Identification of Prebiotic Molecules Containing Peptide-like Bonds in a Hot Molecular Core, G10.47+0.03

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Abstract

After hydrogen, oxygen, and carbon, nitrogen is one of the most chemically active species in the interstellar medium. Nitrogen-bearing molecules are very important as they are actively involved in the formation of biomolecules. Therefore, it is essential to look for nitrogen-bearing species in various astrophysical sources, specifically around high-mass star-forming regions where the evolutionary history is comparatively poorly understood. In this paper, we report on the observation of three potential prebiotic molecules, namely, isocyanic acid (HNCO), formamide (NH₂CHO), and methyl isocyanate (CH₃NCO), which contain peptide-like bonds (–NH–C(=O)–) in a hot molecular core, G10.47 + 0.03 (hereafter, G10). Along with the identification of these three complex nitrogen-bearing species, we speculate on their spatial distribution in the source and discuss their possible formation pathways under such conditions. A rotational diagram method under local thermodynamic equilibrium has been employed to estimate the excitation temperature and the column density of the observed species. The Markov Chain Monte Carlo method was used to obtain the best-suited physical parameters of G10 as well as line properties of some species. We also determined the hydrogen column density and the optical depth for a different continuum observed in various frequency ranges. Finally, based on these observational results, we have constructed a chemical model to explain the observational findings. We found that HNCO, NH₂CHO, and CH₃NCO are chemically linked with each other.

Unified Astronomy Thesaurus concepts: Pre-biotic astrochemistry (2079); Star formation (1568); Interstellar medium (847); Astronomy data analysis (1858); Radiative transfer simulations (1967); Chemical abundances (224); Massive stars (732); High mass x-ray binary stars (733); Protostars (1302)

1. Introduction

Various interdisciplinary studies are involved in the search for the origin of life on Earth. Whether life evolved ab initio here on Earth or came from another part of space is debatable, but it is accepted that our single-celled ancestors formed from the raw materials present at that time somewhere in the universe. When, where, and how the first life came to be is not straightforward to answer. However, in the current era, it is necessary to try explaining how the building blocks of life (simple → complex molecule → biomolecule) could be independently produced in the universe.

Around 200 molecular species have been identified in the interstellar medium or circumstellar shells. Among them are several species marked as the precursor to biomolecules. Study of these prebiotic molecules is always fascinating as they are involved in the formation of amino acids, proteins, and the basic building blocks of life (Chakrabarti & Chakrabarti 2000a, 2000b; Das et al. 2008; Garrod 2013; Chakrabarti et al. 2015; Majumdar et al. 2015; Das et al. 2019). Protein synthesis occurs through peptide-bond formation (Goldman et al. 2010). CN is the first observed nitrogen-bearing species in space (McKellar 1940). Since then, various nitrogen-bearing species have been identified in numerous astronomical objects. Hot-core regions are unique laboratories of complex organic molecules. Forests of molecular lines have been identified in several hot molecular cores (e.g., Belloche et al. 2016; Garrod et al. 2017). Here, we will focus on the observation of a hot molecular core, G10.47 + 0.03 (hereafter, G10), which is located at a distance of 8.6 kpc (Sanna et al. 2014) with a luminosity $5 \times 10^7 L_\odot$ (Cesarini et al. 2010).

Among the prebiotic molecules, methanimine (CH₂NH) and methylamine (CH₃NH₂) are the simple imine and amine, respectively, which play a significant role in the synthesis of the simplest amino acid, glycine (NH₂CH₂COOH) (Allweg et al. 2017; Sil et al. 2018). These molecules have been identified in G10, which strengthens the possibility of the presence of glycine in this source (Ohishi et al. 2019).

Isocyanic acid (HNCO) is the simple molecule with four biogenic elements (C, N, O, and H) making a peptide bond, –NH–C(=O)–. HNCO was observed long ago toward the high-mass star-forming region Sgr B2 (Snyder & Buhl 1972). It has been observed in various astronomical objects such as a translucent molecular cloud (Turner et al. 1999), a dense core (Marcelino et al. 2018), and the low-mass protostar IRAS 16293–2422 (Bisschop et al. 2008). It was also previously detected in G10 (Wyrowski et al. 1999).

Formamide (NH₂CHO) is the simplest possible amide and a potential prebiotic molecule which contains a peptide bond that can link with amino acids and form proteins. NH₂CHO is also a precursor of genetic and metabolic molecules (Saladino et al. 2012). This molecule is one of the key species for the formation of nucleobases and nucleobase analogs. NH₂CHO was observed for the first time toward the high-mass star-forming region Sgr B2 (Rubin et al. 1971). Subsequently, it was identified in other hot cores, such as Orion KL, G327.3 – 0.6, G34-3 + 0.15, NGC 6334 (Turner 1991; Begelund et al. 2019), the solar-type low-mass protostar IRAS 16293–2422 (Kahane et al. 2013), and in the shock of the prestellar core L1157-B1 (Codella et al. 2017). NH₂CHO was previously

1 https://www.astro.uni-koeln.de/cdms/molecules
detected in G10 using millimeter and submillimeter wavelengths with Submillimeter Array (SMA) observation (Rolffs et al. 2011).

Methyl isocyanate (CH$_3$NCO) is another potential prebiotic molecule, which also has a peptide-like bond. It has recently been observed in the high-mass star-forming region Sgr B2 (Cernicharo et al. 2016) and the low-mass star-forming region IRAS 16293–2422 (Ligierink et al. 2017; Martín-Domènech et al. 2017). Here, for the first time, we report the identification of CH$_3$NCO in G10. HNCO has been clearly identified in G10, but for NH$_2$CHO, no clear peak was present in the observed spectra of Rolffs et al. (2011). Recently, HNCO and NH$_2$CHO both have been identified, but CH$_3$NCO has been tentatively identified in the 67P/Churyumov–Gerasimenko comet by the double-focusing mass spectrometer of the ROSINA experiment on ESA’s Rosetta mission (Aalto et al. 2017).

In this paper, we present a combined study of observational analysis and chemical modeling of the peptide-like bond molecules. We report identifications of HNCO, NH$_2$CHO, and CH$_3$NCO in G10. To understand the formation of these three species, we prepare a chemical model which mimics the observed results. We have organized this paper as follows. In Section 2, we describe observational details and data analysis procedures. Observational results are presented in Section 3. A chemical model and results are described in Section 4. Finally, in Section 5, we make concluding remarks.

### 2. Observations, Data Analysis, and Line Identification

In this paper, we have used Atacama Large Millimeter/submillimeter Array (ALMA) cycle 4 archival data of G10 observation (#2016.1.00929.S.). The phase center of the observation is located at α(J2000) = 18$^h$08$^m$38$^s$.232 and δ(J2000) = −19°51′50.4″. Observations were performed with ALMA Band 4 covering four spectral ranges: (i) 129.50–131.44 GHz, (ii) 147.50–149.43 GHz, (iii) 153.00–154.93 GHz, and (iv) 158.49–160.43 GHz. In this observation, the flux calibrator was J1733–1304, the phase calibrator was J1832–2039 and the bandpass calibrator was J1924–2914. The systematic velocity of this source was 67–68 km s$^{-1}$ (Rolffs et al. 2011). An observational summary is given in Table 1. All the analyses, such as spectral and line analyses, were done using CASA 4.7.2 software (McMullin et al. 2007). We have implemented a first-order baseline fit by using the “uvcontsub” command available in the CASA program. We have divided each spectral window into two data cubes: continuum and line emission for the analysis. We did not apply the self-calibration and ALMA missing flux correction. The line identification of all the observed species presented in this paper was carried out using CASSIS software together with the Cologne Database for Molecular Spectroscopy (Müller et al. 2001, 2005) and Jet Propulsion Laboratory (Pickett et al. 1998). To firmly identify a molecular transition corresponding to the observed spectra, we checked line blending, systematic velocity ($V_{LSR}$), upper state energy ($E_{up}$), and the Einstein coefficient. After assigning a molecular species to the observed spectral feature, we used local thermodynamic equilibrium (LTE) modeling to confirm or reject the identification.

### 3. Observational Results

#### 3.1. Continuum Images

Cesaroni et al. (2010) observed G10 with the Very Large Array and identified three distinct H II regions, A, B1, and B2, inside the hot molecular core. The rms noises of these observation were 269 $\mu$Jy/beam, 73 $\mu$Jy/beam, 773 $\mu$Jy/beam, and 227 $\mu$Jy/beam for the 6 cm, 3.6 cm, 2 cm, and 1.6 cm continua. The corresponding synthesized beam and position angles are $0''73 \times 0''42$ and $-11''2$, $0''37 \times 0''19$ and $-15''5$, $0''74 \times 0''39$ and $16''2$, and $0''15 \times 0''092$ and $6''8$, respectively. They referred to B1 and B2 as hypercompact H II regions and A as an ultracompact H II region. Rolffs et al. (2011) observed this source with SMA. They observed continua at three different frequency regions, 201/211 GHz, 345/355 GHz, and 681/691 GHz. However, the beam sizes of the 201/211 GHz and 681/691 GHz frequency ranges were not sufficient to resolve the continua, but the extension can be seen at 345/355 GHz. Here, we also observed continuum maps of G10 at four different frequencies (130.5 GHz, 148.51 GHz, 153.96 GHz, and 159.45 GHz), which are presented in Figure 1. Our observed beam sizes are also not sufficient to resolve the continua. The observed parameters of continuum images such as frequency, position, synthesized beam size, position angle, peak flux, integrated flux, and deconvolved beam size (FWHM) are provided in Table 2. We obtained the peak flux, integrated flux, and the deconvolved beam size by using two-dimensional Gaussian fitting of the continuum images.

#### 3.2. Rotation Diagram Analysis

In this work, we have detected multiple lines of HNCO, NH$_2$CHO, and CH$_3$NCO and carried out rotation diagram analysis to obtain the temperature and column density of the observed species. Assuming the observed transitions of these species are optically thin and are in LTE, we perform rotational diagram analysis. For optically thin lines, the column density

| Source Name | Observation Date | On-source Time | Number of antennas | Frequency Range (GHz) | Channel Spacing (kHz) | Baseline (m) |
|-------------|------------------|----------------|--------------------|-----------------------|-----------------------|-------------|
| G10.47 + 0.03 | 2017 Mar 5 | 01:53:40 | 39 | 129.50–131.44 | 244, 976 | 310 15 |
| | 2017 Jan 28 | 00:33:6 | 40 | 147.50–149.43 | 244, 976 | 272 15 |
| | 2017 Mar 6 | 01:03:5 | 41 | 153.00–154.93 | 244, 976 | 331 15 |
| | 2017 Mar 7 | 00:28:72 | 39 | 158.49–160.63 | 244, 976 | 331 15 |

2 https://cassis.irap.omp.eu

3 http://www.astro.uni-koeln.de/cdms

4 http://spec.jpl.nasa.gov
can be expressed as (Goldsmith & Langer 1999),

$$ N_u^{\text{thin}} / g_u = \frac{3 k_B \int T_{mb} dV}{8 \pi^3 \nu S \mu^2}, $$ (1)

where $g_u$ is the degeneracy of the upper state, $k_B$ is the Boltzmann constant, $\int T_{mb} dV$ is the integrated intensity, $\nu$ is the rest frequency, $\mu$ is the electric dipole moment, and $S$ is the transition line strength. Under LTE conditions, the total column density can be written as

$$ N_u^{\text{thin}} / g_u = \frac{N_{\text{total}}}{Q(T_{\text{rot}})} \exp(-E_u / k_B T_{\text{rot}}), $$ (2)

where $T_{\text{rot}}$ is the rotational temperature, $E_u$ is the upper state energy, and $Q(T_{\text{rot}})$ is the partition function at rotational temperature. Equation (2) can be rearranged as,

$$ \log \left( \frac{N_u^{\text{thin}}}{g_u} \right) = -\frac{E_u}{k_B T_{\text{rot}}} + \log \left( \frac{N_{\text{total}}}{Q(T_{\text{rot}})} \right). $$ (3)

The above equation shows that there is a linear relationship between the upper state energy and column density at the upper level. Using this equation, we can extract both column density and rotational temperature. Line parameters of the observed transitions are estimated with a single Gaussian fit. Observed and Gaussian fitted spectra of various transitions of HNCO, NH2CHO, and CH3NCO are provided in the Appendix. All the line parameters of observed molecules such as molecular transitions (quantum numbers) along with their rest frequency ($\nu$), upper state energy ($E_u$), line width ($\Delta V$), line intensity ($S \mu^2$), and integrated intensity ($\int T_{mb} dV$) are presented in Table 3.

Figure 1. Images of continuum emission observed toward G10 with ALMA at (i) 130.5 GHz ($\sigma = 7$ mJy/beam), (ii) 148.51 GHz ($\sigma = 13$ mJy/beam), (iii) 153.96 GHz ($\sigma = 10$ mJy/beam), and (iv) 159.45 GHz ($\sigma = 9$ mJy/beam). Contours are drawn at $3\sigma$, $9\sigma$, $27\sigma$, and $81\sigma$ for all the continuum maps. The observed beam is shown in the lower left corner of each figure. Black crosses in the continuum images indicate the H II regions B1, B2, and A in a counterclockwise direction starting from the left black cross situated in the white and pink contour of the continuum images (Cesaroni et al. 2010).
We have identified multiple hyperfine transitions of HNCO and NH$_2$CHO. However, with the present spectral resolution it is not possible to resolve these transitions. Since there were various hyperfine transitions corresponding to a single observed spectral profile, we have split the observed intensity flux according to their $S_{\mu}^2$ values. Then we have used the most probable (maximum intensity) hyperfine transitions in rotational diagram analysis. Selected transitions are then used to obtain the rotational temperature and column density from the rotational diagram. We have detected many transitions of CH$_3$NCO but few of them are blended with some other nearby molecular transitions. In Table 3, we have provided all the observed transitions. However, the integrated intensity is estimated only for nonblended transitions of CH$_3$NCO, which are further used in the rotational diagram analysis of it. Rotational diagrams of HNCO, NH$_2$CHO, and CH$_3$NCO are presented in Figure 2.

3.3. Hydrogen Column Density Estimation

Flux density of the dust continuum ($S_{\nu}$) for the optically thin condition can be written as

$$S_{\nu} = \Omega \tau_{\nu} B_{\nu}(T_d),$$

where $\Omega$ is the solid angle of the synthesized beam, $\tau_{\nu}$ is the optical depth, $T_d$ is the dust temperature, and $B_{\nu}(T_d)$ is the Planck function (Whittet 1992). Optical depth can be expressed as

$$\tau_{\nu} = \rho_d \kappa_{\nu} L,$$

where $\rho_d$ is mass density of dust, $\kappa_{\nu}$ is the mass absorption coefficient, and $L$ is the path length. Using the dust-to-gas mass ratio ($Z$), the mass density of the dust can be written as

$$\rho_d = Z \mu_H \rho_\text{H} = Z \mu_H N_{\text{H}_2} 2m_\text{H}/L,$$

where $\rho_\text{H}$ is the mass density of hydrogen, $N_{\text{H}_2}$ is the column density of hydrogen, $m_\text{H}$ is the hydrogen mass and $\mu_\text{H}$ is the mean atomic mass per hydrogen. Here, we used $Z = 0.01$, $\mu_\text{H} = 1.41$ (Cox & Pilachowski 2000), and a dust temperature of 200 K. The measured peak flux density of the dust continuum of the source at different frequencies is noted in Table 2. From the above equations, the column density of molecular hydrogen can be written as

$$N_{\text{H}_2} = \frac{S_{\nu}}{2\kappa_{\nu} B_{\nu}(T_d) Z \mu_H m_\text{H}},$$

According to the extrapolation of the data presented in Ossenkopf & Henning (1994), the mass absorption coefficient per gram of dust at 130.50, 148.51, 153.96, and 159.45 GHz (2.30, 2.02, 1.94, and 1.88 mm respectively) is ~0.20 cm$^2$ g$^{-1}$ for the thin ice condition. If we adopt the formula

| Frequency (GHz) | Position (ICRS 2000) | Synthesized Beam ($'^{\circ}$ $''$) | Position Angle (degrees) | Peak Flux (Jy/beam) | Integrated Flux ($^\circ$) | FWHM (degrees) | rms (mJy/beam) |
|----------------|----------------------|-------------------------------------|------------------------|--------------------|-------------------------|----------------|----------------|
| 130.50         | 18:08:38.23          | $-19.51.50.34$                      | 2.44 $\times$ 1.64     | 63.16              | 1.06(0.007)             | 1.367(0.015)   | 1.04(0.057)    | 7               |
| 148.51         | 18:08:38.24          | $-19.51.50.42$                      | 1.98 $\times$ 1.57     | 64.28              | 1.37(0.012)             | 2.031(0.026)   | 1.22(0.041)    | 13              |
| 153.96         | 18:08:38.24          | $-19.51.50.32$                      | 2.03 $\times$ 1.47     | 73.50              | 1.59(0.001)             | 2.138(0.020)   | 1.00(0.031)    | 10              |
| 159.45         | 18:08:38.23          | $-19.51.50.35$                      | 2.38 $\times$ 1.39     | 77.84              | 1.86(0.014)             | 2.477(0.030)   | 1.01(0.047)    | 9               |

Figure 2. Rotational diagrams of HNCO, NH$_2$CHO, and CH$_3$NCO. Black filled squares are the data points and red lines represent the error bars. Best-fit rotational temperature and column density are mentioned inside the small boxes in the corresponding figures.


\[ k = 0.90(v/230 \text{ GHz})^3 \text{ cm}^2 \text{ g}^{-1} \] (Motogi et al. 2019) in estimating the mass absorption coefficient, where \( k_{230} = 0.90 \text{ cm}^2 \text{ g}^{-1} \) is the emissivity of the dust grains at a gas density of \( 10^5 \text{ cm}^{-3} \) covered by a thin ice mantle at 230 GHz.

The dust spectral index \( \beta \) used is \( \sim 1.6 \) (Friesen et al. 2005). Following the above-mentioned formula, the obtained values of the mass absorption coefficient are 0.36, 0.45, 0.47, and 0.50 for the frequencies 130.5 GHz, 148.5 GHz, 153.96 GHz, and 159.45 GHz respectively. We estimated the hydrogen column density and optical depth of dust for the four frequency regions.

Estimated hydrogen column density and optical depth values are given in Table 4. We take a mean value to find out the resultant column density of the source. By taking the average of these four continuum values, we obtained a column density of \( \sim 1.35 \times 10^{23} \text{ cm}^{-2} \). The observed average hydrogen column density is \( \sim 2 \) times lower (see Table 4) if we consider the mass absorption coefficient values as estimated following Motogi et al. (2019). The optical depth of the dust is estimated to be 0.135. The achieved optical depth suggests that the source is optically thin in this frequency range and with the present angular resolution of the observation.

### 3.4. Results of Observed Species

#### 3.4.1. Isocyanic Acid, HNCO

We have observed numerous hyperfine transitions of HNCO. All the line parameters of perceived transitions are summarized in Table 3. The spatial distribution of the observed HNCO transitions is shown in Figure 3. Here, we have depicted the spatial distribution of two transitions of HNCO with two different upper state energies. To determine the emitting region of various molecular transitions, we have used two-dimensional Gaussian fittings of the first-order moment map image. \( 6_{1,6} - 5_{1,5} \) emission of HNCO is found to be more compact (\( \theta \sim 1.1'' \)) than the \( 7_{1,7} - 6_{1,6} \) transition (\( \theta \sim 1.25'' \)). For \( 7_{0,8} - 6_{0,7} \) and \( 7_{2,6} - 6_{2,5} \) transitions we found a slightly extended region (\( \theta \sim 1.38'' \)). However, the morphological structures of spatial distribution of all transitions are similar. The obtained rotational temperature, column density, and fractional abundances are given in Table 5. From the rotational diagram analysis, we obtained a rotational temperature of about 317 K, and a column density of \( \sim 1.37 \times 10^{17} \text{ cm}^{-2} \). Gibb et al. (2003) estimated the rotational temperature and column density of HNCO in G10 to be 328 K and 6.76 \times 10^{16} \text{ cm}^{-2} \).
Interestingly, it is observed that emission with average value 1.35 \times 10^{13}, 1.88 \times 10^{13}, 1.62 \times 10^{13}, 1.94 \times 10^{13}, 1.48 \times 10^{13}, 2.02 \times 10^{13}, 1.32 \times 10^{13}, 1.48 \times 10^{13}, 1.62 \times 10^{13}, 1.26 \times 10^{13}, 1.62 \times 10^{13}, 1.62 \times 10^{13}, 1.62 \times 10^{13} cm^{-2} optical depth, respectively. Here, we obtained a column density which is about twice as high, and a similar rotational temperature, to those reported in Gibb et al. (2003).

### 3.4.2. Formamide, NH$_2$CHO

We have identified several hyperfine transitions of NH$_2$CHO. All the line parameters of the observed NH$_2$CHO transitions are presented in Table 3. Spatial distribution of the observed NH$_2$CHO transitions are depicted in Figure 3. Spatial distribution of $T_2.6 - T_2.5$ ($E_u = 40.40$ K) and $T_6.1 - T_6.0$ ($E_u = 135.74$ K) transitions show a similar nature. We obtained a higher rotational temperature of $\sim 439$ K. We obtained the column density of NH$_2$CHO of $\sim 3.88 \times 10^{15}$ cm$^{-2}$ which is in good agreement with a previous study (Rolffs et al. 2011). Spatial distribution of NH$_2$CHO is also found to be similar to that of HNCO. The emitting region ($\theta$) of NH$_2$CHO transitions varies between 1$''$18 and 1$''$55.

### 3.4.3. Methyl Isocyanate, CH$_3$NCO

In CH$_3$NCO, there is an internal rotation of the methyl group (CH$_3$, described by quantum number $m$) and a low-frequency CNC bending motion. Estimated energies for the substates $m = 1, 2$ relative to the ground state ($m = 0$) are 8.4 and 36.8 cm$^{-1}$ respectively. For the $m = 3$ substate this estimated relative energy is 79.7 cm$^{-1}$, 80.3 cm$^{-1}$ for the nearly two degenerate $m = 3$ substates and 140.6 cm$^{-1}$ for the $m = 4$ substate. The next higher vibrational state was found to be the first excited state of the CNC bending mode, $V_{cb} = 1$ at 182.2 cm$^{-1}$ (Cernicharo et al. 2016). Observed transitions of CH$_3$NCO and their line parameters are summarized in Table 3. Several transitions of methyl isocyanate have been observed in this work with $m = 0, 1, 2, 3$. The spatial distribution of CH$_3$NCO transitions for $m = 2$ and 3 are depicted in Figure 3. Interestingly, it is observed that emission with $m = 0$ transitions of CH$_3$NCO is compact ($\theta \sim 1''0$) with the continuum emission, whereas for the transitions with a higher value of $m$, the emitting regions are comparatively extended (for $m = 1$, $\theta \sim 1''15$; $m = 2$, $\theta \sim 1''19$). However, these transitions are marginally resolved and it is not possible to draw any conclusions regarding the spatial distribution of these molecules in this source. A high angular and spatial resolution observation can shed some light on this issue more elaborately. The obtained rotational temperature of CH$_3$NCO is 248 K. For another high-mass star-forming region, Cernicharo et al. (2016) observed CH$_3$NCO in the warm gas of Sgr B2 and obtained a rotational temperature of $\sim 200$ K and a column density of $\sim (3 - 5) \times 10^{17}$ cm$^{-2}$. We estimated the column density and fractional abundance of CH$_3$NCO as $1.20 \times 10^{16}$ cm$^{-2}$ and $8.88 \times 10^{-9}$, respectively. Our observed column density of CH$_3$NCO in this source was estimated to be two to four times lower compared to that in the Sgr B2 observation (Cernicharo et al. 2016).

### 3.5. LTE Fitting Using Markov Chain Monte Carlo (MCMC)

We have used the MCMC method to fit the observed line profiles of HNCO, NH$_2$CHO, and CH$_3$NCO toward the hot core G10. We have assumed that the source is under the LTE condition. We have extracted the best-fitted physical parameters (column density, excitation temperature, FWHM, optical depth, and source velocity) from the fitting. We have used the python scripting interface available in CASSIS for our model calculation to find out the best-fitted physical parameters for the astronomical source. To determine the best-fitted set that can fit the observational result, we have used the $\chi^2$ minimization process by considering the N number of spectra. This python script computes $\chi^2$ between the observed and simulated data and finds the minimal value of $\chi^2$ following the relation:

$$ \chi^2 = \sum_{j=1}^{N_{\text{obs}}} \frac{(I_{\text{obs},j} - I_{\text{model},j})^2}{\text{rms}_j^2 + \text{cal}_j \times (I_{\text{obs},j})^2}, $$

where $I_{\text{obs},j}$ and $I_{\text{model},j}$ are the observed and modeled intensity in the channel $j$ of transition $i$, respectively, rms$_j$ is the rms of the spectrum $i$, and cal$_j$ is the calibration error. The reduced $\chi^2$ is computed using the following relation:

$$ \chi^2_{\text{red}} = \frac{1}{\sum_{j=1}^{N_{\text{spec}}} \sum_{i=1}^{N_{\text{obs}}} \chi^2_{ij}}, $$

In the MCMC calculation, the initial physical values are chosen randomly between the minimum ($X_{\text{min}}$) to the maximum ($X_{\text{max}}$) range set by the user during their modeling. The step of MCMC computation ($\psi$) depends on the iteration number $l$ and other parameters ($\alpha$ and $\nu$), where $\psi_{l+1} = \psi_l + \alpha(\nu - 0.05)$ ($\nu$ is a random number between 0 and 1). Here $\alpha$ is defined as

$$ \alpha = \frac{k(X_{\text{max}} - X_{\text{min}})}{k'}, $$

where $k$ is defined as

$$ k = r_c \text{ when } l > c, $$

$$ k = \frac{(r_c - 1)}{c} l + 1 \text{ when } l < c, $$

where $c$ and $r_c$ are the parameter cutoff and ratio at cutoff, respectively, which are set by the user during the modeling. $k'$ is defined as a reduced physical parameter which is set to a value during computation. $\alpha$ determines the amplitude of the steps, which starts with a bigger step at the initial stage of the computation to find a good $\chi^2$ and shorter steps at the end of the computation to extract the value of the potential best $\chi^2$.

LTE model-fitted line parameters of all the observed transitions are provided in Table 6. The observed spectra, along with the fitted one, are shown in Figures 4, 5, and 6 for HNCO, NH$_2$CHO, and CH$_3$NCO, respectively. We found that some transitions of CH$_3$NCO are blended, and thus we do not obtain better fits for those transitions. Some of the spectra shown in these figures contain multiple hyperfine transitions.
For the LTE fitting, we have considered only the transitions which have the highest Einstein coefficient values. Since some of the transitions with the highest Einstein coefficient are slightly offset from the peak position, LTE fitting results show a slight offset from some observational spectra. Extracted physical parameters in Table 6 show that the optical depths ($\tau$) of all the lines are less than 1. Our obtained best-fitted column densities of these three species are shown in Table 6. For this MCMC fitting, we have used the different source sizes for different species, as obtained from their two-dimensional Gaussian fitting. We have obtained higher excitation temperatures by the MCMC calculations (Table 6) which are consistent with the high rotational temperatures of these molecules obtained by the rotational diagram analysis which is described in Section 3.2 (Table 5).

4. Chemical Modeling

We carry out extensive modeling to study the abundance of three peptide-bond-related species in G10. To study the chemical evolution of these species, we used our previous chemical network (Das et al. 2015b, 2015a, 2016; Gorai et al. 2017a, 2017b; Sil et al. 2018). Gas-phase pathways were mainly adopted from the UMIST database (McElroy et al. 2013), whereas ice-phase pathways and binding energies (BEs) of the surface species were taken from the KIDA database unless otherwise stated (Ruaud et al. 2016). We have considered that the diffusion energy of a species is 0.5 times its adsorption energy and nonthermal desorption rate with a fiducial parameter of 0.01 (Gorai et al. 2017a). A cosmic-ray rate of $1.3 \times 10^{-17} \text{ s}^{-1}$ is considered in all our models. For the formation and destruction reactions of these species, we have mainly followed Quénard et al. (2018). In addition, following the recent study of Haupa et al. (2019), we have exclusively included dual-cyclic hydrogen addition and abstraction reactions, which connect NH$_2$CHO, NH$_2$CO, and HNCO. We have shown the chemical linkages among HNCO, NH$_2$CHO, and CH$_3$NCO. Initial abundances of the model are provided in Table 7.
| Species | Frequency (GHz) | Range Used Frequency (GHz) | Range Used FWHM (km s$^{-1}$) | Best-fit FWHM (km s$^{-1}$) | Best-fit Column Density (cm$^{-2}$) | Optical Depth ($\tau$) | Range Used $T_{\text{ex}}$ (K) | Best-fit $T_{\text{ex}}$ | Source Size ($\arcsec$) | Range Used $V_{LSR}$ (km s$^{-1}$) | Best-fitted $V_{LSR}$ (km s$^{-1}$) |
|---------|----------------|---------------------------|-------------------------------|---------------------------|----------------------------------|---------------------|-------------------------|------------------|-------------------|-----------------------|-------------------------|
| HNCO    | 148.223354     | 148.46523–147.53117       | 3–9                           | 8.98                      | $1.3 \times 10^{17}$            | $7.73 \times 10^{-2}$       | 400–600                 | 472.07           | 1.33               | 66.5–67.5             | 67.43                   |
| NH$_3$CHO| 148.599727     | 148.53115–149.46522       | 3–7                           | 7.00                      | $9.5 \times 10^{16}$            | $1.78 \times 10^{-2}$       | 400–550                 | 450.09           | 1.37               | 66.5–67.5             | 67.09                   |
| CH$_3$NCO| 148.833657     | 148.53115–149.46522       | 4–8                           | 7.99                      | $6.9 \times 10^{16}$            | $3.08 \times 10^{-1}$       | 100–300                 | 104.04           | 1.05               | 66.5–67.5             | 67.14                   |

Table 6
Summary of the Best-fitted Line Parameters of Observed Molecules toward G10
4.1. Physical Condition of the Adopted Model

We have considered a three-phase model to study the chemical evolution of these species (Garrod 2013). This model is best suited because G10 is a high-mass star-forming core. The detailed considerations of each phase are discussed below.

First phase: in the first phase, we have considered that the cloud collapses from a low total hydrogen density \( \rho_{\text{min}} = 10^{3} \text{ cm}^{-3} \) to a high total hydrogen density \( \rho_{\text{max}} \). The initial gas temperature \( T_{\text{gas}} \) is assumed to be 40 K, whereas the dust temperature is assumed to remain fixed at an initial ice temperature \( T_{\text{ice}} \). We have considered a time interval of \( t_{\text{coll}} \) years to reach from \( \rho_{\text{min}} \) to \( \rho_{\text{max}} \). Since at the highest density, the gas and dust are well coupled, we have considered the gas temperature \( T_{\text{gas}} \) at the highest density \( \rho_{\text{max}} \), i.e., at \( t = t_{\text{coll}} \). From this stage onward, we have assumed that the temperature of the dust and the gas is the same. Thus, we have considered a negative slope for \( T_{\text{gas}} \) for the collapsing phase. Throughout the first phase, the visual extinction parameter is considered to be constantly increasing from \( A_{V_{\text{min}}} \) to finally at \( A_{V_{\text{max}}} \) in \( t = t_{\text{coll}} \).

Second phase: the second phase of the simulation corresponds to a warm-up phase. Since G10 is a high-mass star-forming region, we consider a moderate warm-up timescale \( t_{w} \) of \( 5 \times 10^{4} \) yr (Garrod 2013). Therefore, during this short period, the temperature of the cloud from \( T_{\text{ice}} \) can reach the highest hot-core temperature \( T_{\text{max}} \). The density, temperature, and visual extinction parameter remain constant at \( \rho_{\text{max}} \), \( T_{\text{max}} \), and \( A_{V_{\text{max}}} \), respectively.

Third phase: this phase belongs to the post-warm-up time. Here, we have considered a post-warm-up timescale \( t_{pw} \) of \( 10^{5} \) yr, so the total simulation time is \( t_{\text{tot}} = t_{\text{coll}} + t_{w} + t_{pw} \). The parameters such as density and visual extinction are assumed to be the same as they were in the warm-up phase.
The temperature of the cloud is kept at $T_{\text{max}}$ throughout the last phase.

4.2. Binding Energies and Reaction Pathways

To study the desorption energy ($BE$) and reaction pathways of three peptide-bond-like species HNCO, NH$_2$CHO, and CH$_3$NCO and their isomers/precursors, we use the Gaussian 09 suite of programs (Frisch et al. 2013). Recently, Das et al. (2018) made an extensive effort to estimate the BE of 100 interstellar species on water-ice surfaces by applying a quantum chemical approach and compared their values with the available experimental results. They found that on average, the computed BE shows a larger deviation from experiments.
### Obtained adsorption energies (BEs) and thermodynamic parameters

We use our calculated scaled BE values of monomers for astrochemical modeling.

- **Wakelam et al. (2017)**
- **Quan et al. (2010)**

#### CHNO

| Species   | Optimized Structure | Calculated BE (K) | Average BE (K) | Scaled BE (K) (x1.416) | Calculated BE (K) using a water hexamer | Available BE (K) in the literatures |
|-----------|---------------------|-------------------|----------------|-------------------------|-----------------------------------------|-----------------------------------|
| HNCO      | ![HNCO structure]   | 3308              | 3308           | 4644                    | 6310, 5554                              | 4400 ± 1320<sup>a</sup>            |
| HCNO      | ![HCNO structure]   | 2640              | 2345           | 3320                    | 6046                                    | 2800<sup>b</sup>                   |
|           |                     |                   |                |                         |                                         |                                   |
| HOCN      | ![HOCN structure]   | 5936              | 4250           | 6018                    | 2153, 8404                              | 2800<sup>b</sup>                   |
|           |                     |                   |                |                         |                                         |                                   |
| HONC      | ![HONC structure]   | 5874              | 4122           | 5837                    | 3387, 8727                              | 2800<sup>b</sup>                   |
|           |                     |                   |                |                         |                                         |                                   |

#### CH₃NH₂O

| Species   | Optimized Structure | Calculated BE (K) | Average BE (K) | Scaled BE (K) (x1.416) | Calculated BE (K) using a water hexamer | Available BE (K) in the literatures |
|-----------|---------------------|-------------------|----------------|-------------------------|-----------------------------------------|-----------------------------------|
| CH₃NCO    | ![CH₃NCO structure] | 3627              | 3091           | 4377                    | 4309                                    | 4700 ± 1410<sup>a</sup>            |
|           |                     |                   |                |                         |                                         |                                   |
| CH₃CNO    | ![CH₃CNO structure] | 2786              | 2786           | 3945                    | —                                        | —                                 |
| CH₃OCN    | ![CH₃OCN structure] | 3534              | 3535           | 5006                    | 6530                                    | —                                 |
|           |                     |                   |                |                         |                                         |                                   |
| CH₃ONC    | ![CH₃ONC structure] | 2949              | 2752           | 3897                    | 4652                                    | —                                 |

#### CNH₃O

| Species   | Optimized Structure | Calculated BE (K) | Average BE (K) | Scaled BE (K) (x1.416) | Calculated BE (K) using a water hexamer | Available BE (K) in the literatures |
|-----------|---------------------|-------------------|----------------|-------------------------|-----------------------------------------|-----------------------------------|
| NH₂CHO    | ![NH₂CHO structure] | 3627              | 3627           | 3862                    | 5468                                    | 6602 ± 1890<sup>a</sup>            |
|           |                     | 2880              | 3862           | 5468                    | 6602                                    |                                   |

---

**Figure 7.** Obtained adsorption energies (BEs) and thermodynamic parameters. We use our calculated scaled BE values of monomers for astrochemical modeling. <sup>a</sup> Wakelam et al. (2017), <sup>b</sup> Quan et al. (2010).
when they considered a single water molecule as a substrate. The deviation is minimal when they used pentamer or hexamer configurations of water clusters. They provided a scaling factor for the extrapolation as the computation was performed with smaller water structures. We carry out a quantum chemical study to find out the BEs of the three peptide-bond-related species considered in this work along with their potentially observable isomers. To estimate the BEs of these species, we have used a similar method and basis set (MP2/aug-cc-pVDZ) as mentioned in Sil et al. (2017) and Das et al. (2018). Our calculated BE values are given in Figure 7. For some cases, we have found multiple probable sites for the adsorption and thus obtained multiple BE values. In that case, we take the average of the multiple BEs. Calculated BEs with a single water molecule are then scaled up by a factor of 1.416 (Das et al. 2018) to have a realistic estimation. Additionally, in Figure 7 we present the BE values for some of these species with a hexamer configuration of water clusters. Since the BEs with the pentamer/hexamer configurations show minimum deviation (Das et al. 2018), one can use these BE values in the model without scaling. We are unable to provide the BE values of all the species with a hexamer configuration and with all the probable sites of adsorption. Thus, for the modeling, we use BE values obtained with a single water molecule with appropriate scaling.

For the formation of ice-phase HNCO, Quénard et al. (2018) considered the reaction between NH and CO. They considered an activation barrier of 4200 K for this reaction (Himmel et al. 2002). For the formation of its other isomers, no such reactions were available. Due to this reason, for the sake of completeness, we run a quantum chemical calculation to check the reaction enthalpy of the following reactions:

\[
\begin{align*}
\text{NH} + \text{CO} & \rightarrow \text{HNCO}, \\
\text{CH} + \text{NO} & \rightarrow \text{HCNO}, \\
\text{CN} + \text{OH} & \rightarrow \text{HOCN}, \\
\text{CN} + \text{OH} & \rightarrow \text{HONC}.
\end{align*}
\]

We have found that the above four reactions are exothermic in nature. Exothermicity values are given in Table 8. The activation barrier for the reaction between NH and CO was known to be 4200 K but for the others it was unknown. The above reactions are mostly between radicals, and finding a true transition state is a difficult task. Instead, we have calculated the reaction enthalpy of these four reactions. Based on the reaction enthalpies, we have prepared the most probable reaction sequence in between these four reactions. Since the activation barrier of the first reaction was known to be 4200 K, we scaled the activation barriers of the rest of the reactions. Though the reaction enthalpy (exothermicity values) is not directly related to the activation barrier of the reaction, it is eventually a better-educated approximation compared to using any crude approximation. Scaled activation barriers are provided in Table 8.

Quénard et al. (2018) studied the peptide-bond-related molecules in the protostar IRAS 16293–2422 and the prestellar core L1554 by using a chemical model. Earlier, it was claimed that HNCO and NHCHO are chemically linked because NHCHO could be formed by the successive hydrogenation reactions of HNCO (HNCO → H₂NCO → NH₂CHO) (Mendoza et al. 2014; López-Sepulcre et al. 2015; Song & Küstner 2016; López-Sepulcre et al. 2019). The first step of this hydrogenation sequence has an activation barrier of 1962 K and the second step is a radical–radical reaction and thus could be barrierless. Recent experimental studies by Noble et al. (2015) and Fedoseev et al. (2015) question this fact. They opposed the formation of NHCHO by the reaction between H₂NCO and hydrogen, rather they proposed that eventually it would return back to HNCO again (H₂NCO + H → HNCO + H₂). Here, we have considered only the formation of NHCHO in our ice-phase network. In order to continue a comparative study between the various isomers of HNCO, we are interested in checking the hydrogenation reactions with the various isomeric forms of HNCO. Thus, we have studied the reaction enthalpies of the following reactions:

\[
\begin{align*}
\text{HNCO} + \text{H} & \rightarrow \text{H}_2\text{NCO}, \\
\text{HCNO} + \text{H} & \rightarrow \text{H}_2\text{CNO}, \\
\text{HOCN} + \text{H} & \rightarrow \text{H}_2\text{OCN}, \\
\text{HONC} + \text{H} & \rightarrow \text{H}_2\text{ONC}.
\end{align*}
\]

However, no valid neutral structure for H₂OCN and H₂ONC were obtained, and thus we did not consider the last two hydrogenation reactions of this sequence. In Table 8, we summarize the obtained reaction enthalpies of reactions 12 and 13. Based on the obtained reaction enthalpy for the second reaction with respect to the first reaction, we scale the activation barrier of the second reaction to 1073 K.

Recently, Haupa et al. (2019) proposed successive hydrogen abstraction reactions to NH₂CHO for the formation of HNCO:

\[
\begin{align*}
\text{NH}_2\text{CHO} + \text{H} & \rightarrow \text{H}_2 + \text{H}_2\text{NCO}, \\
\text{H}_2\text{NCO} + \text{H} & \rightarrow \text{H}_2 + \text{HNCO}.
\end{align*}
\]

They pointed out that reaction 16 has an activation barrier of 240 K–3130 K depending on the level of theory used for the quantum chemical calculation. They found that reaction 17 is barrierless. This reaction is very interesting as it might support

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Table 8

| Reactions                      | Reaction Enthalpy (kcal mol⁻¹) | Types of Reactions | Activation Barrier (K) |
|--------------------------------|---------------------------------|--------------------|------------------------|
| Ice-phase Reactions            |                                 |                    |                        |
| NH + CO → HNCO                 | −139.19                         | Exothermic         | 4200 °C                |
| CH + NO → HCNO                 | −124.62                         | Exothermic         | 4691 K                 |
| CN + OH → HOCN                 | −120.35                         | Exothermic         | 4857 K                 |
| CN + OH → HONC                 | −59.32                          | Exothermic         | 9855 K                 |
| HNCO + H → H₂NCO               | −31.35                          | Exothermic         | 1962 K                 |
| H₂NCO + H → NH₂CHO             | −92.76                          | Exothermic         | 0 K                    |
| H₂NCO + H → HNCO + H₂          | −73.15                          | Exothermic         | 0 K                    |
| HCN + H → H₂CNO                | −57.29                          | Exothermic         | 1073 K                 |
| HCN + H → H₂OCN                | −22.90                          | Exothermic         | 0 K                    |
| HOCN + H → H₂ONC               | −18.80                          | Exothermic         | 0 K                    |
| Gas-phase reactions            |                                 |                    |                        |
| HNCO + O → CO + HNO            | −23.70                          | Exothermic         | ...                    |
| HNCO + O → OH + OCN            | 5.70                            | Endothermic        | ...                    |
| HCN + O → CO + HNO             | −92.52                          | Exothermic         | ...                    |
| HCN + O → OH + CNO             | 0.064                           | Endothermic        | ...                    |
| HOCN + O → OH + OCN            | −22.90                          | Exothermic         | ...                    |
| HONC + O → OH + CNO            | −18.80                          | Exothermic         | ...                    |

Note. a Himmel et al. (2002)
the earlier claim of chemical linkage between HNCO and NH₂CHO. They also performed quantum chemical calculations for the hydrogen addition reactions to H₂NCO and HNCO:

\[
\begin{align*}
H + H₂NCO & \rightarrow NH₂CHO, \\
H + HNCO & \rightarrow H₂NCO.
\end{align*}
\]

They found that reaction 18 is barrierless, whereas reaction 19 has an activation barrier of 2530 K–25050 K depending on the level of theory used for the computation.

For the computation of the gas-phase reaction rate of these four reactions, we have used

\[
\text{rate} = \alpha \left( \frac{T}{300} \right)^\beta \exp(-\gamma/T),
\]

where \(\alpha\), \(\beta\), and \(\gamma\) are the three constants of the reaction. We have considered \(\alpha = 10^{-10}\), \(\beta = 0\), and \(\gamma = 240–3130\) for reaction 16. For reaction 17 and 18, we have considered \(\alpha = 10^{-10}, \beta = 0, \gamma = 0\), and for reaction 19, we have considered \(\alpha = 10^{-10}, \beta = 0, \gamma = 2530–5050\). Since a valid structure for H₂CNO was obtained, we have considered the reaction H + H₂CNO \rightarrow HCN + H₂ in both gas and ice phases.

Quénard et al. (2018) used the gas-phase destruction of HOCN, HNCO, and HONC by an oxygen atom. For all three destruction reactions they considered an activation barrier of 195 K. However, Quan et al. (2010) considered the activation barriers of 2470 K, 195 K and 3570 K, respectively, for these three destruction reactions by oxygen atoms, and these are the default in the UMIST 2012 network. Here, we consider the default destruction reactions as it was used in UMIST 2012. For the destruction of HNCO by an oxygen atom, no reaction was considered. To this effect, we calculate the reaction enthalpies for the reactions HNCO + O \rightarrow CO + HNO and HNCO + O \rightarrow OH + OCN. We have found that the second reaction in this sequence is endothermic, whereas the first one is exothermic, and thus we do not consider the second one. HNCO + O \rightarrow CO + HNO is very similar to HCNO + O \rightarrow CO + HNO, for which a 195 K activation barrier was considered in UMIST 2012. Based on the exothermicity values between HCNO + O and HNCO + O, we have used a scaling factor and obtained an activation barrier of 765 K for HNCO + O. Calculated reaction enthalpies and the activation barriers are noted in Table 8.

### 4.3. Modeling Results

The observed abundances of HNCO, NH₂CHO, and H₂NCO are provided in Table 5. From the chemical modeling, we have seen that our obtained abundance is very much sensitive to the physical parameters (\(T_{\text{ice}}, \rho_{\text{max}}, T_{\text{max}}, t_{\text{coll}}\), and \(t_{\text{pw}}\)) and adopted rate constants. Here, we have made an extensive effort to find out the simultaneous appearance of these three nitrogen-bearing species by varying the sensitive physical parameters and rate constants of some of the key reactions. More precisely, we have prepared two models: Model A and Model B. The difference between the two models is highlighted in Table 9.

### 4.3.1. Results Obtained with Model A

To constrain the best possible model, we have explored the parameter space around which the modeling results are in good agreement with the observational results. To this effect, we run several cases by varying the initial dust temperature (\(T_{\text{ice}}\)) in between 10 K and 25 K and \(\rho_{\text{max}}\) in between 10⁴ and 10⁷ cm⁻³ for Model A. Since G10 is a hot core, a higher density (10⁶–10⁷ cm⁻³) is preferable. It has been previously pointed out that the G10 region is extended by roughly 0.1 pc and has ~10³ solar masses of matter (Cesaroni et al. 1994). From that estimation, the average density of the source is around 10⁷ cm⁻³. It is also interesting to note that our observational analysis suggests that continuum temperatures vary between 19 K to 27 K. Based on the observational results as a preliminary guess, we have used \(\rho_{\text{max}} = 10⁷ \text{ cm}^{-3}\) and \(T_{\text{ice}} = 20 \text{ K}\) for Model A. Initially, we have started with Model A with the rate constants of the gas-phase reactions available in the literature (Skouteris et al. 2017; Quénard et al. 2018; Haupa et al. 2019). Based on some preliminary iterations of our simulation, we have varied the rate constants of the some key gas-phase reactions which are controlling the abundances of the three targeted species. We have obtained a nice
correlation between these three species when the rate constants listed in Table 9 are used. Quénard et al. (2018) considered the reaction between HNCO and CH₃ in the ice phase for the formation of the isomers CH₃NCO and CH₃OCN at the same rate. However, for the gas-phase formation of other isomers of CH₃NCO (CH₃CNO, CH₃OCN, CH₃ONC), Quénard et al. (2018) considered some rate coefficients of $\sim 10^{-20}$ and $5 \times 10^{-11}$ cm$^3$ s$^{-1}$. Here, instead of the rate constant of $5 \times 10^{-11}$ cm$^3$ s$^{-1}$ for some gas-phase reactions and have used a rate of $10^{-20}$ cm$^3$ s$^{-1}$ for those reactions as it was used in Quénard et al. (2018). For the ice-phase formation reactions, we kept it as it was considered by Quénard et al. (2018). To study the abundances of various isomers considered in the network, we thus choose our best-fitted parameters listed in Table 9 for Model A. Time evolution of the abundances of HNCO isomers, C₂H₃NCO isomers, and N₂HCO is shown in Figure 8. Results obtained with the best-fitted rate constants are shown separately in Figure 9 for HNCO, CH₃NCO, and NH₂CHO. They clearly show that around the age of $\sim 1.12 \times 10^{6}$ yr, we have a good correlation between these three species. Parameter space obtained with the best-fitted rate constants.
The chemical evolution of HNCO, CH$_3$NCO, and NH$_2$CHO during the three phases by considering the best-fit parameters of Model A. The best-fitted time zone is also highlighted. Abundance variation by avoiding Haupa et al. a peak abundance of and HOCN. With the best-fitted parameters, we have obtained a good fit between the three targeted nitrogen-bearing species when we have used the parameters listed in Table 9. We found that our model B with $T_{\text{coll}} = (2 - 3) \times 10^5$ yr, $T_{\text{e}} = 5 \times 10^4$ yr and $T_{\text{pw}} = 10^5$ yr is able to explain the observation of these three species simultaneously when we have considered $\rho_{\text{max}} = 10^3$ cm$^{-3}$, $T_{\text{max}} = 200$ K, and $T_{\text{ke}} = 20$ K. The obtained lower timescale with Model B is very interesting because G10 is a high-mass star-forming region. Gas-phase pathways required to establish the linkage between these three species are summarized in Figure 13.

4.3.2. Results Obtained with Model B

For Model B, we did not vary any rate constants. We kept it as it was obtained with the best-fitted Model A which is noted in Table 9. To find out the best-fit physical parameters for Model B, we have started with $T_{\text{e}} = 20$ K and have varied $\rho_{\text{max}}$. Figure 11 shows the variation of HNCO, CH$_3$NCO, and NH$_2$CHO abundance by considering a post-warm-up time ($t_{\text{pw}}$) of $10^7$ yr. Observed abundances are also marked in each panel. We found that the abundance of these three species is highly sensitive to the chosen collapsing timescale ($t_{\text{coll}}$) and the maximum density ($\rho_{\text{max}}$) achieved during the collapsing phase. As we have increased $\rho_{\text{max}}$, abundance significantly decreased. Similarly, as we increased $t_{\text{coll}}$, the abundances gradually decreased. Based on Figure 11, we found that $\rho_{\text{max}} = 10^7$ cm$^{-3}$ and $T_{\text{coll}} \sim 2-3 \times 10^7$ yr are most suitable for explaining the abundance of these three species simultaneously. We further have varied $T_{\text{max}}$ in between 100 K and 400 K by considering $\rho_{\text{max}} = 10^3$ cm$^{-3}$. Figure 12 shows that an increase in $T_{\text{max}}$ from 100 K to 150 K shows a strong increasing trend in the abundance profile. We have a reasonable match when we have used $T_{\text{max}} = 200$ K. In between $T_{\text{max}} = 150$ K–350 K, the abundance profile shows moderate changes. Beyond 350 K the abundances drastically decreased, while we have considered a comparatively longer collapsing timescale. Thus, by considering all types of variation with Model B, we have obtained a good fit between the three targeted nitrogen-bearing species when we have used the parameters listed in Table 9. We found that our model B with $T_{\text{coll}} = (2 - 3) \times 10^5$ yr, $T_{\text{e}} = 5 \times 10^4$ yr and $T_{\text{pw}} = 10^5$ yr is able to explain the observation of these three species simultaneously when we have considered $\rho_{\text{max}} = 10^3$ cm$^{-3}$, $T_{\text{max}} = 200$ K, and $T_{\text{ke}} = 20$ K. The obtained lower timescale with Model B is very interesting because G10 is a high-mass star-forming region. Gas-phase pathways required to establish the linkage between these three species are summarized in Figure 13.

4.3.3. Chemical Linkage between HNCO, NH$_2$CHO, and CH$_3$NCO

Earlier, it was proposed that HNCO and NH$_2$CHO are chemically linked. The successive hydrogenation reactions of HNCO were proposed for the formation of NH$_2$CHO. However, the validity of the second hydrogenation reaction is ruled out by the experimental study of Noble et al. (2015). Recently, a theoretical work by Haupa et al. (2019) proposed dual-cyclic hydrogen addition and abstraction reactions to support the chemical linkage between HNCO and NH$_2$CHO. The chemical evolution of HNCO, NH$_2$CHO, and CH$_3$NCO with Model A are shown in Figure 9. Gradual enhancement in the abundance of ice-phase HNCO and its isomers arises because radicals become mobile enough with the increase in temperature. Beyond 80 K–90 K, the diffusion timescale of the radicals becomes comparable to their desorption timescale and thus they are desorbed back to the gas phase very quickly. Also, HNCO starts to sublimate beyond 90 K, resulting in a sharp decrease in the ice phase. The gas-phase production of CH$_3$NCO mainly occurs by the reaction between CH$_3$ and HNCO. The formation rate of CH$_3$NCO enhances during the later phases of the simulation. In the case of NH$_2$CHO, ice-phase production is sufficient in the collapsing phase, but gas-phase production is not adequate. In the warm-up period, a smooth transfer of NH$_2$CHO from the ice phase to the gas phase can occur. The location of this transfer depends on the adopted BE of NH$_2$CHO. In the warm-up and post-warm-up phase, a major portion of NH$_2$CHO is formed by the gas-phase reaction between NH$_3$ and H$_2$CO. Due to the increased temperature, the activation barrier for the hydrogen abstraction reaction of NH$_2$CHO (by reaction 16) becomes improbable and thus produces HNCO by reaction 17 by the barrierless reaction. To check the effects of the addition of the Haupa et al. (2019) pathways, we have checked with $\alpha = 0$ for the gas-phase reactions 16–19. Figure 9 shows the abundances of these three species by considering $\alpha = 0$ (marked as “NO-Haupa”). We
have noticed that the abundance of gas-phase HNCO is significantly affected with the inclusion of the gas-phase pathways of Haupa et al. (2019). Consideration of reactions 16–19 shows more HNCO at the end and an absence of these pathways (i.e., with \( \alpha = 0 \)) reflects comparatively lower HNCO. In brief, we have found that the pathways proposed by Haupa et al. (2019) are relevant for the gas-phase production of HNCO around the post-warm-up period. In the first phase, CH3NCO is mainly formed in the grain surface by the reaction between CH3 and OCN. CH2NCO may also have formed by the reaction between CH3 and HNCO (Quénard et al. 2018) in the ice phase. However, it is clear from the warm-up and post-warm-up phase that the major contribution of the gas-phase CH3NCO is not coming from the ice phase; instead it is produced inside the gas phase itself. The gas-phase formation is efficient using the HNCO channel at the warm-up and post-warm-up phase.

5. Conclusions

1. We identified three molecules HNCO, NH2CHO, and CH3NCO in G10 which contain peptide-like bonds. Earlier, HNCO and NH2CHO had been identified in G10,
but this is the first identification of CH$_3$NCO in this source.

2. We estimated the hydrogen column density of this source to be $N_\text{H} = 1.35 \times 10^{25}$ cm$^{-2}$. Our estimated optical depth is 0.136, which suggests that the dust is optically thin. Kinetic temperatures of the gas are found to vary between 248 K to 439 K. We estimated the column densities and fractional abundances of three observed peptide-like-bond containing molecules.

3. From the obtained spatial distribution of these three species, we speculated that they are chemically linked. Since all the transitions were marginally resolved, one needs to have high angular and spatial resolution data to make a rigorous comment on their spatial distribution in G10.

4. From our chemical modeling results, we also noticed that these three species are chemically linked. We found that HNCO and NH$_2$CHO are chemically linked by dual-cyclic hydrogen addition and abstraction reactions proposed by Haupa et al. (2019) during the warm-up and post-warm-up phase. HNCO and CH$_3$NCO are also chemically related because HNCO reacts with CH$_3$ to form CH$_3$NCO (Figure 13).

5. Our modeling results suggest that the abundances of HOCN and CH$_2$OCN are significantly higher and could be observed in G10.

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Appendix

Line parameters are obtained using a single Gaussian fitting to the observed lines. Observed and Gaussian fitted spectra of various transitions of HNCO, NH$_2$CHO, and CH$_3$NCO are shown in Figures A1, A2, and A3 respectively.
Figure A2. Gaussian fitting of the observed emission spectra of NH$_2$CHO toward G10. Black lines represent observed emission spectra and red lines represent a Gaussian profile fitted to the observed spectra.
Figure A3. Gaussian fitting of the observed emission spectra of CH$_3$NCO toward G10. Black lines represent observed emission spectra and red lines represent a Gaussian profile fitted to the observed spectra.

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