Study of Complex Nitrogen and Oxygen-bearing Molecules toward the Highmass Protostar IRAS 18089–1732

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Abstract

The observation of oxygen (O)- and nitrogen (N)-bearing molecules gives an idea about the complex prebiotic chemistry in the interstellar medium. Recent millimeter and submillimeter wavelength observations have shown the presence of complex O- and N-bearing molecules in the star formation regions. So, the investigation of those molecules is crucial to understanding the chemical complexity in the star-forming regions. In this article, we present the identification of the rotational emission lines of N-bearing molecules ethyl cyanide (C_2H_5CN) and cyanoacetylene (HC₃N), and O-bearing molecule methyl formate (CH₃OCHO) toward high-mass protostar IRAS 18089–1732 using the Atacama Compact Array. We also detected the emission lines of both the N- and O-bearing molecule formamide (NH₂CHO) in the envelope of IRAS 18089–1732. We have detected the v = 0 and 1 state rotational emission lines of CH₃OCHO. We also detected the two vibrationally excited states of HC₃N (ν 7 = 1 and v7 = 2). The estimated fractional abundances of C₂H₅CN, HC₃N (v7 = 1), HC₃N (v7 = 2), and NH₂CHO toward IRAS 18089–1732 are $(1.40 \pm 0.5) \times 10^{-10}$, $(7.5 \pm 0.7) \times 10^{-11}$, $(3.1 \pm 0.4) \times 10^{-11}$, and $(6.25 \pm 0.82) \times 10^{-11}$ respectively. Similarly, the estimated fractional abundances of CH₃OCHO (v = 0) and CH₃OCHO (v = 1) are $(1.90 \pm 0.9) \times 10^{-9}$ and $(8.90 \pm 0.8) \times 10^{-10}$, respectively. We also created the integrated emission maps of the detected molecules, and the observed molecules may have originated from the extended envelope of the protostar. We show that C_2H_5CN and HC_3N are most probably formed via the subsequential hydrogenation of the CH₂CHCN and the reaction between C_2H_2 and CN on the grain surface of IRAS 18089–1732. We found that NH₂CHO is probably produced due to the reaction between NH₂ and H₂CO in the gas phase. Similarly, CH₃OCHO is possibly created via the reaction between radical CH₃O and radical HCO on the grain surface of IRAS 18089-1732.

Key words: ISM: individual objects (IRA 18089–1732) (except) – ISM: abundances – ISM: kinematics and dynamics – stars: formation – astrochemistry

1. Introduction

The study of complex organic molecules (COMs) from massive stars $(M > 8 M_{\odot})$ is important for understanding the chemical complexity in the interstellar medium (ISM; van Dishoeck & Blake 1998; Herbst & van Dishoeck 2009). Highmass stars generate a significant amount of heavy atomic elements, produce large amounts of ultraviolet (UV) radiation, and inject turbulent energy into the ISM (Zapata et al. 2006). High-mass protostars are located in a rich cluster environment, and it is challenging to understand the physical and chemical formation processes (de Wit et al. 2005). High-mass protostars are highly luminous ($\geq 10^3 L_{\odot}$), and these sources are deeply embedded in massive envelopes that contain a high gas temperature (≥ 100 K) and gas density above 10^6 cm⁻³ (Liu et al. 2021). The study of the physical phenomena of high-mass protostellar disks is a major concern in high-mass star-forming regions. Over the past few years, indirect evidence for the existence of massive disks has accumulated, but there is still no clear proof of massive disks. Additionally, there are several methods for directly studying massive disks. Infrared and millimeter-wavelength continuum observations have revealed several attractive disk candidates, but they are unable to provide kinematic proof of potential accretion disks owing to a lack of velocity information (Shepherd et al. 2000; Chini et al. 2004). On the other hand, class II methanol (CH₃OH) and water (H₂O) maser emission found kinematic signatures from the massive disk candidates, but since maser emission is extremely selective and demands specific conditions, such studies do not permit more statistical analysis of massive disk properties (Torrelles et al. 1996; Pestalozzi et al. 2004). The most likely method to find and investigate disks in high-mass star formations is to detect thermal molecular line emissions, which are predicted to be sensitive to the gas properties and kinematics of the disks. Therefore, spectral line surveys in the millimeter and submillimeter wavelengths are crucial for understanding molecular gas properties, such as column



density and excitation temperature. The best method is to search the rotational emission lines of acetonitrile (CH₃CN) and methyl acetylene (CH₃CCH) because both molecules are known as gas thermometers for interstellar gas in massive protostars, hot molecular cores, and hot corinos (Andron et al. 2018). The prebiotic chemistry of high- and low-mass protostellar candidates may be the same, and a detailed analysis of the chemical evolution of high- and low-mass protostellar sources is not only important for astrochemistry but also crucial for understanding the process of star formation. Over the past decade, a variety of COMs have been discovered in protostellar cores on the scale of a few thousand astronomical units (Sakai & Yamamoto 2013). Two different scenarios were identified: (1) prebiotic chemistry in hot corinos, which is characterized by the richness of saturated COMs (Cazaux et al. 2003; Herbst & van Dishoeck 2009; Caselli & Ceccarelli 2012), and (2) warm carbon chain chemistry, which is characterized by the richness of unsaturated hydrocarbons (Sakai et al. 2008). Studying the chemical evolution of protostellar sources requires the study of isolated sources that are unaffected by nearby protostellar feedback. Isolated protostellar sources are excellent laboratories for theories of both chemical evolution and star formation (Evans et al. 2015).

Most chemical models of protostellar sources and hot molecular cores utilize grain surface chemistry to produce different types of complex organic compounds (Tielens & Charnley 1997; Garrod 2013; Manna & Pal 2024). The hydrogenation of solid oxygen (O), carbon (C), nitrogen (N), and carbon monoxide (CO) in the cold (≤ 20 K) prestellar phase produces CH₃OH and other hydrogenated species such as H₂O, NH₃, and CH₄ (Tielens & Hagen 1982). UV radiation photodissociates these surface ices, and when the cloud core heats up during the protostellar phase, the fragments become mobile. Consequently, complex molecules are formed during the subsequent recombination of the photofragments and evaporate when the grain temperature increases above the ice sublimation temperature of $\geq 100 \text{ K}$ (Garrod & Herbst 2006; Garrod et al. 2008; Manna & Pal 2024). For example, CH₃OCH₃, CH₃OCHO, and C₂H₅OH are formed by UV processing of CH₃OH ice (Öberg et al. 2009). Finally, the hotcore gas phase chemistry between evaporated molecules may cause second-generation species to become more complex (Millar et al. 1991; Charnley et al. 1992). One of the most significant impacts of an equatorial rather than a spherical structure is that UV light may more easily exit from the central source and illuminate the surface layers of the surrounding disk or toroid, as well as the larger-scale envelope (Bruderer et al. 2009, 2010; Isokoski et al. 2013) (Figure 2). This can result in ice-producing COMs that are faster than CH₃OH. Another effect of UV radiation is enhanced photodissociation of gaseous N₂ and CO. Consequently, more atomic N and C are easily accessible for grain surface chemistry, which might

result in an increased abundance of species such as HNCO and NH_2CHO (Garrod 2013).

IRAS 18089-1732 (hereafter IRAS 18089) is a well-known high-mass protostar that contains an ultra-compact (UC) HII region (Liu et al. 2021). That source is located at a distance of 2.34 kpc from the Earth (Xu et al. 2011). The luminosity and gaseous mass of IRAS 18089 are $1.3 \times 10^4 L_{\odot}$ and 1000 M_{\odot} respectively, which are estimated from the single-dish millimeter wavelength continuum emission (Beuther et al. 2002a; Sridharan et al. 2002). Earlier, the emission lines of CH₃OH, SO, SO₂, H₂S, and many other COMs were detected toward IRAS 18089, but no column densities or abundances were reported (Beuther et al. 2004b; Isokoski et al. 2013). Earlier estimated excitation temperature of CH₃CN (~350 K) toward IRAS 18089 indicated that the source is deeply embedded in the hot core (Beuther et al. 2004b). The molecular outflow of SiO (J = 5-4) is also evident toward IRAS 18089, which was detected using the Submillimeter Array (SMA: Beuther et al. 2004b). Additionally, the Goldreich-Kylafis effect was observed for the CO (J = 3-2) emission line, which revealed a linear polarization fraction of up to 8% (Beuther et al. 2010). The H₂O and CH₃OH maser emissions were also detected toward IRAS 18089 (Beuther et al. 2002b). Recently, Qin et al. (2022) conducted a spectral line survey of the rotational emission lines of ethyl cyanide (C₂H₅CN), methyl formate (CH₃OCHO), and methanol (CH₃OH) toward 146 high-mass star-forming regions using the ATOMS survey data (Liu et al. 2020). Qin et al. (2022) mentioned the detection of only two and six transition lines of C2H5CN and CH3OCHO toward IRAS 18089 among which one transition line of C₂H₅CN and two transition lines of CH₃OCHO are blended with other molecules (see supplementary data of Qin et al. 2022). Qin et al. (2022) also do not discuss the abundance and proper gas phase and grain surface chemistry of those molecules toward IRAS 18089. This indicates that another detailed molecular spectral line study is needed to understand the abundance and prebiotic chemistry of different COMs toward IRAS 18089.

In this paper, we present the detection of rotational emission lines of C_2H_5CN , CH_3OCHO , HC_3N , and NH_2CHO toward IRAS 18089. The chemical diagram of those molecules is created using the molecular modeling software Avogadro (Hanwell et al. 2012), as shown in Figure 1. Previously, the emission lines of C_2H_5CN , CH_3OCHO , HC_3N , and NH_2CHO were detected toward hot molecular cores G10.47+0.03 (Gorai & Bhat et al. 2020; Mondal et al. 2021; Manna & Pal 2023; Mondal et al. 2023), G31.41+0.31 (Mininni et al. 2023), Orion KL (Beuther et al. 2005), Sgr B2 (N) (Belloche et al. 2013), and low-mass protostar IRAS 16293-2422 (Jørgensen et al. 2016; Calcutt et al. 2018). The paper is organized in the following manner. The observations and data reduction are presented in Section 2. The result of the detection of emission lines of complex molecules is shown in Section 3. The



Figure 1. Three-dimensional molecular structure of C_2H_5CN , CH_3OCHO , HC_3N , and NH_2CHO . The gray atoms are carbon (C), the red atoms are oxygen (O), the white atoms are hydrogen (H), and the blue atoms are nitrogen (N).



Figure 2. A cartoon diagram of a high-mass protostar with a spherical shape (left) and a protostar with a flattened disk-like structure (right), with increasing UV photons illuminating the walls of the outflow cavity.

Observation Summary of IRAS 18089							
Observation Date (yyyy-mm-dd)	Integration Time (s)	Frequency Range (GHz)	Spectral Resolution (kHz)	Sensitivity (10 km s^{-1}) (mJy beam ⁻¹)	Field of View (FOV) (")		
2017-09-18	5624.64	127.49-128.48	488.28	5.91	74.23		
		129.75-130.75	488.28	5.37			
		139.09-140.09	488.28	5.15			
		140.45-141.45	488.28	5.01			

 Table 1

 Observation Summary of IRAS 18089

discussion and conclusion of the detection of complex molecules are featured in Sections 4 and 5 respectively.

2. Observations and Data Reductions

We used the cycle 4 archival data of IRAS 18089, observed employing the 7 m Atacama Compact Array (ACA) of the Atacama Large Millimeter/submillimeter Array (ALMA) (ID: 2016.2.00005.S. PI: Rivilla, Victor). The observations were performed in Band 4 (frequency range 127.49–141.45 GHz). The observed phase center of IRAS 18089 was (α , δ)_{J2000} = 18:11:51.400, -17:31:28.00. The observation was carried out on 2017 September 18, using eight antennas. The observations were recorded in spectral ranges 127.49–128.48 GHz, 129.75–130.75 GHz, 139.09–140.09 GHz, and 140.45–141.45 GHz, with a corresponding spectral resolution of 488 kHz. During the observation of IRAS 18089, the flux calibrator and bandpass calibrator were J1924–2914, and the phase calibrator was taken as J1833–210B. The observation summary is shown in Table 1.

We used the Common Astronomy Software Application (CASA 5.4.1) with the data reduction automated pipeline for data reduction and spectral imaging of IRAS 18089 (McMullin et al. 2007). For flux calibration of IRAS 18089, we used the



Figure 3. The 2.1 mm continuum map of IRAS 18089 overlaid with black contours. The contour levels start at 3σ , where σ is the rms (26.63 mJy beam⁻¹) of the continuum image. The contour levels increase by a factor of $\sqrt{2}$. The green circle indicates the synthesized beam of the continuum image.

Perley-Butler 2017 flux calibrator model for each baseline to scale the continuum flux density of the flux calibrator using the CASA task SETJY with 5% accuracy (Perley & Butler 2017). Executing the CASA pipeline tasks hifa bandpassflag and hifa flagdata, we create the flux and bandpass calibration after flagging the defective channels and antenna data. After the initial data reduction, we used the CASA task MSTRANSFORM with all available rest frequencies to separate the target data of IRAS 18089. We produced the continuum emission maps of IRAS 18089 for line-free channels using the CASA task TCLEAN with HOGBOM deconvolver. After the production of the continuum images, we used the task UVCONTSUB in the UV plane of separated calibrated data of IRAS 18089 for the continuum subtraction. To create the spectral images of IRAS 18089, we utilized the CASA task TCLEAN with SPECMODE=CUBE parameter and Briggs weighting robust value of 0.5. Both the continuum map and spectral cube were corrected for the primary beam using the CASA IMPBCOR task.

3. Result

3.1. Dust Continuum Emission

The 2.1 mm dust continuum image of IRAS 18089 is depicted in Figure 3. We employ the CASA IMFIT task to estimate parameters of the central core, such as integrated flux density, peak flux density, corresponding position angle, and rms noise level. The estimated peak flux density and integrated

flux density of the source are 274.9 ± 6.5 mJy beam⁻¹ and 346.1 ± 14 mJy, respectively, with an rms noise of 26.63 mJy beam⁻¹. The deconvolved source size is $5.1''14 \times 3.1''59$ at a position angle of $89^{\circ}.8$. The synthesized beam size of the continuum image is $12.1''.78 \times 7.1''20$. Thus, the continuum core is not resolved in the IRAS 18089 region.

3.1.1. Estimation of Hydrogen (H_2) Column Density

For optically thin dust continuum emission, the peak flux density (S_{ν}) can be expressed as

$$S_{\nu} = B_{\nu}(T_d)\tau_{\nu}\Omega_{\text{beam}} \text{ (Gorai et al. 2020)}, \tag{1}$$

where $B_{\nu}(T_d)$ represents the Planck function at dust temperature T_d (Whittet 1992), τ_{ν} indicates the optical depth, and $\Omega_{\text{beam}} = (\pi/4 \ln 2) \times \theta_{\text{major}} \times \theta_{\text{minor}}$ signifies the solid angle of the synthesized beam. The equation of optical depth in terms of the mass density of dust can be written as,

$$\tau_{\nu} = \rho_d \kappa_{\nu} L \text{ (Gorai et al. 2020)}, \qquad (2)$$

where ρ_d represents the mass density of dust, κ_{ν} is the mass absorption coefficient, and *L* defines the path length. The mass density of the dust can be expressed in terms of the dust-to-gas mass ratio (*Z*),

$$\rho_d = Z\mu_{\rm H}\rho_{\rm H_2} = Z\mu_{\rm H}N_{\rm H_2}2m_{\rm H}/L \text{ (Gorai et al. 2020)}, \quad (3)$$

where $\mu_{\rm H}$ defines the mean atomic mass per hydrogen, $\rho_{\rm H_2}$ is the hydrogen mass density, $m_{\rm H}$ represents the mass of hydrogen, and $N_{\rm H_2}$ is the column density of molecular hydrogen. We take the dust temperature $T_d = 30$ K (Sanhueza et al. 2021), $\mu_{\rm H} = 1.41$, and Z = 0.01 (Cox & Pilachowski 2000). The estimated peak flux density of the dust continuum of IRAS 18089 at frequency 140.955 GHz is 274.9 ± 6.5 mJy beam⁻¹. From Equations (1), (2), and (3), the column density of molecular hydrogen can be expressed as,

$$N_{\rm H_2} = \frac{S_{\nu}/\Omega}{2\kappa_{\nu}B_{\nu}(T_d)Z\mu_{\rm H}m_{\rm H}}$$
(Gorai et al. 2020). (4)

For estimation of the mass absorption coefficient (κ_{ν}) , we adopt the formula $\kappa_{\nu} = 0.90(\nu/230 \text{ GHz})^{\beta} \text{ cm}^2 \text{ g}^{-1}$ (Motogi et al. 2019), where $k_{230} = 0.90 \text{ cm}^2 \text{ g}^{-1}$ indicates the emissivity of the dust grains at a gas density of 10^6 cm^{-3} , which is covered by a thin ice mantle at 230 GHz. The dust spectral index (β) of ~1.6 toward IRAS 18089 is adopted from Sanhueza et al. (2021). Using the mass absorption coefficient formula, the estimated value of κ_{ν} is 0.411. Using Equation (4), we estimate the column density of the molecular hydrogen (N_{H_2}) toward IRAS 18089 to be (8.01 ± 0.4) × 10^{23} cm⁻². The earlier estimated column density of molecular H₂ toward IRAS 18089 at wavelength 1.2 mm using the SMA is 9.5×10^{23} cm⁻² (Beuther et al. 2005), which is quite similar to our derived column density of H₂ ((8.01 ± 0.4) × 10^{23} cm⁻²) using the ACA at wavelength 2.1 mm.

3.2. Spectral Line Analysis of IRAS 18089

We extracted the molecular spectrum of the high-mass protostar IRAS 18089 for a 20"2 diameter circular region centered at $(\alpha, \delta)_{J2000} = 18:11:51.400, -17:31:28.00$. The synthesized beam sizes of the spectral images of IRAS 18089 at frequency ranges of 127.49-128.48 GHz, 129.75-130.75 GHz, 139.09-140.09 GHz, and 140.45-141.45 GHz are $12.^{''}82 \times 6.^{''}40$, $12.^{''}90 \times 6.^{''}32$, $12.^{''}66 \times 6.^{''}02$, and $12.^{''}18 \times 12.^{''}82 \times 6.^{''}40$ 6."09 respectively. The systemic velocity (V_{LSR}) of IRAS 18089 is 33.8 km s⁻¹ (Beuther et al. 2005). For identification of the emission line of COMs in the spectra, we use local thermodynamic equilibrium (LTE) model spectra with the Cologne Database for Molecular Spectroscopy (CDMS) molecular database (Müller et al. 2005). For LTE analysis, we use the LTE-RADEX module in CASSIS (Vastel et al. 2015). The LTE assumption is valid in this case as the gas density of the warm inner region of the target is 1.3×10^7 cm⁻³ (Sanhueza et al. 2021). The identification of the different types of COMs is discussed below.

3.2.1. Ethyl Cyanide (C₂H₅CN)

We detected a total of four rotational emission lines of the complex N-bearing molecule C2H5CN toward IRAS 18089 using the LTE-modeled spectra. The upper-state energies (E_u) of the detected emission lines of C₂H₅CN vary between 47.23 and 57.48 K. A Gaussian fit to the observed spectra of C₂H₅CN was performed to estimate the proper FWHM in km s^{-1} and integrated intensity $(\int T_{\rm mb} dV)$ in K km s⁻¹. The resultant LTE and Gaussian fitting of spectral lines of C₂H₅CN are displayed in Figure 4, and the corresponding spectral parameters are listed in Table 2. We also confirmed that the detected emission lines of C₂H₅CN are non-blended, and all detected emission lines of C₂H₅CN exhibit above 5σ significance. The best-fit column density of C₂H₅CN is $(1.13 \pm 0.4) \times 10^{14}$ cm⁻² with an excitation temperature of 200 ± 54 K, which is obtained using the LTE modeling. The fractional abundance of C₂H₅CN toward IRAS 18089 with respect to H₂ is $(1.40 \pm 0.5) \times 10^{-10}$.

3.2.2. Methyl Formate (CH₃OCHO)

We identified a total of sixteen rotational emission lines of CH₃OCHO toward IRAS 18089 using the LTE model with more than 5σ significance level. The resultant LTE and Gaussian-fitted spectral profiles of CH₃OCHO are shown in Figure 4, and the spectral line parameters of CH₃OCHO are presented in Table 2. We observed the $V_t = 0$ and $V_t = 1$ states in the transitions of the CH₃OCHO. The $V_t = 0$ and $V_t = 1$ states correspond to the ground and first torsionally excited states of CH₃OCHO. We find that the upper state energies (E_u) of the detected emission lines of CH₃OCHO ($V_t = 0$) vary between 40.71 and 114.60 K. Similarly, the upper state energies (E_u) of the CH₃OCHO ($V_t = 1$) vary between 223.32

and 235.0 K. We also observe the torsional substates A and E in the transitions of CH₃OCHO due to the internal rotation of the methyl (CH₃) group. During the spectral fitting using the LTE model, we observed that the J = 17(6,11) - 17(5,12)A transition line of CH₃OCHO ($V_t = 0$) is not fitted well because that emission line is blended with CH₃OCH₃. In Table 2, the transitions of CH₃OCHO are presented corresponding to $V_t = 0$ and $V_t = 1$ states. Using the LTE model, the best-fit column density of the CH₃OCHO $V_t = 0$ is $(1.5 \pm 0.3) \times 10^{15} \text{ cm}^{-2}$ and $V_t = 1$ is $(7.1 \pm 0.5) \times 10^{14} \text{ cm}^{-2}$ with corresponding excitation temperatures of 200 ± 48 K and 196 ± 74 K. The column density of CH₃OCHO varies between the $V_t = 0$ and $V_t = 1$ torsional excited states because the first torsional excited state ($V_t = 1$) of CH₃OCHO is located at about 132 cm⁻¹ above the ground state ($V_t = 0$), where $1 \text{ cm}^{-1} = 1.438 \text{ K}$ (Tudorie et al. 2012). The estimated abundances of CH₃OCHO with respect to H₂ toward IRAS 18089 are $(1.90 \pm 0.9) \times 10^{-9}$ (for $V_t = 0$ and $(8.90 \pm 0.8) \times 10^{-10}$ (for $V_t = 1$).

3.2.3. Cyanoacetylene (HC_3N)

We detected two vibrationally excited states of HC₃N (v7 = 1and v7 = 2) toward IRAS 18089. Using the LTE-modeled spectra, we identified two rotational emission lines of v7 = 1 state and three rotational emission lines of v7 = 2 states of HC₃N. The detected vibrationally excited HC₃N emission lines exhibit the higher upper-state energies of $E_{\rm up}/{\rm k}$ ~366.80–366.86 K (for v7 = 1) and ~687.82-691.10 K (for v7 = 2). The higher vibrational states of HC₃N (v7 = 1 and v7 = 2) with higher upper state energies have the ability to trace the inner hot gas near the central star. The resultant detected spectral lines of HC₃N (v7 = 1 and v7 = 2) are shown in Figure 4, and the spectral line parameters of HC₃N (v7 = 1 and v7 = 2) are presented in Table 2. Using the LTE model, the best-fit column density of HC₃N with v7 = 1and v7 = 2 excited states are $(6.02 \pm 0.5) \times 10^{13} \text{ cm}^{-2}$ and $(2.50 \pm 0.3) \times 10^{13} \text{ cm}^{-2}$ respectively, with excitation temperatures of 160 ± 25 K and 180 ± 20 K. The estimated fractional abundances of HC₃N toward IRAS 18089 are $(7.5 \pm 0.7) \times 10^{-11}$ (for v7 = 1) and $(3.1 \pm 0.4) \times 10^{-11}$ (for v7 = 2).

3.2.4. Formamide (NH_2CHO)

We have detected a single transition line of NH₂CHO toward IRAS 18089 using the LTE-modeled spectra. We detected the J = 6(2,4)-5(2,3), F = 6-5 transition line of NH₂CHO. We do not observe any other transition lines of NH₂CHO in the entire data. The upper-state energy (E_u) of the detected emission line of NH₂CHO is 33.38 K. To estimate the proper FWHM in km s⁻¹ and integrated intensity ($\int T_{mb}dV$) in K km s⁻¹ of the emission line of NH₂CHO, we fitted the Gaussian model over the observed spectra of NH₂CHO. The resultant LTE and Gaussian fitting spectral lines of NH₂CHO are shown in Figure 4, and the corresponding spectral parameters are listed in Table 2. We observed that the detected emission lines of



Figure 4. Rotational emission lines of C₂H₅CN, CH₃OCHO (both $V_t = 0$ and $V_t = 1$), HC₃N (both v7 = 1 and v7 = 2), and NH₂CHO toward IRAS 18089 with different transitions. The black lines present the observed millimeter-wavelength spectra of IRAS 18089 and the blue synthetic spectra correspond to the LTE model spectra of C₂H₅CN, CH₃OCHO ($V_t = 0$ and $V_t = 1$), HC₃N (v7 = 1 and v7 = 2), and NH₂CHO. The red spectrum indicates the Gaussian model which is fitted over the detected molecular spectra. The green vertical lines indicate the rest frequency positions of the detected transitions of C₂H₅CN, CH₃OCHO (both $V_t = 0$ and $V_t = 1$), HC₃N (both v7 = 1 and v7 = 2), and NH₂CHO.

Molecule	Observed Frequency ^a (GHz)	Transition ^a	E_u^{a} (K)	A_{ij}^{a} (s ⁻¹)	FWHM ^b (km s ⁻¹)	$\int T_{\rm mb} dV^{\rm b}$ (K km s ⁻¹)	Column Density (cm ⁻²)	Excitation Temperature (K)	Remark ^c
C ₂ H ₅ CN	127.520 127.618 129.795 139.335	$\begin{array}{c} 14(2,12){-}13(2,11)\\ 14(1,13){-}13(1,12)\\ 15(1,15){-}14(1,14)\\ 16(0,16){-}15(0,15) \end{array}$	50.02 47.23 51.09 57.48	$\begin{array}{c} 1.69 \times 10^{-4} \\ 1.72 \times 10^{-4} \\ 1.82 \times 10^{-4} \\ 2.26 \times 10^{-4} \end{array}$	$\begin{array}{c} 5.52 \pm 0.24 \\ 5.16 \pm 0.28 \\ 4.82 \pm 0.64 \\ 5.16 \pm 0.22 \end{array}$	0.587 0.563 0.255 0.621	$(1.13 \pm 0.4) \times 10^{14} \mathrm{cm}^{-2}$	$200\pm54~{\rm K}$	Non blended Non blended Non blended Non blended
CH ₃ OCHO, <i>v</i> _t = 0	130.010 130.016 139.565 139.569 141.037 141.044 141.244 141.260 141.350 141.354	$\begin{array}{c} 11(2,10)-10(2,9)E\\ 11(2,10)-10(2,9)A\\ 11(2,10)-10(1,9)E\\ 11(2,10)-10(1,9)A\\ 12(2,11)-11(2,10)E\\ 12(2,11)-11(2,10)A\\ 11(3,8)-10(3,7)E\\ 11(3,8)-10(3,7)A\\ 17(6,11)-17(5,12)A\\ 17(6,11)-17(5,12)E\\ \end{array}$	40.71 40.70 40.71 40.70 47.48 47.47 47.77 47.75 114.59 114.60	$\begin{array}{c} 3.12\times10^{-5}\\ 3.12\times10^{-5}\\ 3.82\times10^{-6}\\ 4.01\times10^{-5}\\ 4.01\times10^{-5}\\ 4.01\times10^{-5}\\ 3.87\times10^{-5}\\ 3.87\times10^{-5}\\ 4.09\times10^{-6}\\ 3.98\times10^{-6} \end{array}$	$\begin{array}{c} 3.36 \pm 0.35 \\ 3.56 \pm 0.42 \\ 3.10 \pm 0.36 \\ 3.23 \pm 0.28 \\ 3.72 \pm 0.29 \\ 4.22 \pm 0.89 \\ 3.90 \pm 0.31 \\ 4.01 \pm 0.35 \\ 5.86 \pm 1.09 \\ 3.37 \pm 0.50 \end{array}$	$\begin{array}{c} 0.284\\ 0.293\\ 0.063\\ 0.081\\ 0.784\\ 0.875\\ 0.995\\ 0.846\\ 0.199\\ 0.054 \end{array}$	$(1.5 \pm 0.3) \times 10^{15} \mathrm{cm}^{-2}$	$200 \pm 48 \text{ K}$	Non blended Non blended Non blended Non blended Non blended Non blended Non blended Blended with CH ₃ OCH ₃ Non blended
$\overline{\text{CH}_{3}\text{OCHO}, v_{t}} = 1$	127.836 128.273 139.381 139.635 140.020 140.622	10(2,8)–9(2,7)A 10(2,8)–9(2,7)E 11(3,8)–10(3,7)A 11(3,8)–10(3,7)E 12(2,11)–11(2,10)A 11(2,9)–10(2,5)E	223.96 223.32 233.19 232.67 235.00 230.07	$\begin{array}{c} 2.95 \times 10^{-5} \\ 2.99 \times 10^{-5} \\ 3.70 \times 10^{-5} \\ 3.72 \times 10^{-5} \\ 3.92 \times 10^{-5} \\ 3.98 \times 10^{-5} \end{array}$	$\begin{array}{c} 4.59 \pm 0.78 \\ 3.96 \pm 0.69 \\ 4.63 \pm 0.86 \\ 4.36 \pm 0.44 \\ 4.05 \pm 0.23 \\ 4.81 \pm 0.73 \end{array}$	$\begin{array}{c} 0.102 \\ 0.076 \\ 0.133 \\ 0.124 \\ 0.144 \\ 0.253 \end{array}$	$(7.1 \pm 0.5) \times 10^{14} \mathrm{cm}^{-2}$	$196\pm74~{ m K}$	Non blended Non blended Non blended Non blended Non blended Non blended
HC ₃ N, $v7 = 1$	127.680 127.863	J = 14-13, l = 1e J = 14-13, l = 1f	366.80 366.86	$\begin{array}{c} 1.61 \times 10^{-4} \\ 1.62 \times 10^{-4} \end{array}$	$\begin{array}{c} 7.22 \pm 0.30 \\ 6.98 \pm 0.22 \end{array}$	1.258 1.072	$(6.02 \pm 0.5) \times 10^{13} \mathrm{cm}^{-2}$	$160\pm25~\mathrm{K}$	Non blended Non blended
$HC_3N, v7 = 2$	128.169 128.175 128.182	J = 14-13, l = 0 J = 14-13, l = 2e J = 14-13, l = 2f	687.82 691.09 691.10	$\begin{array}{c} 1.63 \times 10^{-4} \\ 1.60 \times 10^{-4} \\ 1.60 \times 10^{-4} \end{array}$	$\begin{array}{c} 3.61 \pm 0.53 \\ 3.89 \pm 0.82 \\ 3.96 \pm 0.68 \end{array}$	0.112 0.233 0.349	$(2.50\pm0.3)\times10^{13}\text{cm}^{-2}$	$180 \pm 20 \text{ K}$	Non blended Non blended Non blended
NH ₂ CHO	128.102	J = 6(2,4)-5(2,3), F = 6-5	33.38	1.28×10^{-4}	5.20 ± 0.86	0.429	$(5.01 \pm 0.2) \times 10^{13} \mathrm{cm}^{-2}$	$180\pm62~{\rm K}$	Non blended

Table 2 Summary of the Line Properties of the Detected Molecules toward IRAS 18089

Notes.

 $\overline{}$

^a Frequency, transitions, E_u and A_{ij} are obtained from the LTE modeling. ^b FWHM and $\int T_{mb} dV$ are an estimate from the Gaussian fitting over the molecular lines. ^c Blended and non-blended effects in the observed spectral lines are verified by the LTE modeling and online molecular line list database Splatalogue.

NH₂CHO are non-blended and exhibit above 5σ significance. Using the LTE spectral modeling, the best-fit column density of NH₂CHO, based on the single transition line, is $(5.01 \pm 0.2) \times 10^{13}$ cm⁻² with an excitation temperature of 180 ± 62 K. The fractional abundance of NH₂CHO with respect to H₂ toward IRAS 18089 is $(6.25 \pm 0.8) \times 10^{-11}$.

3.3. Spatial Distribution of Detected COMs

We create the integrated intensity maps of the non-blended transitions of C₂H₅CN, CH₃OCHO ($V_t = 0$ and $V_t = 1$), HC₃N (v7 = 1 and v7 = 2), and NH₂CHO using the CASA task IMMOMENTS toward IRAS 18089. The integrated intensity maps of detected COMs toward IRAS 18089 are created by integrating the spectral data cubes over carefully determined channel ranges where COMs are detected (see Figure 5). We notice that the integrated intensity maps of different COMs have a peak at the position of the continuum. From the integrated emission maps, it is clear that the emission lines of different COMs may have arisen from the extended envelope of IRAS 18089. We also estimated the emitting regions of COMs toward IRAS 18089 by fitting the two-dimensional (2D) Gaussian over the integrated intensity maps using the CASA IMFIT task. The deconvolved beam size of the emitting region of COMs is estimated by using the following equation,

$$\theta_{\rm S} = \sqrt{\theta_{\rm 50}^2 - \theta_{\rm beam}^2},\tag{5}$$

where $\theta_{50} = 2\sqrt{A/\pi}$ denotes the diameter of the circle with area, A is the area that encloses 50% of the peak intensity, and θ_{beam} is the half-power width of the synthesized beam of the integrated emission maps (Rivilla et al. 2017). The value of θ_{50} is estimated using the task IMFIT. The estimated emitting regions of COMs are shown in Table 3. The emitting regions of C₂H₅CN vary between 12".09 (29.43 pc) and 12".12 (29.50 pc). The emitting regions of CH₃OCHO with $V_t = 0$ and $V_t = 1$ states vary between 12"07 (29.38 pc)-12".15 (29.57 pc) and 12".07 (29.38 pc)-12".14 (29.55 pc). The emitting regions of HC_3N with vibrationally excited states v7 = 1 and v7 = 2 vary between $12''_{...}11$ (29.47 pc)-12.''12 (29.50 pc) and 12.''10 (29.45 pc)-12.''11 (29.47 pc). Similarly, the emitting region of NH₂CHO is 12."13 (29.52 pc). A smaller emitting region of COMs in comparison to the synthesized beam size implies that the emitting area of COMs is spatially unresolved in the current data set. Further high-resolution observations of these lines are required, possibly using the ALMA 12 m array, to examine the distribution and chemical morphology of COMs in the IRAS 18089 region.

4. Discussion

4.1. Possible Formation Mechanism of COMs

4.1.1. Ethyl Cyanide (C₂H₅CN)

The N-bearing molecule, C₂H₅CN, is formed on the grain surface of high-mass protostars and hot molecular cores (see

Mehringer et al. 2004; Garrod 2013; Garrod et al. 2017, 2022, for details). Garrod (2013) showed that the subsequential hydrogenation of HC₃N in the freefall collapse phase can form vinyl cyanide (CH₂CHCN) (HC₃N + 2H \rightarrow CH₂CHCN). The subsequential hydrogenation of the CH2CHCN forms C2H5CN on the grain surface of the hot molecular cores and high-mass protostars (CH₂CHCN + 2H \rightarrow C₂H₅CN; Garrod 2013), through barrierless and exothermic radical-radical reactions (Singh et al. 2021). This particular chemical reaction is demonstrated to be the most efficient way for the formation of C₂H₅CN toward Sgr B2, G10.47+0.03, G31.41+0.31, and other molecular cores (Belloche et al. 2009; Manna & Pal 2023; Mininni et al. 2023). This reaction may be most efficient toward IRAS 18089 because HC₃N acts as a possible precursor of C₂H₅CN, and we detected the emission lines of HC₃N from this source, which we already discussed in this paper.

4.1.2. Methyl Formate (CH₃OCHO)

In this article, we present the first detection of CH₃OCHO with $V_t = 0$ and $V_t = 1$ states toward IRAS 18089 using the ACA. In the hot molecular cores and high-mass protostars, the CH₃OCHO molecule can efficiently be formed by the reaction of CH₃O and HCO radicals on the surface of dust grains $(CH_3O + HCO \rightarrow CH_3OCHO)$ (see Garrod et al. 2008, and references therein). Earlier, Manna & Pal (2022) showed that the reactions between radical CH₃O and radical HCO produce CH₃OCHO toward the hot molecular core IRAS 18566+0408. Garrod (2013) showed the chemical reaction between CH₃O and HCO is mobile between 30 and 40 K, and this chemical reaction is the most efficient pathway to the formation of CH₃OCHO toward the hot molecular cores and high-mass protostars. According to the chemical modeling of Garrod (2013), the gas phase CH₃OCHO mainly comes from the ice phase of massive protostars. Earlier, Gorai et al. (2021) reported that the UV photodissociation of CH₃OH leads to the formation of CH₂O, CH₃O, and CH₃ at around a temperature of 40 K, and these molecules create the COMs, like CH₃OCHO and CH₃OCH₃. At temperature $T \sim 40$ K in the gas phase, the reaction of protonated CH₃OH and H₂CO creates $H_5C_2O_2^+$ (Gorai et al. 2021). The CH₃OCHO is created in the hot molecular cores and massive protostars via the electron recombination of $H_5C_2O_2^+$ ($H_5C_2O_2^+ + e^- \rightarrow CH_3OCHO + H$) (Bonfand et al. 2019; Gorai et al. 2021). Earlier, Balucani et al. (2015) proposed an efficient gas phase reaction of CH₃OCHO in a cold environment where CH₃OCH₃ behaves as a possible precursor of CH₃OCHO. Therefore, it is evident that CH₃OCHO can be produced through both grain surface and gas phase reactions in the hot molecular cores and high-mass protostars. Note that Beuther et al. (2005) detected CH₃OCH₃ with transition J = 19(1,18) - 18(2,17) AA toward IRAS 18089 using SMA. However, such detection of a single transition line



Figure 5. Integrated intensity maps of C₂H₅CN, CH₃OCHO (both $V_t = 0$ and $V_t = 1$), HC₃N (both v7 = 1 and v7 = 2), and NH₂CHO toward IRAS 18089, which are overlaid with the 2.1 mm continuum emission map of IRAS 18089 (black contours). The contour levels are at 20%, 40%, 60%, 80%, and 100% of the peak flux. The red circles represent the synthesized beam of the integrated emission maps.

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Figure 5. (Continued.)

Molecule	Observed Frequency	Transition	Emitting Region	Physical Scale ^a
	(GHz)		(")	(pc)
C ₂ H ₅ CN	127.520	14(2,12)–13(2,11)	12.09 ± 0.61	29.43
	127.618	14(1,13)-13(1,12)	12.10 ± 0.65	29.45
	129.795	15(1,15)-14(1,14)	12.12 ± 0.59	29.50
	139.335	16(0,16)–15(0,15)	12.11 ± 0.60	29.47
CH ₃ OCHO, $v_t = 0$	130.010	11(2,10)-10(2,9)E	12.08 ± 0.58	29.40
	130.016	11(2,10)–10(2,9)A	12.07 ± 0.57	29.38
	139.565	11(2,10)-10(1,9)E	12.09 ± 0.59	29.43
	139.569	11(2,10)–10(1,9)A	12.11 ± 0.61	29.47
	141.037	12(2,11)-11(2,10)E	12.14 ± 0.58	29.55
	141.044	12(2,11)-11(2,10)A	12.09 ± 0.55	29.43
	141.244	11(3,8)–10(3,7)E	12.15 ± 0.59	29.57
	141.260	11(3,8)–10(3,7)A	12.11 ± 0.58	29.47
	141.354	17(6,11)–17(5,12)E	12.08 ± 0.61	29.40
CH ₃ OCHO, $v_t = 1$	127.836	10(2,8)–9(2,7)A	12.11 ± 0.58	29.48
	128.276	10(2,8)–9(2,7)E	12.10 ± 0.61	29.45
	139.381	11(3,8)–10(3,7)A	12.14 ± 0.59	29.55
	139.635	11(3,8)–10(3,7)E	12.07 ± 0.57	29.38
	140.020	12(2,11)-11(2,10)A	12.11 ± 0.60	29.47
	140.622	11(2,9)–10(2,5)E	12.09 ± 0.56	29.43
$HC_{3}N, v7 = 1$	127.680	$J = 14-13, \ l = 1e$	12.11 ± 0.62	29.47
	127.863	$J = 14 - 13, \ l = 1f$	12.12 ± 0.63	29.50
HC ₃ N, $v7 = 2$	128.169	$J = 14 - 13, \ l = 0$	12.10 ± 0.58	29.45
	128.175	$J = 14-13, \ l = 2e$	12.11 ± 0.60	29.47
	128.182	$J = 14-13, \ l = 2f$	12.10 ± 0.59	29.45
NH ₂ CHO	128.102	J = 6(2,4) - 5(2,3), F = 6 - 5	12.13 ± 0.62	29.52

 Table 3

 Estimated Emitting Regions of Detected COMs Toward IRAS 18089

Note.

^a During the estimation of the physical scale of the emitting regions of different molecules, we used the cosmological parameters from Plank with Hubble constant $H_0 = 0.6731$, $\Omega_M = 0.315$, and $\Omega_L = 0.685$ (Aghanim et al. 2020).

of one complex molecule could not be considered as conclusive evidence of the presence of the molecule in high-mass protostars.

4.1.3. Cyanoacetylene (HC₃N)

In the ISM, acetylene (C_2H_2) is one of the known compounds that is formed on the grain surfaces (Chapman et al. 2009). After the evaporation of C_2H_2 from the grains, there are two possible scenarios.

1. When the UV field is strong, like in photodissociation regions (PDRs), then C_2H_2 photodissociates into the ethynyl radical (C_2H) ($C_2H_2 + h\nu \rightarrow C_2H + H$) (Cherchneff et al. 1993; Meier & Turner 2005).

2. In the weak UV field regime (without a PDR) in the presence of the cyano radical (CN), C_2H_2 reacts with CN to create HC_3N ($C_2H_2 + CN \rightarrow HC_3N + H$) (Fukuzawa & Osamura 1997; Meier & Turner 2005; Chapman et al. 2009). Recently, Taniguchi et al. (2022) claimed that the HC_3N is created in high-mass protostars and UC H II regions when C_2H_2

immediately reacts with the CN. The HC_3N molecule is associated with highly dense, warm, and shielded gas in the star-forming regions or high-mass protostars (Taniguchi et al. 2022).

In the star-forming regions, with the presence of UV radiation, the HC₃N molecule is easily destroyed by reacting with C+ ions (Rodriguez-Franco et al. 1998; Meier & Turner 2005). After the destruction, HC₃N converts into C₂H or C₃N if HC₃N is photodissociated (Cherchneff et al. 1993). Similarly, HC₃N converts into C₃H⁺ or C₄N⁺ if HC₃N reacts with C+ (Bohme & Raksit 1985). The possible destruction reactions are:

$$\mathrm{HC}_{3}\mathrm{N} + h\nu \to \mathrm{C}_{2}\mathrm{H} + \mathrm{CN},\tag{6}$$

$$\mathrm{HC}_{3}\mathrm{N} + h\nu \to \mathrm{C}_{3}\mathrm{N} + \mathrm{H},\tag{7}$$

$$HC_3N + C^+ \to C_3H^+ + CN, \qquad (8)$$

$$\mathrm{HC}_{3}\mathrm{N} + \mathrm{C}^{+} \to \mathrm{C}_{4}\mathrm{N}^{+} + \mathrm{H}. \tag{9}$$

The rates of the above reaction are reported in Cherchneff et al. (1993), and Taniguchi et al. (2022) showed that these

destruction pathways are the most efficient toward high-mass protostars and UC H II regions.

4.1.4. Formamide (NH₂CHO)

In the ISM, the formation pathways of NH₂CHO are still a topic of debate in both gas phase and solid state ice mantle formation routes (Garrod et al. 2008). Previously, Garrod (2013) showed that NH₂CHO is created in the gas phase barrierless reaction between NH₂ and H₂CO (NH₂ + H₂CO \rightarrow NH₂CHO + H). Earlier, Garrod (2013) and Suzuki et al. (2018) showed that this reaction is the most efficient for the formation of NH₂CHO toward hot molecular cores. After that, Gorai & Bhat et al. (2020) claimed that the reaction is responsible for the production of NH₂CHO toward G10.47+0.03.

4.2. Comparison between the Observed and Modeled Abundance of COMs

Here we compare the estimated fractional abundances of C₂H₅CN, CH₃OCHO, HC₃N, and NH₂CHO toward IRAS 18089 with the existing three-phase warm-up chemical model abundances of Suzuki et al. (2018). For chemical modeling, Suzuki et al. (2018) used the gas-grain chemical kinetics code NAUTILUS in the environment of hot molecular cores and massive protostars. During the chemical modeling of complex molecules, Suzuki et al. (2018) assumed an isothermal collapse phase after a static warm-up phase. In the first phase, the gas density increases from 3×10^3 to 2×10^7 cm⁻³ and dust temperature decreases from 16 to 8K under the freefall collapse (Suzuki et al. 2018). In the second phase, known as the warm-up phase, the dust temperature increases from 8 to 400 K, and the gas density remains fixed at 2×10^7 cm⁻³. For the chemical modeling, Suzuki et al. (2018) used the following reactions on the grain surfaces to produce the C₂H₅CN, CH₃OCHO, and HC₃N:

$$CH_2CHCN + 2H \rightarrow C_2H_5CN, \tag{10}$$

$$CH_3O + HCO \rightarrow CH_3OCHO,$$
 (11)

$$C_2H_2 + CN \rightarrow HC_3N + H, \qquad (12)$$

$$NH_2 + H_2CO \rightarrow NH_2CHO + H.$$
 (13)

We explain reactions (10), (11), (12), and (13) in Section 4.1. The three-phase warm-up chemical modeling of Suzuki et al. (2018) is appropriate for explaining the chemical abundance and evolution of COMs toward IRAS 18089 because the gas density of IRAS 18089 is 1.3×10^7 cm⁻³ (Sanhueza et al. 2021) and the gas temperature is above 100 K (Beuther et al. 2004a). After the chemical modeling, Suzuki et al. (2018) determined the modeled abundance of C₂H₅CN, CH₃OCHO, HC₃N, and NH₂CHO to be 6.3×10^{-10} , 4.9×10^{-9} , 1.1×10^{-11} , and 4.0×10^{-11} respectively using the fast warm-up model with the help of reactions (10), (11), (12), and (13) on the grain surfaces and gas phases of hot molecular cores and

massive prostars. Our estimated abundances of C_2H_5CN , CH_3OCHO ($V_t = 0$), HC_3N , and NH_2CHO are reported in Section 3.2. We find that our estimated abundances of C_2H_5CN , CH_3OCHO , HC_3N , and NH_2CHO are quite similar to the chemical modeling abundances of Suzuki et al. (2018). This result indicates that reactions (10), (11), (12), and (13) may be responsible for the production of C_2H_5CN , CH_3OCHO , HC_3N , and NH_2CHO toward IRAS 18089.

5. Conclusion

In this article, we present the identification of the rotational emission lines of C₂H₅CN, CH₃OCHO ($V_t = 0$ and $V_t = 1$), HC₃N (v7 = 1 and v7 = 2), and NH₂CHO toward IRAS 18089. The estimated abundance of C2H5CN toward IRAS 18089 is $(1.40 \pm 0.5) \times 10^{-10}$. The estimated abundance of CH₃OCHO with respect to H_2 is $(1.90\pm0.9)\times10^{-9}$ and $(8.90\pm$ $0.8) \times 10^{-10}$ for $V_t = 0$ and $V_t = 1$, respectively. The abundance of HC₃N toward IRAS 18089 is $(7.5 \pm 0.7) \times 10^{-11}$ (for v7 = 1) and $(3.1 \pm 0.4) \times 10^{-11}$ (for v7 = 2). Similarly, the abundance of NH₂CHO toward IRAS 18089 is $(6.25 \pm 0.8) \times$ 10^{-11} . We created the integrated emission maps of detected COMs, and we observed that the detected emission lines of different COMs arise from the extended envelope of the protostar. We also compared the estimated abundances of C₂H₅CN, CH₃OCHO, HC₃N, and NH₂CHO with the existing three-phase warm-up modeling abundances of those molecules. After the comparisons, we noticed that the observed and modeled abundances are quite similar. So, the N-bearing molecules C₂H₅CN and HC₃N are most probably created via the subsequential hydrogenation of CH₂CHCN and the reactions between C2H2 and CN on the grain surface of IRAS 18089. The O-bearing molecule CH₃OCHO is probably created via the reactions between radical CH₃O and radical HCO on the grain surface of IRAS 18089. Similarly, the O- and N-bearing molecule NH₂CHO is most probably formed between the reactions of NH₂ and H₂CO in the gas phase of IRAS 18089. The prebiotic chemistry of C₂H₅CN, CH₃OCHO, HC₃N, and NH₂CHO toward IRAS 18089 suggests that both gas phase and grain surface chemistry are efficient for the production of other COMs in that protostar, including those molecules that are chemically connected with those detected molecules. The detections of both N- and O-bearing molecules toward IRAS 18089 indicate that IRAS 18089 is a reservoir of several other COMs. A spectral line survey is needed using the ALMA 12 m array to understand the prebiotic chemistry in this high-mass protostar, which will be carried out in our follow-up study.

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Conflicts of Interest

The authors declare no conflict of interest.

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