
0.6535171862569978	0.9920708306439862	0.0159535054489979
0.9868505195900009	0.9920708306439862	0.0159535054489979
0.2186901232590020	0.0615218340180011	0.0955531191689971
0.5520234565920040	0.0615218340180011	0.0955531191689971
0.8853567899249992	0.0615218340180011	0.0955531191689971
0.2186901232590017	0.2615218340179939	0.0955531191689971
0.5520234565920039	0.2615218340179939	0.0955531191689971
0.8853567899249992	0.2615218340179939	0.0955531191689971
0.2186901232590017	0.4615218340179942	0.0955531191689971
0.5520234565920040	0.4615218340179942	0.0955531191689971
0.8853567899249994	0.4615218340179942	0.0955531191689971
0.2186901232590009	0.6615218340179913	0.0955531191689971
0.5520234565920039	0.6615218340179913	0.0955531191689971
0.8853567899249991	0.6615218340179913	0.0955531191689971
0.2186901232590008	0.8615218340179863	0.0955531191689971
0.5520234565920035	0.8615218340179863	0.0955531191689971
0.8853567899249959	0.8615218340179863	0.0955531191689971
0.0648350526889984	0.1155063811579976	0.1115066246180021
0.3981683860230021	0.1155063811579976	0.1115066246180021
0.7315017193559983	0.1155063811579976	0.1115066246180021
0.0648350526889978	0.3155063811579962	0.1115066246180021
0.3981683860230020	0.3155063811579962	0.1115066246180021
0.7315017193559979	0.3155063811579962	0.1115066246180021
0.0648350526889977	0.5155063811579899	0.1115066246180021
0.3981683860230019	0.5155063811579899	0.1115066246180021

0.7315017193559954	0.5155063811579899	0.1115066246180021
0.0648350526889973	0.7155063811579874	0.1115066246180021
0.3981683860230018	0.7155063811579874	0.1115066246180021
0.7315017193559961	0.7155063811579874	0.1115066246180021
0.0648350526889969	0.9155063811579812	0.1115066246180021
0.3981683860230018	0.9155063811579812	0.1115066246180021
0.7315017193559956	0.9155063811579812	0.1115066246180021
0.9630059972156535	0.5844663602720731	0.1919697254881338
0.9632531614147863	0.7847133107167844	0.1922316948278515
0.6303743986707857	0.3854040100488663	0.1926331186904188
0.9634391887734779	0.3853167940638696	0.1926395303448984
0.9631572247025129	0.1847506594918687	0.1926258085359761
0.6306202249434690	0.1855763234466113	0.1924949002495389
0.9639406586182804	0.9848778197691896	0.1927172007067399
0.6308648926428864	0.5841792875234905	0.1928146762313848
0.2966043039859975	0.5851171783464509	0.1930494449617061
0.2968366421874627	0.7847118514447158	0.1928872860804677
0.2970241879274089	0.9849334826760373	0.1929894571856383
0.6302300933325530	0.9844946819725218	0.1929396261974872
0.6307740083149134	0.7847117016012712	0.1930052540798657
0.2968663026027313	0.1847168063730345	0.1934578699648607
0.2962683396353537	0.3852415858044251	0.1936435840589323
0.1436118949910796	0.2386100227803515	0.2080325189922415
0.1429942554397087	0.8385245213883263	0.2079233608479724
0.4769353065367021	0.0381505218750677	0.2079636410936149
0.8105045183755004	0.0380062019792155	0.2081194138567377
0.8102909427356956	0.2378755877955703	0.2081849879171866
0.8104248104684297	0.6379622288336092	0.2084210728308577
0.4769763774714498	0.8379576722958224	0.2081098608677723
0.8099299159222507	0.4384121352878961	0.2083966817364442
0.1431920576355918	0.6380439744885866	0.2082659049159413
0.1432449803824098	0.4385447833900807	0.2084460869482334
0.1436321852649654	0.0389415060853653	0.2085536445712279
0.4773777605506826	0.2397635689673707	0.2092996976656656
0.4764363664789987	0.6368099526470502	0.2085713888683637
0.8087820940246495	0.8372085076566143	0.2088477581769249
0.4756099445636692	0.4374548313024135	0.2090595620286307
0.3724914359970181	0.1050464319851586	0.2851052703435375
0.0382390161841331	0.3072760612527470	0.2853513911254103
0.0368783228781847	0.5060786033843284	0.2856181788603169
0.0377693839032094	0.7061080302260654	0.2856013970586472
0.7052891762991506	0.1067448686961361	0.2854699295306329
0.7046758406484099	0.3045809257947202	0.2847199237515345
0.3715406167125622	0.7089563914186511	0.2855726386974809

0.3718405738652394	0.9067532926206695	0.2856303756693785
0.0379656849829329	0.1074472171442862	0.2858321240777840
0.0396456546456768	0.9078128601705309	0.2857998349241027
0.7032266263536797	0.5079606841017628	0.2874353164824673
0.7054126492988839	0.9079048516128524	0.2860572607457834
0.3681476436003241	0.3020908470973728	0.2872595724280556
0.7058106547902550	0.7080609633026762	0.2875248775572788
0.3704625403609493	0.5086637453622203	0.2883277734186719
0.8892378306625766	0.7648844106721450	0.2981755358724524
0.5525026795100983	0.7635984303424893	0.2984568764538498
0.5542254032982743	0.1585914073708022	0.2985663865957631
0.8876982715481359	0.9630774939886569	0.2989026759591547
0.2166970803018434	0.5657475746923391	0.2988752974614935
0.8865502482915356	0.3598296284784163	0.2991393536662285
0.2200638386915456	0.9607027995709946	0.2991403897177925
0.8867779841287906	0.1614593359202510	0.2992744682390847
0.2195336454854422	0.7627354959583471	0.2990743064496603
0.5511077986364152	0.5659372973733837	0.2996490784885767
0.5537241408836330	0.9618173582379539	0.2994234863219685
0.2167400822377322	0.1552327228283158	0.2998221441103499
0.2143121383297426	0.3623252676107231	0.3017103018476909
0.8888771616854652	0.5629351363514113	0.3029278349417504
0.5510697570906099	0.3577581488735638	0.3050423409491831

Ru: Initial state state for ArCH(COOMe)CH_2 and H coupling
(*E* -1236.7738 eV, *ZPE* = 4.9261704885 eV, *S***T* = 1.38575945360879 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
12 10 2 120
Selective dynamics
Direct

0.7990144712016302	0.6351523013640409	0.3238557790921574
0.4759096376109092	0.5462312942130567	0.4027038635777714
0.6860557669081382	0.4833249901008155	0.3968001492509544
0.3866086988797925	0.2185758306815772	0.4041734054347191
0.3218762299178182	0.5563965996254282	0.4098515117415188
0.2265499483052785	0.2278234914066216	0.4117260998271420
0.1946783493372354	0.3978455820624315	0.4228320700323842
0.6030086445629108	0.5517530448558624	0.3969663600604055
0.6885503271801461	0.1670254075403162	0.4249526394937086
0.7834962318712346	0.2773733251606171	0.4397451548402171
0.5464853491891102	0.3863931788170200	0.4581708052285503
0.6783262083487228	0.2585281340404356	0.4835538521633130
0.4250893102632717	0.4801132384860465	0.3834523886399012
0.4472072244809463	0.3801142835698677	0.3843168444416548
0.3313600360457056	0.4853439410444726	0.3905489021896915
0.3716267332949449	0.2893351384502211	0.3893549324147179
0.5783747015689239	0.2892779187101822	0.3849467041558815
0.6166665723096759	0.4801973643324771	0.3794485229447452
0.2773453256351718	0.2958159447940792	0.3941519956278658
0.2562992959331996	0.3926150316453645	0.3981743756353912
0.5456837740903884	0.3835629664706275	0.4065320017576851
0.7085902402683438	0.2481796027514797	0.4383763164756480
0.6787557283336421	0.3105916755687345	0.3922818254775154
0.5333646123931122	0.1948724498180522	0.3971141747483283
0.1407055901600970	0.1380862835040199	0.0000000000000000
0.4740389234927777	0.1380862835040199	0.0000000000000000
0.8073722568255945	0.1380862835040199	0.0000000000000000
0.1407055901609501	0.3380862835039297	0.0000000000000000
0.4740389234927747	0.3380862835039297	0.0000000000000000
0.8073722568259011	0.3380862835039297	0.0000000000000000
0.1407055901599990	0.5380862835040792	0.0000000000000000
0.4740389234928012	0.5380862835040792	0.0000000000000000
0.8073722568260924	0.5380862835040792	0.0000000000000000

0.1407055901599334	0.7380862835032062	0.0000000000000000
0.4740389234930277	0.7380862835032062	0.0000000000000000
0.8073722568252162	0.7380862835032062	0.0000000000000000
0.1407055901597954	0.9380862835041772	0.0000000000000000
0.4740389234925578	0.9380862835041772	0.0000000000000000
0.8073722568266777	0.9380862835041772	0.0000000000000000
0.3201838529237411	0.1920708306439943	0.0159535054489979
0.6535171862582497	0.1920708306439943	0.0159535054489979
0.9868505195887536	0.1920708306439943	0.0159535054489979
0.3201838529240688	0.3920708306438155	0.0159535054489979
0.6535171862571523	0.3920708306438155	0.0159535054489979
0.9868505195900884	0.3920708306438155	0.0159535054489979
0.3201838529240035	0.5920708306435506	0.0159535054489979
0.6535171862569916	0.5920708306435506	0.0159535054489979
0.9868505195897481	0.5920708306435506	0.0159535054489979
0.3201838529237477	0.7920708306439772	0.0159535054489979
0.6535171862566179	0.7920708306439772	0.0159535054489979
0.9868505195900010	0.7920708306439772	0.0159535054489979
0.3201838529241964	0.9920708306452186	0.0159535054489979
0.6535171862564080	0.9920708306434328	0.0159535054489979
0.9868505195906592	0.9920708306434328	0.0159535054489979
0.2186901232588694	0.0615218340179681	0.0955531191689971
0.5520234565910362	0.0615218340179681	0.0955531191689971
0.8853567899250356	0.0615218340179681	0.0955531191689971
0.2186901232588606	0.2615218340180336	0.0955531191689971
0.5520234565923413	0.2615218340180336	0.0955531191689971
0.8853567899257324	0.2615218340180336	0.0955531191689971
0.2186901232591009	0.4615218340178255	0.0955531191689971
0.5520234565911807	0.4615218340178255	0.0955531191689971
0.8853567899255904	0.4615218340178255	0.0955531191689971
0.2186901232588392	0.6615218340178596	0.0955531191689971
0.5520234565908002	0.6615218340178596	0.0955531191689971
0.8853567899254560	0.6615218340178596	0.0955531191689971
0.2186901232580557	0.8615218340176555	0.0955531191689971
0.5520234565915989	0.8615218340176555	0.0955531191689971
0.8853567899250854	0.8615218340176555	0.0955531191689971
0.0648350526889985	0.1155063811578972	0.1115066246180021
0.3981683860227253	0.1155063811578972	0.1115066246180021
0.7315017193560439	0.1155063811578972	0.1115066246180021
0.0648350526889702	0.3155063811584176	0.1115066246180021
0.3981683860229169	0.3155063811584176	0.1115066246180021
0.7315017193558551	0.3155063811584176	0.1115066246180021
0.0648350526890769	0.5155063811580765	0.1115066246180021
0.3981683860232990	0.5155063811580765	0.1115066246180021

0.7315017193555857	0.5155063811580765	0.1115066246180021
0.0648350526888646	0.7155063811574039	0.1115066246180021
0.3981683860229656	0.7155063811574039	0.1115066246180021
0.7315017193561566	0.7155063811574039	0.1115066246180021
0.0648350526891310	0.9155063811577384	0.1115066246180021
0.3981683860229881	0.9155063811577384	0.1115066246180021
0.7315017193561940	0.9155063811577384	0.1115066246180021
0.9637651479324418	0.3847841647886946	0.1924534117430367
0.9635415697408207	0.7848404754751528	0.1925342029281902
0.9642049237619827	0.5850279785344327	0.1923529225857087
0.6307537977667985	0.3850128639662764	0.1919473301058054
0.9630369743387702	0.1851631603034423	0.1928493411822828
0.6310166159068886	0.5852498364389537	0.1925950275237984
0.6303876532616587	0.7853819105746673	0.1926472412557189
0.6300329761986656	0.9851822823472484	0.1929513601872074
0.9632068315643727	0.9847943373430136	0.1928905387978921
0.2971153447200174	0.5846050751834780	0.1931001327145845
0.2969453992115337	0.7850361401323840	0.1929145373546253
0.2969294267963530	0.9846680959152324	0.1930288695899235
0.6306470963107492	0.1854235769485670	0.1932601975150628
0.2969525105471105	0.3847446495079229	0.1936780969569005
0.2974163427230661	0.1852240297107141	0.1937431065916328
0.8099156573375288	0.6375038517042472	0.2071979398892488
0.1429135608165985	0.8381827184863864	0.2081288676134792
0.4764937004949588	0.8387993309547743	0.2081584542876479
0.8100844778668401	0.8386552233672947	0.2084242810100160
0.8100280929579328	0.0383044699195506	0.2084028429161983
0.4776400563956356	0.0399953257061272	0.2088682300137616
0.1439063232364728	0.2381030485070098	0.2081694550882603
0.4741573210601113	0.4394174889181409	0.2076230351699528
0.1440825292147216	0.6375148919765140	0.2085697560873594
0.8084458041739656	0.2391396691720948	0.2091216329432216
0.1445263110471486	0.4376000460302911	0.2086935854450858
0.1437471324754927	0.0391604779082714	0.2086709292309145
0.4765388481735525	0.6371599246089990	0.2089069861598999
0.4772925805440102	0.2393755855945309	0.2089900089442578
0.8080178808343046	0.4370569713819504	0.2095437435597287
0.3697752689067280	0.1041928657509069	0.2852141068899305
0.7041890064970749	0.1057754466921071	0.2855476718576352
0.3725149746498539	0.7095548091510998	0.2855488754246971
0.0388281745668699	0.5072234308214927	0.2855973547004461
0.7060771753473245	0.7103223724629231	0.2860036860090344
0.0366750905774147	0.1071921369110804	0.2856720415101324
0.3710875687826113	0.9068529047758147	0.2857264450153001

0.0378047396923698	0.9069925622014500	0.2858229211023409
0.0397907487532743	0.7079749194232827	0.2859182199983804
0.7055866530569943	0.9079059620081973	0.2859156255501693
0.0378786722982904	0.3064420656230964	0.2858574815247031
0.7067336293971032	0.5096993564692485	0.2877229825551521
0.3738852424589597	0.3050560525091010	0.2881499052304028
0.7082978864034637	0.3059385603639396	0.2890545349423701
0.3716677538741405	0.5082764190084782	0.2900031835770175
0.8890508230384092	0.3628153722875191	0.2985876477052493
0.2185654211595809	0.5651367651873497	0.2986885888064401
0.5539777197166869	0.7631364620213962	0.2985779317908613
0.5535119670127276	0.9601320062214219	0.2992666454714173
0.8860337049363288	0.1616137260952723	0.2992888260335952
0.2193783816823980	0.9607743979866502	0.2992167988808015
0.8867528398198489	0.9621521410506041	0.2993908534882996
0.2164016675276775	0.1570267684549915	0.2994298125811111
0.2200209481187609	0.7621033265443743	0.2994995617270563
0.5560650371506605	0.5666431313672312	0.2992262817535273
0.8896597721766001	0.5619642566455456	0.2992478135263747
0.5564757733622123	0.3630347162170647	0.2985954222774541
0.8880856940238296	0.7629459809542619	0.3001612937826714
0.5474399042287106	0.1577481800044263	0.3019332869905579
0.2150661570517867	0.3594223970426653	0.3023031379805345

Ru: Transition state state for ArCH(COOMe)CH_2 and H coupling
(*E* = -1235.7104 eV, *ZPE* = 4.92177565499999 eV, *S***T* = 1.37727084756014 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
12 10 2 120
Selective dynamics
Direct
0.6526957111158911 0.5746510980279479 0.3500282722142252
0.4803119677632395 0.5547777778208467 0.3997140633736603
0.6906599395262820 0.4774002746887330 0.4051128960513469
0.3918536308318931 0.2268053162249209 0.4044552184565812
0.3247786183042595 0.5629453694574631 0.4079371839243189
0.2314986347207312 0.2342171309055850 0.4122899769449489
0.1988553670884362 0.4040288416041374 0.4227198609895612
0.6163374208885033 0.5511869775172281 0.4296496103972187
0.6884081618754628 0.1671216533268513 0.4299626303282197
0.7800784822537365 0.2785971065988515 0.4495678243827466
0.5463923785248741 0.3664813862715836 0.4525744104972403
0.6692449832992645 0.2571520550983111 0.4864574018437015
0.4290987361925073 0.4879983620748380 0.3807777018629783
0.4511910101689635 0.3885674643942025 0.3836411219674582
0.3345403206088096 0.4920952595578720 0.3885100815055084
0.3759829519914361 0.2967881795584102 0.3890345048707640
0.5848519268123730 0.2858128739041449 0.3799623986422433
0.6236366695446489 0.4921319827306019 0.3965706292422480
0.2816822015557067 0.3023527160380994 0.3943744528610341
0.2600940245162998 0.3987519626949844 0.3976162077120606
0.5480088527537856 0.3911926979204151 0.4035165344649487
0.7058800158691191 0.2480535364879695 0.4435990441280892
0.6813130646078251 0.3103479220716505 0.3949721737867256
0.5361002032179162 0.1965979275525165 0.3981931696746457
0.1407055901600567 0.1380862835039474 0.0000000000000000
0.4740389234929795 0.1380862835039474 0.0000000000000000
0.8073722568262085 0.1380862835039474 0.0000000000000000
0.1407055901609773 0.3380862835039840 0.0000000000000000
0.4740389234930552 0.3380862835039840 0.0000000000000000
0.8073722568261485 0.3380862835039840 0.0000000000000000
1.1407055901601297 0.5380862835037752 0.0000000000000000
0.4740389234930317 0.5380862835037752 0.0000000000000000
0.8073722568260653 0.5380862835037752 0.0000000000000000

1.1407055901599403	0.7380862835037176	0.0000000000000000	
0.4740389234930995	0.7380862835037176	0.0000000000000000	
0.8073722568260457	0.7380862835037176	0.0000000000000000	
1.1407055901594552	0.9380862835037282	0.0000000000000000	
0.4740389234931193	0.9380862835037282	0.0000000000000000	
0.8073722568258801	0.9380862835037282	0.0000000000000000	
0.3201838529240384	0.1920708306439835	0.0159535054489979	
0.6535171862580356	0.1920708306439835	0.0159535054489979	
0.9868505195891355	0.1920708306439835	0.0159535054489979	
0.3201838529239434	0.3920708306439518	0.0159535054489979	
0.6535171862572209	0.3920708306439518	0.0159535054489979	
0.9868505195899140	0.3920708306439518	0.0159535054489979	
0.3201838529240035	0.5920708306438688	0.0159535054489979	
0.6535171862570449	0.5920708306438688	0.0159535054489979	
0.9868505195900116	0.5920708306438688	0.0159535054489979	
0.3201838529240059	0.7920708306437820	0.0159535054489979	
0.6535171862573990	0.7920708306437820	0.0159535054489979	
0.9868505195902231	0.7920708306437820	0.0159535054489979	
0.3201838529240065	-0.0079291693561326	0.0159535054489979	F
0.6535171862571099	0.9920708306429984	0.0159535054489979	
0.9868505195900468	0.9920708306429984	0.0159535054489979	
0.2186901232590252	0.0615218340180142	0.0955531191689971	
0.5520234565909872	0.0615218340180142	0.0955531191689971	
0.8853567899256268	1.0615218340185235	0.0955531191689971	
0.2186901232590331	0.2615218340178888	0.0955531191689971	
0.5520234565920610	0.2615218340178888	0.0955531191689971	
0.8853567899248875	0.2615218340178888	0.0955531191689971	
0.2186901232589631	0.4615218340180085	0.0955531191689971	
0.5520234565919568	0.4615218340180085	0.0955531191689971	
0.8853567899248784	0.4615218340180085	0.0955531191689971	
0.2186901232589959	0.6615218340179048	0.0955531191689971	
0.5520234565910407	0.6615218340179048	0.0955531191689971	
0.8853567899250798	0.6615218340179048	0.0955531191689971	
1.2186901232581095	0.8615218340178284	0.0955531191689971	
0.5520234565920541	0.8615218340178284	0.0955531191689971	
0.8853567899240649	0.8615218340178284	0.0955531191689971	
1.0648350526893799	1.1155063811585295	0.1115066246180021	
0.3981683860230169	0.1155063811579831	0.1115066246180021	
0.7315017193561762	0.1155063811579831	0.1115066246180021	
1.0648350526890160	0.3155063811578807	0.1115066246180021	
0.3981683860228455	0.3155063811578807	0.1115066246180021	
0.7315017193561942	0.3155063811578807	0.1115066246180021	
1.0648350526889976	0.5155063811577725	0.1115066246180021	
0.3981683860230213	0.5155063811577725	0.1115066246180021	

0.7315017193560065	0.5155063811577725	0.1115066246180021	
1.0648350526886174	0.7155063811581660	0.1115066246180021	
0.3981683860230540	0.7155063811581660	0.1115066246180021	
0.7315017193559734	0.7155063811581660	0.1115066246180021	
1.0648350526892405	0.9155063811570047	0.1115066246180021	
0.3981683860230048	0.9155063811570047	0.1115066246180021	
0.7315017193558611	0.9155063811570047	0.1115066246180021	
0.9636253431828834	0.3848081998876397	0.1923093989479739	
0.9631046641543595	0.7845118098970758	0.1927388443834738	
0.9636404875456255	0.5849355724818043	0.1926215774236919	
0.6304928423731140	0.3846902349567925	0.1921330265641658	
0.9629333012523809	0.1851524379826501	0.1927095107507009	
0.6303793595862177	0.5843459646646481	0.1929067529869710	
0.6303204406415572	0.7850251682731686	0.1925237891301397	
0.6299319108173214	0.9849457846941444	0.1927743724818419	
0.9630661138795080	0.9848023821780656	0.1928553832270875	
0.2967990883686553	0.5848635845236830	0.1929364120537703	
0.2970531880372997	0.7849389524330728	0.1928730507001284	
0.2968658363745540	-0.0152237359852764	0.1929224084572417	T
0.6305735928565810	0.1848152001700271	0.1932499523978632	
0.2963715712624290	0.3845636689437025	0.1934884100284480	
0.2972273930059570	0.1851785456154801	0.1935982700600689	
0.8093298191047061	0.6375834890675823	0.2084039639219517	
1.1428469241483268	0.8381437091337476	0.2080410221376709	
0.4766440592093161	0.8386528731654265	0.2080686929037188	
0.8097065824338562	0.8382489445425330	0.2083509108526734	
0.8099689845368816	1.0381651853263856	0.2083468521603464	
0.4773281025415498	0.0393529276638176	0.2085458798283012	
0.1436856022272826	0.2380300379686212	0.2080635725412449	
0.4740332805271753	0.4382889303770877	0.2074694669170998	
1.1436964203858115	0.6378408353608375	0.2083652129077832	
0.8087912184650081	0.2388782707564948	0.2087731600110980	
0.1440024040458518	0.4378685075789961	0.2085773995178669	
1.1435110843731646	1.0391771695087735	0.2087175832361951	
0.4766227097486976	0.6366267478538675	0.2085243783574630	
0.4771738847149169	0.2395544246714776	0.2090254240806399	
0.8075392627135626	0.4369153093280333	0.2095342194578504	
0.3697959882021467	0.1043308064508582	0.2851485076693683	
0.7049063269578876	0.1054515407982685	0.2853988642222290	
0.3729513375903352	0.7096202961783069	0.2852446978522938	
1.0384874703295801	0.5070370706896714	0.2855449446053709	
0.7061590072721349	0.7100162845672690	0.2860397744678621	
1.0367739338170323	1.1074590963423645	0.2856735677619974	
0.3708897861948425	0.9068049977673108	0.2856957612606632	

1.0380124976675504	0.9074088824450335	0.2857882938950118
1.0392120758389773	0.7077632143185536	0.2858645581060358
0.7052598533375400	0.9069321044687630	0.2858784135597038
1.0380479990081171	0.3067061997582589	0.2857895455248236
0.7079116824490088	0.5086956558327473	0.2879021559763503
0.3730550442300202	0.3052701896757813	0.2878102371477421
0.7090302050572344	0.3053848202211462	0.2885832386869996
0.3700156710128697	0.5085398221147615	0.2884970160817603
0.8888932254207234	0.3629073693080334	0.2986963961265796
0.2177710072654619	0.5657583621803021	0.2986588812904218
0.5537817214101810	0.7639409871441833	0.2986433976248288
0.5535679151778559	0.9600928794218453	0.2990536832893494
0.8861799657604145	0.1616812570909491	0.2992070639664219
1.2192819687111496	0.9608806673623661	0.2991248553118999
0.8865715939275900	0.9621422124023251	0.2993924492384852
0.2161524126370575	0.1568763619560001	0.2993692912482138
0.2199640626957914	0.7621136324944496	0.2992094719917411
0.5530897424511947	0.5654702435684832	0.2999775226331976
0.8887784898695794	0.5631020295905442	0.2988779241880716
0.5547630444906704	0.3589711616678310	0.2997813864544698
0.8872970866005407	0.7621450415988480	0.2993240367570819
0.5484042780595072	0.1554890551994159	0.3015989330121849
0.2147229962793112	0.3598798944102256	0.3025259867550623

Ru: Final state state for ArCH(COOMe)CH_2 and H coupling
(*E* = -1236.865 eV, *ZPE* = 5.1493929735 eV, *S***T* = 1.48245648273949 eV)
AutoCreatByScript: H C O Ru
1.00000000000000
15.1228015700000000 0.0000000000000000 0.0000000000000000
-3.6418149199999998 13.0568463000000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.5088567099999999
H C O Ru
12 10 2 120
Selective dynamics
Direct
0.4356934705325813 0.6049308383362487 0.4052646644915771
0.7571221472380379 0.1539818089389538 0.4075275011548428
0.2971244330821840 0.4632566051937868 0.4088392013978738
0.4559285227695382 0.2470083622021752 0.4033138809467479
0.3086366841842201 0.2852710660660466 0.4095516187058446
0.7207942749069991 0.5231244971019460 0.3938890525503220
0.5816477127674314 0.5682626344328059 0.4215335444130500
0.7623240163368307 0.4576609426201596 0.4538150966989470
0.8474771030986850 0.2543550529875962 0.4412368807738519
0.6022897802868238 0.3423704994177061 0.4702732289367770
0.7358254574524977 0.2165233846279862 0.4777402956244603
0.6801295666426038 0.5260186803968109 0.4712608109060614
0.6536160914950901 0.2974565386782851 0.3863187074607226
0.3572814746681496 0.4484583195255743 0.3864030549498348
0.3639680033655474 0.3424684017610882 0.3866385549387253
0.4414180075722305 0.5304936695327823 0.3895726836198496
0.4541078779450580 0.3234938992483244 0.3890093600738020
0.5382270224698982 0.4047247718353648 0.3959472699318907
0.5301791410412904 0.5103544862027943 0.3963275902761547
0.6229991831662414 0.3803592573991075 0.4248419956850975
0.7732688722353248 0.2268962297905147 0.4333848183331254
0.7007176482256290 0.4766214503163501 0.4368606974002823
0.5986556165866899 0.2022890211342784 0.3921036351102477
0.7500593988843351 0.3072061415430891 0.3980851269363072
0.1407055901600090 0.1380862835039923 0.0000000000000000
0.4740389234930064 0.1380862835039923 0.0000000000000000
0.8073722568240146 0.1380862835039923 0.0000000000000000
0.1407055901579997 0.3380862835039966 0.0000000000000000
0.4740389234929924 0.3380862835039966 0.0000000000000000
0.8073722568249713 0.3380862835039966 0.0000000000000000
0.1407055901600086 0.5380862835049637 0.0000000000000000
0.4740389234930137 0.5380862835049637 0.0000000000000000
0.8073722568280020 0.5380862835049637 0.0000000000000000

0.1407055901600049	0.7380862835040013	0.0000000000000000
0.4740389234930325	0.7380862835040013	0.0000000000000000
0.8073722568259869	0.7380862835040013	0.0000000000000000
0.1407055901599948	0.9380862835039349	0.0000000000000000
0.4740389234930014	0.9380862835039349	0.0000000000000000
0.8073722568259926	0.9380862835039349	0.0000000000000000
0.3201838529240124	0.1920708306439962	0.0159535054489979
0.6535171862569937	0.1920708306439962	0.0159535054489979
0.9868505195870019	0.1920708306439962	0.0159535054489979
0.3201838529240029	0.3920708306440009	0.0159535054489979
0.6535171862569908	0.3920708306440009	0.0159535054489979
0.9868505195890283	0.3920708306440009	0.0159535054489979
0.3201838529240035	0.5920708306439728	0.0159535054489979
0.6535171862569755	0.5920708306439728	0.0159535054489979
0.9868505195900175	0.5920708306439728	0.0159535054489979
0.3201838529240111	0.7920708306449945	0.0159535054489979
0.6535171862569871	0.7920708306439583	0.0159535054489979
0.9868505195919874	0.7920708306419231	0.0159535054489979
0.3201838529240119	0.9920708306439144	0.0159535054489979
0.6535171862569817	0.9920708306439144	0.0159535054489979
0.9868505195890059	0.9920708306439144	0.0159535054489979
0.2186901232590025	0.0615218340179963	0.0955531191689971
0.5520234565919805	0.0615218340179963	0.0955531191689971
0.8853567899250226	0.0615218340179963	0.0955531191689971
0.2186901232590013	0.2615218340179785	0.0955531191689971
0.5520234565919716	0.2615218340179785	0.0955531191689971
0.8853567899249952	0.2615218340179785	0.0955531191689971
0.2186901232590018	0.4615218340179602	0.0955531191689971
0.5520234565919724	0.4615218340179602	0.0955531191689971
0.8853567899249488	0.4615218340179602	0.0955531191689971
0.2186901232589849	0.6615218340169950	0.0955531191689971
0.5520234565920040	0.6615218340169950	0.0955531191689971
0.8853567899240151	0.6615218340169950	0.0955531191689971
0.2186901232599897	0.8615218340179431	0.0955531191689971
0.5520234565920161	0.8615218340179431	0.0955531191689971
0.8853567899250021	0.8615218340179431	0.0955531191689971
0.0648350526890062	0.1155063811579869	0.1115066246180021
0.3981683860230023	0.1155063811579869	0.1115066246180021
0.7315017193540072	0.1155063811579869	0.1115066246180021
0.0648350526889974	0.3155063811579679	0.1115066246180021
0.3981683860230064	0.3155063811579679	0.1115066246180021
0.7315017193550013	0.3155063811579679	0.1115066246180021
0.0648350526889927	0.5155063811589610	0.1115066246180021
0.3981683860230060	0.5155063811589610	0.1115066246180021

0.7315017193559994	0.5155063811589610	0.1115066246180021
0.0648350526890109	0.7155063811579524	0.1115066246180021
0.3981683860230066	0.7155063811579524	0.1115066246180021
0.7315017193559543	0.7155063811579524	0.1115066246180021
0.0648350526889876	0.9155063811579294	0.1115066246180021
0.3981683860230023	0.9155063811579294	0.1115066246180021
0.7315017193560438	0.9155063811579294	0.1115066246180021
0.6307892314000183	0.5859748865998370	0.1920017484647686
0.9626085903686098	0.3849436259763598	0.1925441752208800
0.6302461161648711	0.9855765205714764	0.1928555917369169
0.6304394958861336	0.7849417903347568	0.1926201046932505
0.9635051916339307	0.7852393189667676	0.1928522351798913
0.9633253723667178	0.1853125500823997	0.1926257075544399
0.9634376192515107	0.5853526924347530	0.1926012733129634
0.9634316315515042	0.9850479509933354	0.1927813231345014
0.6304789167095194	0.1859324135545004	0.1942455046866401
0.2969300677302963	0.9852703354575690	0.1930093205263683
0.2969107725070684	0.5851775512441925	0.1929497904150939
0.2968848347644991	0.7850067067951729	0.1931029652149360
0.2967400103726546	0.1849620093744148	0.1927776384538970
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