



The JWST Proto-PAH Project: Detection of the Methyl Radical CH₃ in the Highly Evolved C-rich Object SMP LMC 011

Jialu Li^{1,2} , D. A. García-Hernández^{1,2} , A. Manchado^{1,2,3} , Debayan Das⁴ , J. Cami^{4,5} , Els Peeters^{4,5} , G. C. Sloan^{6,7} , B. Aringer^{8,9} , J. Bernard-Salas^{10,11} , C. Bhatt^{4,5} , Nicholas Clark^{4,5} , Harriet L. Dinerstein¹² , M. A. Gómez-Muñoz^{13,14} , Kathleen E. Kraemer¹⁵ , M. Matsuura¹⁶ , R. Sahai¹⁷ , N. C. Sterling¹⁸ , Kevin Volk⁶ , G. M. Wahlgren⁶ , and A. A. Zijlstra¹⁹

¹ Instituto de Astrofísica de Canarias, C/Vía Láctea s/n, E-38205 La Laguna, Spain; jialu.li@iac.es

² Departamento de Astrofísica, Universidad de La Laguna (ULL), E-38206 La Laguna, Spain

³ Consejo Superior de Investigaciones Científicas (CSIC), Spain

⁴ Department of Physics and Astronomy, The University of Western Ontario, London, ON N6A 3K7, Canada

⁵ Institute for Earth and Space Exploration, The University of Western Ontario, London, ON N6A 3K7, Canada

⁶ Space Telescope Science Institute, 3700 San Martin Drive, Baltimore, MD 21218, USA

⁷ Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC 27599-3255, USA

⁸ Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden

⁹ Department of Astrophysics, University of Vienna, Türkenschanzstraße 17, 1180 Wien, Austria

¹⁰ ACRI-ST, Centre d'Etudes et de Recherche de Grasse (CERGA), 10Av. Nicolas Copernic, 06130 Grasse, France

¹¹ INCLASS Common Laboratory, 10 Av. Nicolas Copernic, 06130 Grasse, France

¹² Department of Astronomy, University of Texas at Austin, 2515 Speedway, Stop C1400, Austin, TX 78712-1205, USA

¹³ Departament de Física Quàntica i Astrofísica (FQA), Universitat de Barcelona (UB), C/Martí i Franqués 1, E-08028 Barcelona, Spain

¹⁴ Institut de Ciències del Cosmos (ICCUB), Universitat de Barcelona (UB), C/Martí i Franqués 1, E-08028 Barcelona, Spain

¹⁵ Institute for Scientific Research, Boston College, 140 Commonwealth Avenue, Chestnut Hill, MA 02467, USA

¹⁶ Cardiff Hub for Astrophysics Research and Technology (CHART), School of Physics and Astronomy, Cardiff University, The Parade, Cardiff, CF24 3AA, UK

¹⁷ Jet Propulsion Laboratory, MS 183-900, 4800 Oak Grove Dr., California Institute of Technology, Pasadena, CA 91109, USA

¹⁸ University of West Georgia, 1601 Maple Street, Carrollton, GA 30118, USA

¹⁹ Jodrell Bank Centre for Astrophysics, Department of Physics & Astronomy, The University of Manchester, Oxford Road, Manchester, M13 9PL, UK

Received 2026 June 18; revised 2026 August 27; accepted 2026 September 14; published 2026 September 30

Abstract

We report the first detection of the neutral methyl radical CH₃ in a highly evolved C-rich object, SMP LMC 011, using the Mid-Infrared Instrument (MIRI) Medium-Resolution Spectrometer (MRS) on JWST. CH₃ is well fitted by an excitation temperature of $T_{\text{ex}} \simeq 190$ K and a column density of $N_{\text{tot}}(\text{CH}_3) \simeq 5.6 \times 10^{17} \text{ cm}^{-2}$. We also report the nondetection of ethane (C₂H₆), consistent with CH₃ reacting preferentially with unsaturated radicals rather than self-recombination, which may be inefficient in SMP LMC 011. Combined with the exceptionally large benzene column density of SMP LMC 011, this supports a methyl-addition route from benzene toward alkyl-substituted aromatics. We propose that the high CH₃ abundance is driven by the erosion of hydrogenated amorphous carbon (HAC) dust grains in the dense warm torus by UV photons from the central star and/or by shocks, which release CH₃ directly into the gas phase. These results establish CH₃ as a key reactive intermediate in the formation of complex hydrocarbons in C-rich circumstellar environments. Chemical models that incorporate methyl-addition reactions are needed for a better understanding of polycyclic aromatic hydrocarbon (PAH) formation pathways in evolved stars. The potential detection of alkyl-substituted aromatics such as toluene (C₇H₈) and ethylbenzene (C₈H₁₀) in C-rich evolved stars would provide direct confirmation of CH₃-driven aromatic growth in circumstellar environments.

Unified Astronomy Thesaurus concepts: Small molecules (2267); Circumstellar gas (238); Astrochemistry (75); Interstellar medium (847); Planetary nebulae (1249)

1. Introduction

Carbon-rich pre-planetary nebulae (PPNe) and young planetary nebulae (PNe) are extraordinary chemical laboratories. As C-rich stars evolve from the asymptotic giant branch (AGB) toward the PN phase, the increasing UV radiation field from the warming central star transforms the circumstellar chemistry. Photochemical reactions in the neutral layers of the photodissociation region (PDR) are expected to produce high abundances of polyynes (C_{2n}H₂), cyanopolyynes (HC_{2n+1}N), methylpolyynes (CH₃C_{2n}H), and crucially benzene (C₆H₆), the basic building block of polycyclic aromatic hydrocarbons (PAHs; e.g.,

J. Cernicharo et al. 2001a, 2001b; J. Cernicharo 2004). Revealing the reactive intermediates that drive the molecular chemistry is central to understanding the formation and growth of the complex C-rich molecules (e.g., PAHs) observed from Galactic objects to very distant galaxies.

A key species in this chemistry is the methyl radical, CH₃. As a highly reactive open-shell intermediate in interstellar ion-molecule reaction networks, CH₃ is believed to be formed via hydrogen abstraction reactions starting from C⁺ and H₂ (e.g., E. Herbst & W. Klemperer 1973) and through photodissociation of methane (e.g., H. Feuchtgruber et al. 2000).²⁰ Thus, it may play a dual role. Its reactions with C⁺ represent one of the



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²⁰ The ion-molecule initiation is endothermic and requires high temperatures or vibrationally excited H₂ to proceed; in the UV-irradiated torus of SMP LMC 011, gas-phase CH₃ is therefore expected to be produced mainly by methane photodissociation (see text).

most important steps in the buildup of complex hydrocarbons, while its addition to aromatic radicals such as *ortho*-benzynes ($\text{o-C}_6\text{H}_4$) provides a bottom-up pathway to five-membered rings (J. Bouwman et al. 2023) and alkyl-substituted aromatics (B. Shukla & M. Koshi 2010; G. Santoro et al. 2020). The CH_3 radical is also expected to play a key role in HCN formation in PDRs (e.g., A. Sternberg & A. Dalgarno 1995).

Despite this central role, CH_3 is notoriously difficult to detect. Being planar (D_{3h} symmetry), it has no permanent electric dipole moment and no accessible pure rotational spectrum. Its detection has mainly relied on the ν_2 out-of-plane bending mode near $16.5\ \mu\text{m}$, a spectral window blocked by the Earth's atmosphere. The first detection of CH_3 was made with the Infrared Space Observatory (ISO) toward Sagittarius A* in the Galactic center (H. Feuchtgruber et al. 2000). In the JWST era, CH_3 has been identified in the protoplanetary disk around the very low-mass star ISO-ChaI 147 (A. M. Arabhavi et al. 2024) and the extragalactic buried nucleus of IRAS 07251–0248 (I. García-Bernete et al. 2026). Beyond the neutral radical, the methyl cation CH_3^+ has now been detected in several UV-irradiated environments, including a protoplanetary disk in the Orion star-forming region (O. Berné et al. 2023; P. B. Changala et al. 2023), the Orion Bar PDR (M. Zannese et al. 2026), the transition disks TW Hya (T. Henning et al. 2024) and GM Aur (M. Volz et al. 2026), as well as the O-rich PN NGC 6302 (C. Bhatt et al. 2025). However, a detection of the neutral methyl radical CH_3 in a C-rich evolved stellar environment has remained elusive until now.

SMP LMC 011 is uniquely suited for this search. It has been classified as a young PN in the Large Magellanic Cloud (LMC; N. Sanduleak et al. 1978; J. Bernard-Salas et al. 2006). Its Spitzer Infrared Spectrograph (IRS; J. R. Houck et al. 2004) spectrum reveals an exceptionally rich molecular absorption spectrum, including C_2H_2 , C_4H_2 , CH_4 , C_2H_4 , HC_3N , propyne ($\text{CH}_3\text{C}_2\text{H}$), and most remarkably benzene (C_6H_6 ; J. Bernard-Salas et al. 2006; S. E. Malek et al. 2012). SMP LMC 011 is one of only two highly evolved C-rich objects in which benzene has been detected (the other being the Galactic PPN AFGL 618, the Westbrook Nebula; J. Cernicharo et al. 2001b), and it harbors by far the largest known benzene column density ($N_{\text{tot}}(\text{C}_6\text{H}_6) \simeq 6.3 \times 10^{17}\ \text{cm}^{-2}$; S. E. Malek et al. 2012), with a benzene-to-acetylene ratio roughly 20 times higher than in AFGL 618 (S. E. Malek et al. 2012).

These anomalous abundances, inconsistent with current photochemical models of C-rich PPN outflows, point to unusual chemistry operating within a dense, warm, edge-on torus (J. Cernicharo 2004; S. E. Malek et al. 2012). Hubble Space Telescope imaging by R. A. Shaw et al. (2006) revealed a compact bipolar morphology analogous to AFGL 618, and the central star (or possibly a binary system; see G. C. Sloan et al. 2026, hereafter Paper I) is entirely obscured by the optically thick dusty torus, with the total mid-IR flux dominated by warm dust emission (S. E. Malek et al. 2012).

The presence of methyl-bearing species such as $\text{CH}_3\text{C}_2\text{H}$, combined with the high column density of benzene, makes SMP LMC 011 the most compelling environment in which to search for CH_3 as the key reactive intermediate linking small hydrocarbons to the aromatic chemistry. Here we report the first detection of the methyl radical CH_3 in SMP LMC 011 using JWST Mid-Infrared Instrument (MIRI) Medium-Resolution Spectrometer (MRS) observations, which represents the

first secure detection and quantitative characterization of this species in an evolved stellar object.

2. JWST Observations and Data Reduction

SMP LMC 011 was observed on 2025 May 27 under JWST GO Cycle 3 program 4678, using the MRS (I. Argyriou et al. 2023) of MIRI (G. S. Wright et al. 2023). All three grating settings were employed to achieve continuous spectral coverage from 4.9 to $28.7\ \mu\text{m}$, and a four-point dither pattern optimized for point sources was used. The program was designed to reach a signal-to-noise ratio of 100 or better over the 4.9 – $20\ \mu\text{m}$ range. Full details of the observing strategy are given in Paper I.

SMP LMC 011 is unresolved in the integral field unit data, and the spectra were reduced using a development version of the JWST calibration pipeline (v1.20.2dev) together with the point fixed-pattern correction (PFPC; K. D. Gordon & D. R. Law 2026).²¹ The PFPC extracts spectra from each of the four dither positions independently and calibrates them against JWST standard-star observations.²² This approach effectively removes residual fringing and flat-field errors from the extracted spectra (see Paper I for details). Discontinuities between the 12 spectral subbands were corrected by applying scalar multiplicative factors in the overlap regions between adjacent segments, propagating outward in both directions from Band 3A ($12.57\ \mu\text{m}$); these stitching corrections were generally smaller than 1%.

We constructed a continuum-normalized MIRI/MRS spectrum over 5 – $20\ \mu\text{m}$ for the molecular analysis presented below. The continuum was estimated with a smooth spline interpolation through selected continuum windows outside the strongest molecular absorption bands. Specifically, the broad absorption complexes at 6.65 – 8.35 and 12.0 – $17.5\ \mu\text{m}$ were excluded from the continuum fit, together with the narrower absorption region at 10.25 – $10.85\ \mu\text{m}$. The observed spectrum was then divided by the fitted continuum, and the resulting normalized flux and propagated uncertainties were used for the molecular identification and spectral modeling described in Section 3.

3. Molecular Identification and Spectral Modeling

3.1. Model Construction

We adopted the spectroscopic parameters for CH_3 and C_2H_6 from the HITRAN database (L. S. Rothman 2021) and modeled their molecular absorption bands using the foreground-slab model, which is commonly used for mid-IR absorption spectra. We neglect the source-function contribution from the slab itself and assess the impact of this approximation in Section 3.2. For an isothermal slab covering a fraction f_c of the background continuum, the observed intensity is

$$I_\nu = I_c[1 - f_c(1 - e^{-\tau_\nu})], \quad (1)$$

where I_c is the continuum intensity and τ_ν is the optical depth of the absorbing gas. For a given excitation temperature T_{ex} , total column density N_{tot} , Doppler parameter b , and velocity shift ($263.5\ \text{km s}^{-1}$ for the LMC; D. H. Morgan &

²¹ <https://github.com/STScI-MIRI/MRS-PFPC>

²² All SMP LMC 011 spectra presented here were calibrated using standard stars from the CALSPEC database (K. D. Gordon et al. 2022).

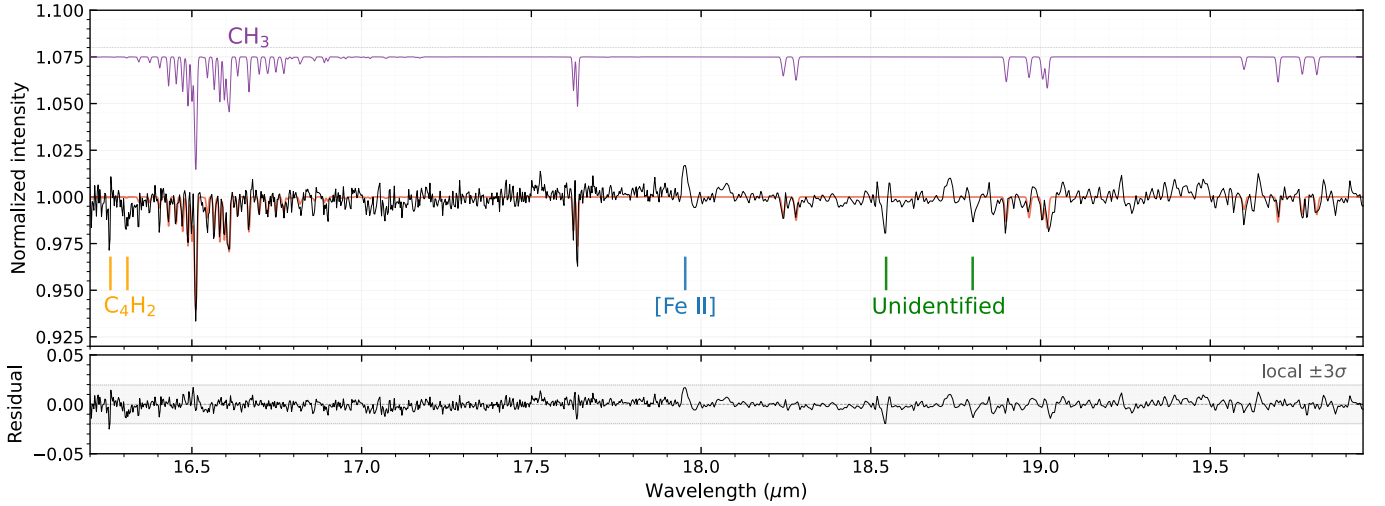


Figure 1. Top panel: continuum-normalized 16.2–20 μm JWST/MIRI MRS spectrum of SMP LMC 011 (black), compared with the adopted CH_3 model (red shaded region). The offset purple spectrum shows the CH_3 model separately. The orange markers indicate the C_4H_2 absorption after subtracting the broad C_4H_2 plateau (see Figure A1 in the Appendix A), the blue marker marks $[\text{Fe II}]$ identified in Paper I, and the green markers denote unidentified absorption features. Bottom panel: residual after subtracting the CH_3 model from the normalized spectrum. The gray band indicates the local $\pm 3\sigma$ uncertainty, estimated as 3 times the median-normalized MRS uncertainty over the 17–20 μm region.

Q. A. Parker 1998), we computed the lower-state column density, N_l , of each transition, assuming LTE:

$$N_l = N_{\text{tot}} \frac{g_l}{Q(T_{\text{ex}})} \exp\left(-\frac{E_l}{k_B T_{\text{ex}}}\right), \quad (2)$$

where g_l and E_l are the lower-state statistical weight and energy, $Q(T_{\text{ex}})$ is the partition function, and k_B is the Boltzmann constant.

The optical-depth profile of each transition was calculated from

$$\tau_\nu = \tau_p \phi_\nu = \sqrt{\pi} e^2 / (m_e c) N_l f_{lu} (\lambda/b) \phi_\nu, \quad (3)$$

where e is the electron charge, m_e is the electron mass, c is the speed of light, f_{lu} is the oscillator strength, and b is the Doppler parameter in velocity space (A. Tielens 2021). τ_p is the peak optical depth, and the profile function ϕ_ν is a Voigt profile normalized to unity at line center, $\phi_{\nu_0} = 1$, and consists of a Doppler core and a negligible Lorentzian damping wing (J. Li et al. 2024). The model spectrum was then calculated using Equation (1) and convolved to the wavelength-dependent MIRI/MRS resolving power. We adopted the linear resolving-power relations $R(\lambda) = A + B\lambda$ given by K. M. Pontoppidan et al. (2024, their Table 3) using the appropriate coefficients for Channels 3C and 4A over the corresponding wavelength intervals. The convolution was performed locally with a Gaussian line-spread function whose width varies with wavelength according to the adopted $R(\lambda)$.

3.2. Line Identification and Physical Constraints

The 16.2–20 μm region provides the clearest window for identifying CH_3 in the MIRI/MRS spectrum, although CH_3 has predicted absorption features throughout the broader 12–20 μm range. Compared with the more complex 12–16 μm region (Paper I; D. Das et al. 2026, in preparation), the 16.2–20 μm spectrum contains several groups of recognizable CH_3 absorption features extending from ~ 16.3 to 20 μm , together with a broad C_4H_2 plateau below 17 μm

(previously identified in SMP LMC 011; J. Bernard-Salas et al. 2006; S. E. Malek et al. 2012), and several absorption features still unidentified here. Figure 1 compares our representative CH_3 model with the continuum-normalized MRS spectrum.

CH_3 . The line identification and model comparison were carried out iteratively. We first used the predicted CH_3 line positions and relative strengths to identify wavelength intervals in which CH_3 is expected to contribute. The adopted intervals are 16.3–16.9, 17.6–17.65, 18.2–18.32, 18.8–19.05, and 19.55–19.85 μm . These intervals avoid the short-wavelength region most strongly affected by the C_4H_2 plateau and exclude near-continuum regions that contain little molecular signal and are more sensitive to continuum uncertainties.

Within these intervals, we selected a fixed set of diagnostically important absorption features and compared the observed and modeled fluxes in narrow windows centered on their local minima. We then performed a grid search over $T_{\text{ex}} = 50\text{--}350$ K, $\log[N_{\text{tot}}(\text{CH}_3)/\text{cm}^{-2}] = 16.0\text{--}19.5$, $b = 5\text{--}15$ km s $^{-1}$, and $f_c = 0.1\text{--}0.25$, using a feature-based χ^2 -like statistic that measures how well each model reproduces the relative depths of the selected CH_3 features. Appendix A describes the empirical motivation for the adopted b and f_c ranges, together with the details of the statistic, uncertainty treatment, and parameter degeneracies. Because the fit quality changes only modestly along these degeneracies, we adopt the global minimum of the feature-based statistic as a representative solution rather than as a unique physical model.

This solution has $T_{\text{ex}} = 190^{+25}_{-20}$ K, $\log[N_{\text{tot}}(\text{CH}_3)/\text{cm}^{-2}] = 17.75^{+0.05}_{-0.05}$, $b = 10$ km s $^{-1}$, and $f_c = 0.1$ (Appendix A). The quoted uncertainties are the projections of the joint 68.3% T_{ex} and $\log N_{\text{tot}}$ region for this fixed (b, f_c) pair. They therefore represent only the formal uncertainties within this adopted model and do not include the broader systematic uncertainty associated with the poorly constrained b , f_c , continuum placement, and model assumptions. For the representative solution adopted here, the omitted source-function term changes the continuum-normalized intensity by at most $\sim 1\%$ in the optically thick limit, and by less for unsaturated

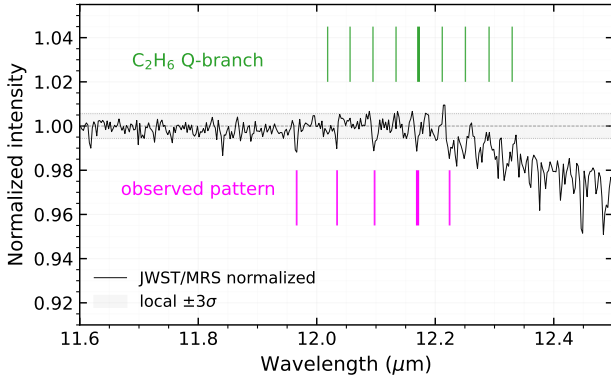


Figure 2. The 11.6–12.5 μm JWST/MIRI MRS spectrum of SMP LMC 011 (solid black), with the gray band indicating the local $\pm 3\sigma$ uncertainty. Green vertical markers show the predicted positions of the C_2H_6 Q-branch absorption features, while magenta markers show the observed quasi-regular narrow absorption pattern. The thicker markers indicate the predicted central Q-branch minimum near 12.172 μm (green) and the nearest observed feature at 12.170 μm (magenta). Although this central observed feature lies close to the expected Q-branch center, the spacing of the observed pattern does not match the predicted C_2H_6 Q-branch structure, supporting the nondetection of C_2H_6 .

lines. For this solution, the strongest individual CH_3 transition in the fitted wavelength range has a peak optical depth of $\tau_p \simeq 11.5$ at 16.513 μm . We note that this fitted T_{ex} characterizes the rotational population sampled by the ν_2 absorption band rather than providing a direct measurement of the gas kinetic temperature. Both collisional redistribution and radiative pumping by the mid-IR continuum can contribute to setting the CH_3 rotational populations, so T_{ex} cannot be identified uniquely with T_{kin} without a full non-LTE treatment, which is beyond the scope of this Letter.

The present constraints on b and f_c are not independent of the adopted CH_3 model. A future simultaneous analysis of multiple molecular species or spectral bands in this dataset may provide tighter and more physically motivated constraints on these parameters and reduce the associated degeneracies (e.g., D. Das et al. 2026, in preparation).

C_2H_6 . C_2H_6 has several bands from the near- to the mid-IR. However, the C–H stretching bands near 3.3 μm fall within the NIRSpec spectral range analyzed by D. Das et al. (2026, in preparation). On the other hand, the CH_3 -deformation band near 6.8 μm is heavily blended with C_6H_6 and HCN absorption (S. E. Malek et al. 2012; D. Das et al. 2026, in preparation). We therefore focus on the ν_9 band near 12.2 μm , which provides the cleanest constraint on C_2H_6 .

An absorption feature at 12.170 μm with a depth of $\sim 1.14\%$ is present near the predicted central Q branch of the $\text{C}_2\text{H}_6\nu_9$ band at 12.172 μm , but the local pattern is inconsistent with C_2H_6 (Figure 2). A search of the relevant spectroscopic databases and literature did not yield a convincing identification. If the quasi-regular spacing of $4.41 \pm 0.57 \text{ cm}^{-1}$ corresponds to consecutive P- or R-branch lines of a near-rigid linear molecule, it would imply a rotational constant of approximately $B \sim 2.2 \text{ cm}^{-1}$. A more extensive investigation of this unidentified carrier will be presented by D. Das et al. (2026, in preparation).

We place a conservative upper limit on the C_2H_6 column density using the local 3σ uncertainty of the continuum-normalized MRS spectrum in a region free of absorption features near the central Q branch of the ν_9 band, where the model predicts the strongest C_2H_6 absorption. The local 3σ level is

0.56% in normalized intensity. Adopting the same b , f_c , and 1σ T_{ex} range for CH_3 ($b = 10 \text{ km s}^{-1}$, $f_c = 0.10$, and $T_{\text{ex}} = 190^{+25}_{-20} \text{ K}$), we obtain $\log[N_{\text{tot}}(\text{C}_2\text{H}_6)/\text{cm}^{-2}] \lesssim 17.64^{+0.04}_{-0.05}$, or $N_{\text{tot}}(\text{C}_2\text{H}_6)/N_{\text{tot}}(\text{CH}_3) \lesssim 0.8$.

4. Discussion

4.1. Implications for the Hydrocarbon Chemistry of SMP LMC 011

The detection of CH_3 in SMP LMC 011 has significant implications for our understanding of the formation of small hydrocarbons in C-rich circumstellar environments. The methyl radical occupies a uniquely central position in the reaction network of the PDR associated with the dense torus. CH_3 is simultaneously a product of photodissociation, a building block for more complex molecules, and a reactive intermediate that bridges aliphatic and aromatic chemistry. A more complete analysis of the molecular inventory of SMP LMC 011 based on the JWST MIRI/MRS data, including detailed spectral modeling of all detected species, is presented by D. Das et al. (2026, in preparation). Here we focus on the specific chemical implications of the CH_3 detection.

4.2. The Origin of the CH_3 Reservoir: Grain Erosion in a Warm, Irradiated Torus?

The detection of CH_3 in SMP LMC 011 provides the first secure, quantitative measurement of gas-phase CH_3 in highly evolved C-rich stars. Whether CH_3 is comparably abundant in the prototypical C-rich AGB star IRC +10216 and the PPN AFGL 618 (the two sources with comparable molecular richness) cannot presently be established. The diagnostic $\sim 16.5 \mu\text{m}$ $\text{CH}_3 \nu_2$ band region is compromised in the archival SWSISO Short-Wave Spectrometer (SWS) spectra of both sources by strong fringing or by its location at the edge of two segments, so these data can neither confirm nor exclude CH_3 at column densities comparable to, or below, that derived here. In IRC +10216, the circumstellar chemistry is dominated by C_2H_2 , HCN, and carbon-chain radicals (C_nH), while in AFGL 618, the UV field from the central star drives the photopolymerization of acetylene into polyynes, cyanopolyynes, and methylpolyynes; the available carbon is channeled exclusively through unsaturated, progressively dehydrogenated species (J. Cernicharo 2004). In both cases, current photochemical models of these environments predict a negligible steady-state CH_3 abundance (see below).

The CH_3 column density derived here, $N_{\text{tot}}(\text{CH}_3) \simeq 5.6 \times 10^{17} \text{ cm}^{-2}$, establishes CH_3 as an abundant reactive intermediate in the hydrocarbon chemistry within the torus. Pure gas-phase photodissociation of CH_4 , a minor but established constituent of C-rich AGB envelopes (e.g., J. J. Keady & S. T. Ridgway 1993), cannot alone account for the observed CH_3 abundance. In the photochemical models of J. Cernicharo (2004), CH_3 is rapidly photodissociated and the neutral reactions that could replenish it have low rates at the standard 300 K reference temperature used in those models, implying a negligible steady-state abundance. This suggests that an additional source of CH_3 may be required in the torus. Independently, SMP LMC 011 shows C–H absorption associated with aliphatic material (i.e., hydrogenated amorphous carbon, HAC-like), while laboratory experiments demonstrate that energetic processing of such material can release CH_3 and other small hydrocarbons (see below). We therefore suggest that

erosion of HAC-like dust grains by UV photons from the central star (or binary system; Paper I) and/or by shocks driven by the fast ($\sim 122 \text{ km s}^{-1}$) bipolar outflow (S. E. Malek et al. 2012) provides a physically motivated additional source of CH_3 . The dense, warm torus of SMP LMC 011, directly irradiated by a hot central star ($>35 \text{ kK}$; J. Bernard-Salas et al. 2006; R. A. Shaw et al. 2006; Paper I), may provide the favorable conditions for efficient grain surface erosion and release of radicals into the gas phase.

Our suggested interpretation is consistent with the detection of aliphatic (HAC-like) C–H stretching modes in absorption at $3.4\text{--}3.5 \mu\text{m}$ toward SMP LMC 011, together with the lack of any PAH-related emission (Paper I). Moreover, recent laboratory simulations of dust formation under AGB star conditions demonstrate that HAC-like grains with C–H bonds in aliphatic CH_2/CH_3 groups are the expected dust product of C-rich AGB envelopes (G. Tajuelo-Castilla et al. 2026), thus providing the carbonaceous precursor material for UV and/or shock-driven CH_3 release in the subsequent PPN phase. As mentioned above, laboratory experiments show that UV irradiation and sputtering of HAC grains efficiently release aliphatic CH groups and small radical fragments, primarily CH_3 and CH_4 , into the gas phase (e.g., I. Alata et al. 2015; W. W. Duley et al. 2015; E. Dartois et al. 2017) as the C–C bonds are preferentially photocleaved over the C–H bonds (G. Tajuelo-Castilla et al. 2024).

Interestingly, the molecular inventory of SMP LMC 011 shows a striking resemblance to that of the ultraluminous IR galaxy IRAS 07251–0248, in which I. García-Bernete et al. (2026) recently detected the same set of hydrocarbons at similar excitation temperatures, attributing their high abundances to erosion of HAC grains or PAHs by cosmic rays. In SMP LMC 011, grain erosion would instead be driven by UV photons and/or shocks. The nondetection of C_2H_6 in both sources could suggest that CH_3 is preferentially channeled into reactions with unsaturated radicals rather than predominantly undergoing self-recombination (see below). This may point to similar methyl radical chemistry in grain-erosion environments despite different physical drivers.

4.3. CH_3 as the Key Intermediate: From Grain Erosion to Benzene and Alkyl-substituted Aromatics

From the nondetection of C_2H_6 , we derive a conservative upper limit of $N_{\text{tot}}(\text{C}_2\text{H}_6)/N_{\text{tot}}(\text{CH}_3) \lesssim 0.8$. This limit alone does not fix the branching of CH_3 , since the $\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_6$ stoichiometry caps the C_2H_6 yield at half the CH_3 consumed and any C_2H_6 formed may itself be photodissociated. In the dense torus, CH_3 produced by grain erosion and CH_4 photolysis may find two possible fates (the full network is summarized in Figure B1): self-recombination ($\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_6$) and reaction with the unsaturated radicals (C_{2n}H). However, self-recombination seems to be disfavored on physical grounds. It has no exothermic bimolecular exit channel ($\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_5 + \text{H}$ is strongly endothermic and opens only at temperatures of $\sim 1000\text{--}2500 \text{ K}$; P. Stewart et al. 1989), so the C_2H_6 adduct must be stabilized by a collision or by photon emission. The density of the torus ($n(\text{H}_2) \approx 10^7 \text{ cm}^{-3}$ in the analogous AFGL 618 torus; J. Cernicharo et al. 2001a; J. Cernicharo 2004) is far below that at which three-body stabilization becomes competitive for such neutral–neutral associations (e.g., E. Herbst 1980, 2021), so only the pressure-independent radiative channel remains. Radiative association becomes efficient at low pressure only for sufficiently large

adducts (e.g., those with roughly four or more carbon atoms; V. Vuitton et al. 2012) and has a strong inverse temperature dependence (e.g., J. Tennis et al. 2021); for an adduct as small as C_2H_6 at the dust temperature ($\simeq 425 \text{ K}$; S. E. Malek et al. 2012) of the torus, it is therefore expected to be inefficient. Reactions of CH_3 with unsaturated radicals, by contrast, access exothermic, largely barrierless bimolecular channels and are not so bottlenecked. Indeed, CH_3 additions to radicals such as phenyl are estimated to be much faster than CH_3 self-recombination (e.g., V. Vuitton et al. 2012). Although reaction-specific rate coefficients for $\text{CH}_3 + \text{C}_{2n}\text{H}$ are not yet available, the same rapid behavior is measured experimentally for the analogous unsaturated radical C_2H_3 (e.g., A. Fahr et al. 1991). We thus suggest that reactions with unsaturated radicals dominate the fate of CH_3 , placing it at the root of a rich and branching chemical network (Figure B1).

The first branch of this network is the methylpolyyne pathway. The reaction of CH_3 with C_{2n}H radicals is expected to produce the methylpolyynes $\text{CH}_3\text{C}_{2n}\text{H}$, of which propyne ($\text{CH}_3\text{C}_2\text{H}$, $n = 1$) is detected in SMP LMC 011 (S. E. Malek et al. 2012; D. Das et al. 2026, in preparation). Its significantly higher abundance compared to AFGL 618 (S. E. Malek et al. 2012) may be a direct consequence of a large CH_3 reservoir in SMP LMC 011, i.e., at every step of the polyacetylenic ladder, CH_3 competes with C_2H_2 for the available C_{2n}H radicals, redirecting carbon from the pure polyynes chain into the methylpolyyne branch.

The second and chemically more significant branch is the aromatic pathway. SMP LMC 011 harbors an exceptionally large benzene column density, with a $\text{C}_6\text{H}_6/\text{C}_2\text{H}_2$ ratio ~ 20 times higher than in AFGL 618 (S. E. Malek et al. 2012). The origin of the anomalously high $\text{C}_6\text{H}_6/\text{C}_2\text{H}_2$ ratio remains an open question;²³ we note however that benzene destruction via CN could be inhibited in SMP LMC 011 by the marginal HCN abundance (the parent species of CN, as suggested by S. E. Malek et al. 2012), which may contribute to benzene accumulation independent of the formation route.

Once benzene is formed, the abundant CH_3 drives its growth toward alkyl-substituted aromatics through a hydrogen abstraction (here driven by UV photodissociation rather than thermally) followed by barrierless methyl addition (see G. Santoro et al. 2020, and references therein). For example, vacuum ultraviolet (VUV) photodissociation of benzene yields the phenyl radical (C_6H_5) as its dominant channel (e.g., V. V. Kislov et al. 2004), which then reacts with CH_3 in a barrierless step to form toluene (C_7H_8); further methyl additions to larger photochemically generated aromatic radicals propagate the growth of alkyl-substituted PAHs (see Figure 11 in G. Santoro et al. 2020). Similarly, *ortho*-benzynes (*o*- C_6H_4) can form via several channels: the barrierless, exoergic $\text{C}_2\text{H} + \text{C}_4\text{H}_4$ reaction (provided vinylacetylene is available; F. Zhang et al. 2011), H loss from phenyl, or (to a minor extent) H_2 loss from benzene, and then reacts with CH_3 in a barrierless addition step to form the benzyl radical (C_7H_7), with subsequent H-atom loss yielding five-membered ring species (J. Bouwman et al. 2023).

²³ Such a discrepancy remains a puzzle that neither the neutral acetylenic polymerization route of J. Cernicharo (2004) nor the ionic benzene formation route (e.g., P. M. Woods et al. 2002, 2003) has been able to fully explain (see S. E. Malek et al. 2012).

Both CH_3 -driven pathways simultaneously consume benzene, producing more complex aromatic species and creating a self-amplifying cycle in which the large benzene reservoir is continuously processed toward higher molecular complexity. SMP LMC 011 is therefore a unique target for the detection of the simplest alkyl-substituted aromatics such as toluene (C_7H_8) and ethylbenzene (C_8H_{10}) in an evolved star. However, their detection with JWST/MIRI is currently hampered by the absence of gas-phase rovibrational line lists at astrophysically relevant temperatures. New laboratory spectroscopic measurements or theoretical line-list computations for these species are therefore urgently needed.

5. Summary and Conclusions

We report the first secure detection of the methyl radical CH_3 in a C-rich evolved star, SMP LMC 011. CH_3 is well fitted by an excitation temperature of $T_{\text{ex}} \simeq 190$ K and a column density of $N_{\text{tot}}(\text{CH}_3) \simeq 5.6 \times 10^{17} \text{ cm}^{-2}$. We also report the nondetection of ethane (C_2H_6), consistent with CH_3 reacting preferentially with unsaturated radicals rather than recombining with itself. The high CH_3 abundance may require an additional source, which we tentatively attribute to the erosion of carbonaceous (HAC-like) dust grains by UV photons and/or shocks in the dense, warm, directly irradiated torus, i.e., with grain erosion acting as a direct driver of aromatic chemistry in evolved stars. Once benzene is formed through the acetylenic and/or ionic routes, the abundant CH_3 would drive its growth toward alkyl-substituted aromatics (e.g., through hydrogen abstraction and methyl addition) and/or five-membered ring species, with profound implications for PAH formation. SMP LMC 011 is therefore a unique target for searching for alkyl-substituted aromatics and five-membered ring species in evolved stars, which would provide direct confirmation of CH_3 -driven aromatic growth, provided that gas-phase rovibrational line lists for these species become

available. Our results thus call for updated chemical models incorporating CH_3 -addition reactions to understand PAH formation in C-rich circumstellar environments.

Acknowledgments

J.L., D.A.G.H., and A.M. acknowledge support from the State Research Agency (AEI) of the Spanish Ministry of Science, Innovation, and Universities (MICIU) of the Government of Spain, and the European Regional Development fund (ERDF), under grant PID2023-147325NB-I00/AEI/10.13039/501100011033. This publication is based upon work from COST Action CA21126 – Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology). This work is based on observations made with the NASA/ESA/CSA James Webb Space Telescope. All of the data presented in this Letter were obtained from the Mikulski Archive for Space Telescopes (MAST) at the Space Telescope Science Institute. The data of this specific observing program can be accessed via the JWST Proto-PAH project (doi:[10.17909/zs5n-2t21](https://doi.org/10.17909/zs5n-2t21)). D.D., J.C., E.P., C.B., and N.C. acknowledge support from the Canadian Space Agency (CSA) [24JWGO3B01], and the Natural Sciences and Engineering Research Council of Canada. G.C.S., H.L.D., K.E.K., R.S., N.S., and G.M.W. were supported in part for program 4678 through grants from the STScI under NASA contract NAS5-03127. R.S.'s contribution to the research described here was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with NASA (80NM0018D0004).

Facility: JWST (MIRI).

Appendix A

CH_3 Fitting Constraints and Parameter Uncertainties

Figure A1 shows the region covering the C_4H_2 plateau subtracted in Figure 1.

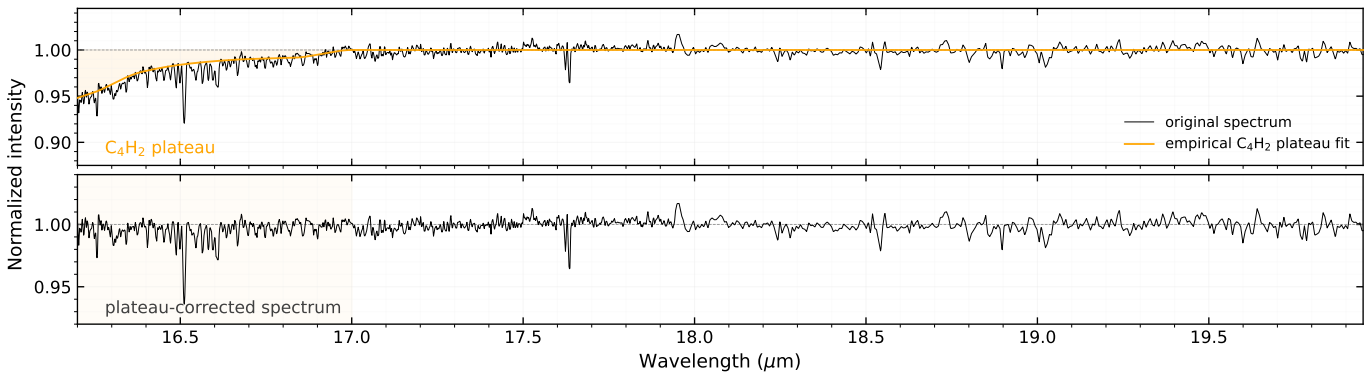


Figure A1. Empirical removal of the broad C_4H_2 plateau from the 16.2–20 μm spectrum. Top panel: original continuum-normalized JWST/MIRI MRS spectrum of SMP LMC 011, with the smooth empirical baseline adopted for the C_4H_2 plateau shown in orange. This baseline was obtained by fitting a smooth spline to the binned broad short-wavelength residual after subtracting the representative CH_3 model and is not intended as a physical C_4H_2 model. Bottom panel: plateau-corrected normalized spectrum used for the CH_3 model comparison in Figure 1.

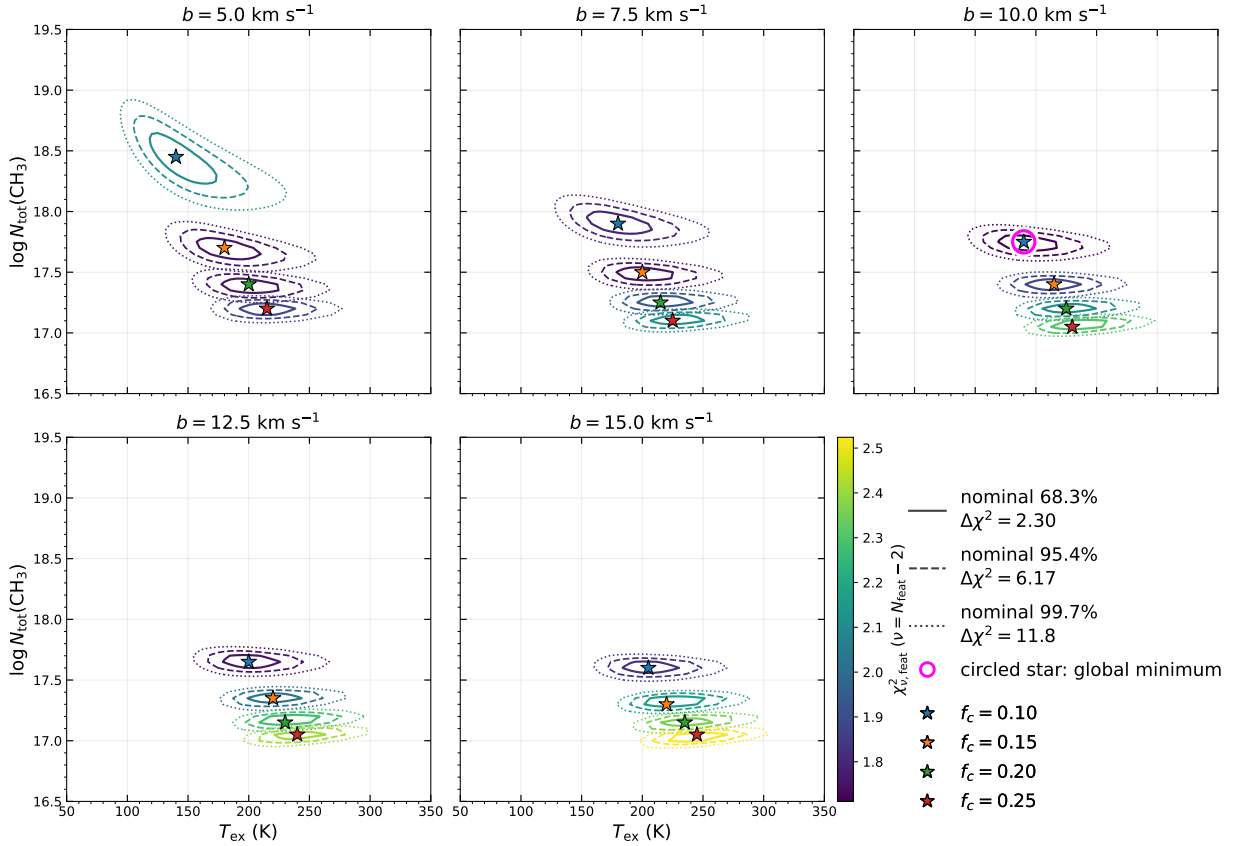


Figure A2. Joint constraints on the CH₃ excitation temperature, T_{ex} , and column density, $N_{\text{tot}}(\text{CH}_3)$, for fixed values of the intrinsic line width, b , and covering factor, f_c . Each panel corresponds to a different value of b , while the colored stars mark the minimum feature-based statistic for the four adopted values of f_c . The solid, dashed, and dotted contours represent the nominal joint 68.3%, 95.4%, and 99.7% regions, corresponding to $\Delta\chi^2 = 2.3$, 6.17, and 11.8 relative to the minimum within each fixed (b, f_c) slice. The contour color indicates the reduced feature-based statistic at the slice minimum, with lower values corresponding to better fits. The open circle marks the global minimum over the full grid.

For the spectral fitting of CH₃, a unique best-fitting model is difficult to identify using a conventional channel-by-channel χ^2 fitting alone. Strong or broad features dominate the fitting process (e.g., see Figure A1), but they are affected by saturation, blending, and parameter degeneracies. Their absorption depths no longer increase linearly with column density, while they may still exhibit apparently Gaussian-like profiles at the MIRI resolving power. In contrast, weaker and more optically thin features contribute relatively little to the total statistic (J. Li et al. 2024), even though they provide more direct constraints on the column density. Robust constraints on the intrinsic line width, b , and covering fraction, f_c , would ideally come from a simultaneous analysis of multiple molecular species or spectral bands, but such an analysis will be presented in D. Das et al. (2026, in preparation). We therefore focus on characterizing the degeneracies among the model parameters and identifying the parameter ranges that remain consistent with the observed CH₃ spectrum.

To do so, we evaluate the CH₃ models using a fixed set of diagnostically important feature windows, each centered on an individual absorption minimum identified in the observed spectrum. Each window spans 1.5 instrumental resolution elements at the local wavelength-dependent resolving power $R(\lambda)$ adopted in Section 3, which is broad enough to sample the local absorption feature over multiple spectral channels while remaining narrow enough to limit contamination from neighboring spectral structure. We then calculate a feature-based statistic for the selected windows. This statistic has the

form of a χ^2 , but is used primarily as an empirical measure of how well each model reproduces the relative depths of the observed features.

Figure A2 presents the resulting constraints in the $T_{\text{ex}}\text{--}\log N_{\text{tot}}$ plane for fixed values of b and f_c . Although all four parameters could formally be fitted simultaneously, the lack of constraints on b and f_c as well as the continuum uncertainties make the resulting posterior sensitive to the adopted priors and error model. We therefore use a grid-based analysis to display the parameter degeneracies directly. Specifically, our exploration shows that models outside $b = 5\text{--}15 \text{ km s}^{-1}$ or $f_c > 0.25$ provide poor matches to the observed spectral profiles: Larger values of b excessively broaden and blend the CH₃ features, smoothing out the observed local minima. In addition, larger values of f_c require column densities that are too low to reproduce the weaker absorption features and their relative depths. We note that the covering fraction also has a direct lower limit of approximately $f_c = 0.075$ within the adopted partial-coverage model, as set by the depth of the strongest observed CH₃ absorption. Even for a fully saturated line, the maximum absorption depth cannot exceed f_c . We therefore examine the joint constraints on T_{ex} and $\log N_{\text{tot}}$ for fixed (b, f_c) pairs.

Figure A2 reveals several trends in the model parameters. (1) f_c and N_{tot} are strongly degenerate. As f_c increases, a smaller column density is required to reproduce the same absorption depth, as expected from the approximate scaling of optically thin absorption with $f_c N$. (2) The preferred column

density does not decrease without limit at large f_c , because a sufficiently large column is still required to reproduce the weaker features and the relative depths among features with different optical depths. (3) Larger values of b generally produce poorer fits, indicating that excessively broad profiles smooth out the observed feature structure and increase blending among neighboring transitions. (4) Temperature is less tightly constrained than the other parameters. Most of the competitive solutions remain near $T_{\text{ex}} \sim 200$ K, while modest changes in T_{ex} can be compensated by corresponding adjustments in N_{tot} .

Since several combinations of T_{ex} , N_{tot} , b , and f_c produce comparably good fits, the global minimum should not be interpreted as a unique physical solution. We nevertheless adopt it as a representative best-fitting model and quote the corresponding joint $T_{\text{ex}}\text{--}\log N_{\text{tot}}$ constraints for the fixed (b, f_c) pair. The minimum feature-based statistic is obtained for $T_{\text{ex}} = 190$ K, $\log[N_{\text{tot}}(\text{CH}_3)/\text{cm}^{-2}] = 17.75$, $b = 10 \text{ km s}^{-1}$, and $f_c = 0.1$. For this fixed (b, f_c) pair, the nominal joint 68.3% region gives $T_{\text{ex}} = 190^{+25}_{-20}$ K and $\log[N_{\text{tot}}(\text{CH}_3)/\text{cm}^{-2}] = 17.75^{+0.05}_{-0.05}$. These ranges are the projections of the joint two-dimensional $T_{\text{ex}}\text{--}\log N_{\text{tot}}$ contour corresponding to $\Delta\chi^2 = 2.3$. We note that since the selected features are not guaranteed to be statistically independent and their uncertainties include an empirical continuum removal, we tested the nominal $\Delta\chi^2 = 2.3$ threshold with slice-by-slice parametric Monte Carlo simulations and verified that the calibrated 68.3% thresholds were close to the nominal two-parameter value. These confidence regions should therefore not be interpreted as the full uncertainty on the physical parameters, but rather as conditional constraints within each adopted (b, f_c) model.

Appendix B

CH₃ Chemical Network in the Warm, UV-irradiated Torus of SMP LMC 011

Figure B1 displays a simplified schematic of the CH₃ chemical network in the warm, UV-irradiated torus of SMP LMC 011. Species are color-coded: blue = detected in this source (or, for the methylpolyynes, detected via CH₃C₂H); gray dashed = searched for but not detected; purple dashed = predicted but not yet detected; cream = transient reactive intermediates or reactants. CH₃ is supplied by erosion of HAC grains (UV photons and/or shocks) and, more minorly, by CH₄ photodissociation. It then follows three competing routes: (i) self-recombination to C₂H₆ (disfavored at the low density of the torus; see Section 4.3); (ii) addition to unsaturated carbon-chain radicals C_{2n}H to form methylpolyynes (CH₃C_{2n}H; e.g., propyne, CH₃C₂H), in competition with C₂H₂; and (iii) an aromatic-growth branch. In the latter, VUV photodissociation of benzene generates the phenyl radical (C₆H₅) by H-atom loss, to which CH₃ adds barrierlessly to form toluene (C₇H₈); successive H abstraction/photolysis and CH₃ additions then build ethylbenzene (C₈H₁₀) and larger alkyl-substituted aromatics. In parallel, *ortho*-benzynes (*o*-C₆H₄) may form via (i) the barrierless C₂H + C₄H₄ reaction, (ii) H loss from phenyl, or (iii) direct H₂ loss from benzene (a minor channel). The barrierless reaction *o*-C₆H₄ + CH₃ then yields the transient benzyl radical (C₇H₇), which by ring contraction and H-atom loss produces five-membered-ring species (e.g., fulvenallene and ethynylcyclopentadienes; J. Bouwman et al. 2023). Note that benzene itself is supplied by acetylenic/ionic routes rather than by CH₃ (see Section 4.3).

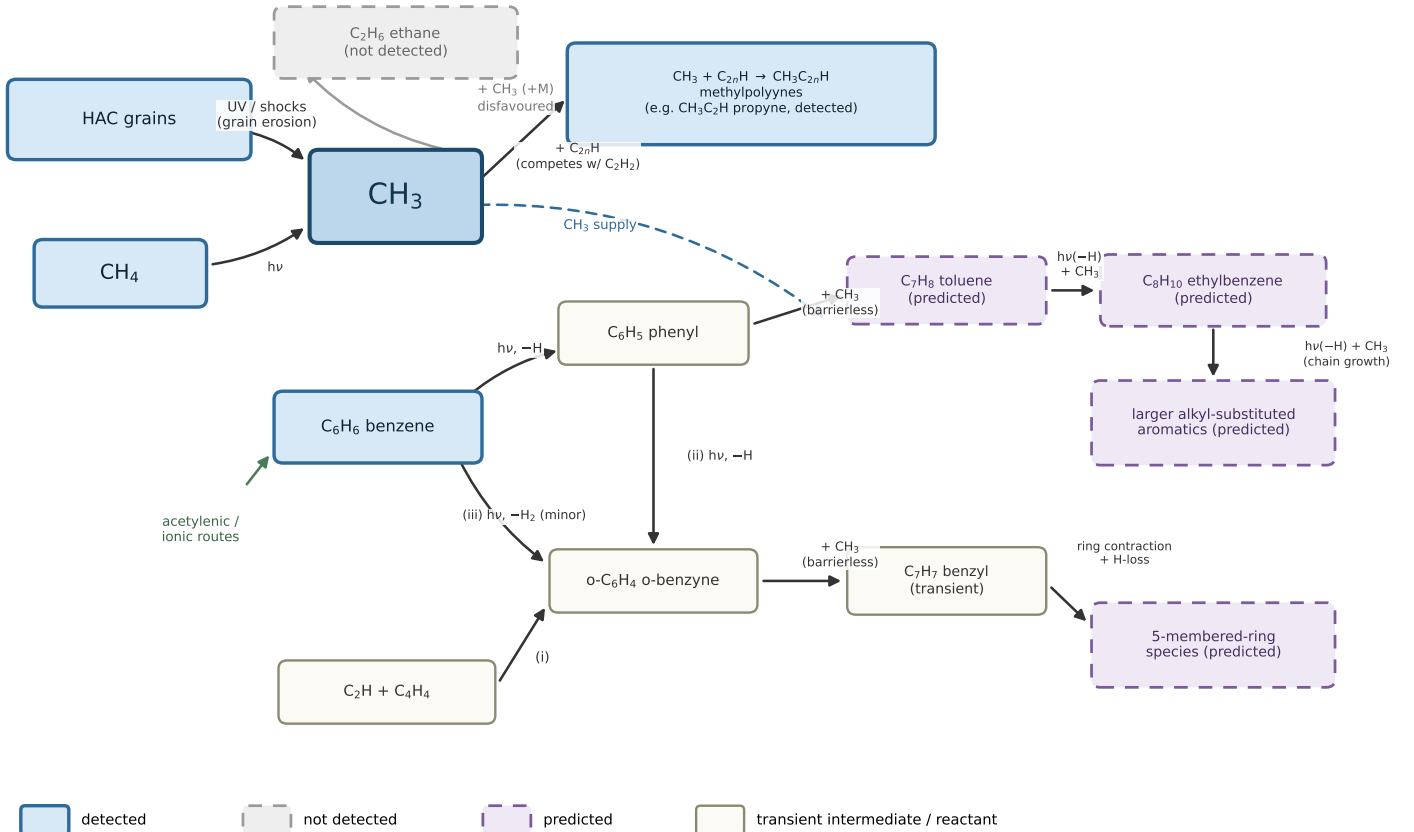


Figure B1. Simplified schematic of the CH₃ chemical network in the warm, UV-irradiated torus of SMP LMC 011 (see text).

ORCID iDs

Jialu Li  <https://orcid.org/0000-0003-0665-6505>
 D. A. García-Hernández  <https://orcid.org/0000-0002-1693-2721>
 A. Manchado  <https://orcid.org/0000-0002-3011-686X>
 Debayan Das  <https://orcid.org/0009-0001-4100-9218>
 J. Cami  <https://orcid.org/0000-0002-2666-9234>
 Els Peeters  <https://orcid.org/0000-0002-2541-1602>
 G. C. Sloan  <https://orcid.org/0000-0003-4520-1044>
 B. Aringer  <https://orcid.org/0000-0001-9848-5410>
 J. Bernard-Salas  <https://orcid.org/0000-0002-8452-8675>
 C. Bhatt  <https://orcid.org/0009-0000-0191-6756>
 Nicholas Clark  <https://orcid.org/0009-0009-4643-2734>
 Harriet L. Dinerstein  <https://orcid.org/0000-0002-4017-5572>
 M. A. Gómez-Muñoz  <https://orcid.org/0000-0002-3938-4211>
 Kathleen E. Kraemer  <https://orcid.org/0000-0002-2626-7155>
 M. Matsuura  <https://orcid.org/0000-0002-5529-5593>
 R. Sahai  <https://orcid.org/0000-0002-6858-5063>
 N. C. Sterling  <https://orcid.org/0000-0002-9604-1434>
 Kevin Volk  <https://orcid.org/0000-0002-3824-8832>
 G. M. Wahlgren  <https://orcid.org/0000-0002-6570-4776>
 A. A. Zijlstra  <https://orcid.org/0000-0002-3171-5469>

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