Differential Deuterium Enrichment of Multiple Molecular Species and Gaseous CO Depletion in Infrared Dark Cloud G 011.0970–0.1093

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Abstract

Using molecular line mapping with the Institut de Radioastronomie Millimétrique (IRAM) 30 m radio telescope in the 1.3–4.0 mm band, combined with 70–870 m continuum data and mapping of the $ {NH}_3$(J, K) = (1, 1) and (2, 2) lines with the Green Bank Telescope (GBT) (where J is the total angular momentum quantum number and K describes the component of angular momentum along the molecular principal axis), we observed a pair of neighboring clumps at the end of the G 011.0970–0.1093 filamentary molecular cloud. Although both appear associated with continuum flux peaks at 870 m, they exhibit contrasting bright and faint characteristics at 70 m. Comparative analysis of these two clumps reveals: (1) the gas and dust temperatures are highly coupled in this very early-stage massive star-forming region; (2) the gas-dust temperature of the 70 m bright clump shows a decreasing trend from the center (约17 K) to the envelope edge, suggesting that protostar formation may already be occurring inside the clump; the center of the 70 m faint clump is colder (约11 K) and denser (约$5 \times 10^{22}\,\mathrm{cm}^{-2}$) than its edge, and a strong anti-correlation exists between the H_2 column density and dust temperature, indicating that external radiation may dominate the heating of this clump; (3) on parsec scales, the depletion rate $f_D(C^{18}O)$ of gaseous $ {C}^{18}{O}$ is strongly positively correlated with the deuteration fraction of HCO^+, and gaseous $C^{18}O$ in the cold and dense DCO^+-dominated clump has a depletion $f_D(C^{18}O)$ as high as 7; (4) in environments where the gas-dust temperature varies from 10 K to 20 K and the H_2 column density ranges from $10^{22}\,\mathrm{cm}^{-2}$ to $10^{23}\,\mathrm{cm}^{-2}$, the deuteration fractions of HCO^+, N_2H^+, and $ {HNC}$ show significant enhancement in denser, colder, and darker environments, while $ {HCN}$ exhibits greater deuteration enhancement in slightly warmer and 70 m bright environments, and the deuteration fraction of $ {NH}_3$ shows no significant change in this environment. These differences in deuteration

enhancement among different molecules may originate from differences in their gas-dust reaction pathways.

Full Text

Preamble

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The Differentiation in Molecular Deuteration and CO Depletion towards the Infrared Dark Cloud G 011.0970–0.1093

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Abstract

Using the Institut de Radioastronomie Millimétrique (IRAM) 30 m radio telescope for a molecular line imaging survey at 1.3–4.0 mm, combined with continuum data spanning 70–870 m and Green Bank Telescope (GBT) observations of NH3 (J;K) = (1;1) and (2;2) lines (where J is the total angular momentum quantum number and K describes the projection of angular momentum onto the molecular principal axis), we observed a pair of neighboring clumps at the terminus of the filamentary molecular cloud G 011.0970−0.1093. Although both clumps coincide spatially with the continuum emission peak at 870 m, they exhibit contrasting brightness characteristics at 70 m—one bright and one faint. Comparative analysis reveals: (1) The gas and dust temperatures are tightly coupled in this extremely early-stage high-mass star-forming region; (2) The gas-dust temperature of the 70 m bright clump decreases from the center (17 K) toward the envelope edge, suggesting that protostar formation may have already begun within the clump; the 70 m dark clump is colder at its center (11 K) and denser than at its edge, with a strong anti-correlation between H2 column density and dust temperature, indicating that external radiation likely dominates heating of this clump; (3) At parsec scales, the deuterium fractionation of gaseous DCO+ shows a strong positive correlation with that of N2H+, with the deuterium fraction of DCO+ reaching as high as 7; (4) In environments where gas-dust temperature varies from 10 K to 20 K and H2 column density ranges from 1022 cm−2 to 1023 cm−2, warm and 70 m bright regions exhibit greater deuterium fractionation enhancement, while NH3 shows no significant change in deuteration across this temperature range. These differential deuteration enhancements among various molecules likely originate from differences in

their gas-dust reaction pathways.

Keywords stars: formation, ISM: clouds, ISM: lines and bands, ISM: molecules, submillimeter: ISM

1 Introduction

Infrared Dark Clouds (IRDCs) are the products of gravitational and turbulent magnetic field equilibrium in diffuse molecular clouds. With number densities exceeding 104 cm−3 and temperatures below 25 K, these molecular clouds exhibit substantial dust extinction and consequently show no prominent infrared emission, hence the name "infrared dark clouds" [1−3]. IRDCs serve as cradles of star formation, potentially harboring low-mass prestellar cores, massive starless cores, and massive young stellar objects [4−5].

IRDCs are crucial for studying the physical and chemical evolution during the earliest stages of star formation. In these dense (nH > 104 cm−3), cold (T < 25 K) regions, stellar heating and feedback activities have not yet emerged on large scales, thus preserving the dynamical and chemical characteristics of early molecular clouds [6]. These properties are essential for understanding the physical and chemical evolution of star formation. Molecular deuteration and gaseous CO depletion are two important chemical processes during this stage and constitute the focus of this study. In interstellar media, deuterium primarily exists in the form of HD; the deuteration process releases deuterium atoms from HD through cosmic-ray-driven ion-molecule reactions in cold, dense environments, enabling isotope exchange with H3+ to form H2D+, D2H+, and other ions [8−11]. These ions further react with other molecules to produce species such as N2D+, DCO+, and DCN [12]. Gaseous CO depletion refers to the process where heavy-element molecules like CO become adsorbed onto dust grain surfaces, reducing the abundance of gaseous CO [13−18]; the degree of gaseous CO depletion can be measured by the ratio between the expected gaseous CO abundance and the observed gaseous CO abundance. For a long time, observed gaseous CO depletion in molecular clouds has primarily been concentrated in subparsec-scale clumps [14−15, 19−20], with only a few detections on parsec-scale molecular clouds [21−22].

Previous extensive observations of simple molecules such as N2H+, HCO+, HCN, and HNC have shown that their deuterium fractionation in dense (nH > 104 cm−3), cold (T < 25 K) environments is several orders of magnitude higher than in diffuse interstellar media [8, 23]. As protostars form, molecular deuteration decreases. However, Feng et al. [6, 24] conducted high-sensitivity, wide-bandwidth "control" spectral line imaging observations of two neighboring (1 pc) dense clumps at the terminus of the filamentary infrared dark cloud G 28.34+0.06, both peaking at 870 m continuum but with bright and faint 70 m continuum emission respectively. They found: (1) Not all molecules show greater deuteration enhancement in relatively cold environments (<20 K) compared to relatively warm environments (>20 K); some molecules like NH3

show no significant deuteration enhancement at 14–22 K, likely due to differences in their gas-dust reaction pathways; (2) At parsec scales, gaseous CO depletion and DCO+ deuteration fraction show a strong positive correlation in spatial distribution, possibly resulting from HCO+ chemistry.

To investigate whether these two chemical phenomena in G 28.34+0.06 molecular cloud arise from the particularity of its physical-chemical environment or represent universal characteristics of these chemical processes in extremely early-stage high-mass star-forming molecular clouds, Feng et al. [24] initiated the MIAO (The Multiwavelength Line-Imaging Survey of the 70 m Dark and Bright Clouds) survey program. This project selected 24 cold (dust temperature <20 K), dense (pc-scale mean density nH 105 cm−3), nearby (kinematic distance 5 kpc) molecular regions located at the tails of filamentary infrared dark clouds. To minimize statistical uncertainties caused by external environmental differences, each region in this survey covers a pair of clumps that both peak at 870 m continuum but appear bright and dark respectively at 70 m continuum.

In the MIAO survey, the pair of 70 m bright and dark clumps at the terminus of molecular cloud G 011.0970–0.1093 shares remarkable physical-chemical environmental similarities with the pilot study source [6]—the pair of 70 m bright and dark clumps at the terminus of molecular cloud G 28.34+0.06: (1) The mass of this pair (Mc 870 M) exceeds the empirical threshold for massive star formation (Mc $\geq$ 0.2 g cm−2, or surface density $\Sigma > 0.05$ g cm−2) according to the McKee & Tan [25] criterion; (2) The projected separation between the pair is 1.0 pc in G 011.0970–0.1093; (3) The 70 m dark clump has a luminosity of 108 L and a luminosity-to-mass ratio less than one solar luminosity per solar mass (Lbol/Mc < 1 L /M).

This paper presents imaging observations and comparative analysis of the physical properties (dust and gas temperature and density) and low-temperature chemistry (differential deuteration of multiple molecules and gaseous CO depletion) of these paired clumps, aiming to test whether the conclusions from the pilot study source G 28.34+0.06 are universal. The structure of this paper is as follows: Section 2 introduces the observational data, Section 3 describes the observed spectral line profiles and spatial distributions of key molecules, Section 4 discusses possible correlations among various physical-chemical parameters across the region, and Section 5 lists the conclusions drawn from analyzing this source.

2 Observational Data Sources

Between August 2017 and May 2018, we used the Institut de Radioastronomie Millimétrique (IRAM) 30 m radio telescope to conduct a molecular line imaging survey of the G 011.0970–0.1093 molecular cloud at 1.3 mm, 3.4 mm, and 4.0 mm wavelengths. We employed the Eight MIxer Receiver (EMIR) and Fast Fourier Transform Spectrometers (FTS)–200 backend, covering 16 GHz bandwidth in each band (i.e., 70.718–78.501 GHz, 82.056–94.183 GHz, and 217.122–

224.842 GHz), achieving a frequency resolution of 200 kHz (corresponding to a velocity resolution of 0.637 km s−1 at 93.173 GHz, i.e., for the C18O (1–0) transition). Using On-The-Fly (OTF) mapping mode, we mapped a region centered at α(J2000) = 18h10m25s.70, δ(J2000) = (–19°22 59 .5) with a step size of 5 . [Figure 1: see original paper] shows the continuum and molecular line imaging toward the tail of G 011.0970–0.1093 molecular cloud, revealing a pair of neighboring (1 pc) clumps whose continuum peaks both appear at 870 m but show bright and faint contrast at 70 m. For pointing and flux calibration, we used Mars and Saturn as calibrators.

At 1.3 mm, 3.4 mm, and 4.0 mm wavelengths, considering forward efficiencies (Feff) of 93%, 95%, and 95% respectively, and main beam efficiencies (Beff) of 60%, 81%, and 81% respectively, the observed antenna temperature (TA∗) can be converted to main beam temperature (TMB) using TMB = (Feff/Beff) × TA∗. During observations, weather conditions were good, with atmospheric opacity (τ225GHz) below 0.6 at 255 GHz. Consequently, the rms noise levels at 1.3 mm, 3.4 mm, and 4.0 mm wavelengths were 0.14–0.54 K, 0.02–0.04 K, and 0.02–0.06 K respectively [24]. Subsequently, we used the GILDAS software package to preprocess and conduct preliminary analysis of the observed data (stored as three-dimensional cubes in Right Ascension–Declination–velocity space).

[Figure 1: see original paper] The multi-wavelength continuum and molecular spectral line image towards the tail of G 011.0970–0.1093. Subfigure (a) depicts the dust distribution measured by Herschel at 70 m (flux density, F70 m), with a black circle in the top right corner indicating a resolution of 10 .2. Subfigure (b) shows a two-color plot presenting the integrated intensities of C18O (2–1) (displayed in cyan, with an angular resolution of 11 .8) and DCO+ (1–0) (displayed in red, with an angular resolution of 36 .0) within the same velocity range (15–45 km s−1). Inside the magenta dashed circle is the 70 m bright and DCO+-dominated region, while outside the magenta dashed circle is the 70 m faint and C18O-dominated region. White contours in both subfigures represent the continuum radiation observed by APEX at 870 m [28], starting from 5σ (σ = 5.6 MJy sr−1) and increasing in steps of 5σ, with an angular resolution of 18 .2. The 870 m peaks are marked with gray ‘x’ symbols, while PDCO+ and PC18O markers are placed here.

Additionally, we utilized the following telescope archives to quantify the physical properties (i.e., gas and dust temperature and density) of the observed region. Dust continuum data were obtained from Herschel space telescope’s Hi-GAL (Herschel Infrared Galactic Plane Survey) program (wavelengths of 70 m, 160 m, 250 m, 350 m, and 500 m, with corresponding angular resolutions of 13 .5, 13 .5, 24 .9, 36 .4, and 36 .4 respectively) [29], as well as from the Atacama Pathfinder Experiment (APEX) telescope at 870 m wavelength with an angular resolution of 19 .2 [28].

NH3 (J;K) = (1;1) and (2;2) transition line data (where J is the total angular momentum quantum number and K describes the projection of angular momentum onto the molecular principal axis) were obtained from the Radio Ammonia

Mid-plane Survey (RAMPS) program [30], observed with the Green Bank Telescope (GBT) at an angular resolution of 34 .7, with a velocity resolution of 0.018 km s−1 per channel across the observed region, and an rms noise level of 0.11 K in TMB for each velocity sampling channel.

3 Results

3.1 Molecular Spectral Line Profiles

In cold (T < 20 K) and dense (nH > 104 cm−3) environments, high-energy-level molecular transitions may not be excited. Therefore, the target spectral lines observed with IRAM 30 m include isotopologue pairs containing 12C and 13C, hydrogen-bearing and deuterium-bearing isotopologue pairs, and NH3 lines. Among these, molecules containing 12C have the highest abundance and are easiest to detect.

However, 12C-containing spectral lines often exhibit strong self-absorption features [6−24, 31], primarily caused by large optical depths due to high abundances of 12C-containing molecules. Meanwhile, low-energy transitions of 12C-containing molecules in the observed region show line wings with multiple velocity components from Galactic spiral arms [32]. In contrast, molecules containing rare isotopes such as 13C or C18O, as well as deuterated isotopologues, are less affected by these factors. Therefore, this work focuses on ground-state rotational transitions of rare isotopologues and their deuterated counterparts, which have critical densities greater than 104 cm−3 at temperatures of 10–20 K [33−35], making them effective probes of dense gas. presents the chemical composition and observational characteristics of the molecular lines studied toward the 70 m bright and dark clump pair at the terminus of G 011.0970–0.1093.

Chemical and observational characteristics of molecular lines towards the 70 m bright and dark clouds pair in G 011.0970–0.1093

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[Figure 2: see original paper] shows the molecular spectral lines toward the 70 m bright and dark clump pair at the terminus of G 011.0970–0.1093. Comparing the beam-averaged molecular line profiles extracted at the 870 m continuum peak reveals that the line-center velocities (Vlsr) and line widths (FWHM) of the 70 m bright and faint clumps are less than 0.8–3.3 km s−1, confirming that this pair of clumps are spatially adjacent and located within the same filamentary molecular cloud. Notably, due to the large span of observed wavelengths, the spatial and velocity resolutions are not uniform across different bands. Considering the hyperfine structures of these molecular lines, their line-center velocities, velocity dispersions, line-center intensities, and integrated intensities along the velocity axis were obtained through fitting with the PySpecKit software package [40] (assuming Gaussian profiles, see the best-fit parameters for each molecular line in).

[Figure 2: see original paper] The beam-averaged line profiles towards the 70

m bright and dark clumps pair in G 011.0970–0.1093. Black lines represent observational data (with a frequency resolution of 200 kHz), and red lines represent Gaussian profile fits using the PySpecKit software package [40]. Two gray vertical dashed lines indicate the velocity integration ranges: 5–55 km s−1 for NH3 (to preserve contributions from hyperfine structure components), and 15–45 km s−1 for other molecular lines to reduce noise. Blue vertical dashed lines indicate the systemic velocity of the source, Vsys = 29.8 km s−1.

Best-fit parameters of molecular lines towards the 70 m bright and dark clumps pair in G 011.0970–0.1093

[The table content is preserved exactly as in the original]

3.2 Integrated Intensities

By integrating the common velocity ranges for each molecular spectral line shown in [Figure 2: see original paper] (with a velocity integration range of 15–45 km s−1 for lines other than NH3), we obtained the integrated intensity maps of the relevant molecules toward the terminus of G 011.0970–0.1093 molecular cloud, as shown in [Figure 3: see original paper]. To facilitate spatial correspondence between dust radiation and gas distribution in this source, the 870 m continuum measured by APEX is overlaid on each subfigure [28]. Notably, because the hyperfine structure components of NH3 cover a larger velocity range (5–55 km s−1) than other target molecular lines (see [Figure 2: see original paper]), Figure 3: see original paper shows the total flux integrated over all hyperfine components, which is approximately 15% higher than the flux integrated over the 15–45 km s−1 range.

In the wide-band imaging, the DCO+ (1–0) integrated intensity map has the highest signal-to-noise ratio (S/N) at each pixel compared to other deuterated molecular lines (S/N > 5). However, compared to the C18O (2–1) molecular line, the integrated intensity of DCO+ (1–0) shows a clear spatial offset, consistent with the findings of Feng et al. [24] in G 28.34+0.06. For subsequent quantitative analysis, we overlaid the integrated intensity maps of C18O and DCO+ as a cyan-red two-color plot (see Figure 1: see original paper), using a magenta dashed circle to delineate the boundary between the two regions: the cyan region (outside the magenta dashed circle) is C18O-dominated, while the red region (inside the magenta dashed circle) is DCO+-dominated. The 870 m peaks in each region are marked and labeled.

Integrating Figure 1: see original paper–(b) shows that PC18O and PDCO+ respectively resemble the spatial distribution of the 70 m dark and bright regions. [Figure 3: see original paper] also demonstrates that while the integrated intensity maps of hydrogenated isotopologue ground-state transitions such as C18O, H13CN, HN13C, H13CO+, and N2H+ are highly consistent with the spatial distribution of 870 m continuum radiation, the integrated intensity maps of their deuterated counterparts show diversity: relatively strong DCO+ and DNC integrated intensities are mainly distributed in the 70 m dark re-

gion (i.e., C18O-dominated region), while relatively strong N2D+ and NH2D integrated intensities are mainly distributed in the 70 m bright region (i.e., DCO+-dominated region).

[Figure 3: see original paper] The integrated intensity of molecular lines towards the end of G 011.0970–0.1093 molecular cloud. The velocity range for intensity integration for each line is given in [Figure 2: see original paper]. In each subfigure, red contours indicate regions with S/N > 3, with the black circle in the top right corner indicating the corresponding angular resolution (see). White contours represent the continuum emission observed by APEX at 870 m [28], starting from 5σ (σ = 5.6 MJy sr−1) and increasing in steps of 5σ, with an angular resolution of 18 .2. The 870 m continuum peaks are marked with gray 'x' symbols, while PC18O and PDCO+ markers are placed here.

3.3 Physical Parameters

3.3.1 Dust Temperature and H2 Column Density Using the multi-wavelength continuum data mentioned in Section 2, we can derive hydrogen molecular column density (NH2) and dust temperature (Tdust) by fitting the Spectral Energy Distribution (SED) of an ideal blackbody spectrum. The process is as follows: first, smooth (convolve) multi-band data to a uniform beam, then subtract foreground and background fluxes from the observed region, and finally organize the data for SED fitting. Details of this process are described below.

Using the Astropy convolution package [41], we smoothed data from different bands to achieve a common angular resolution, specifically Herschel's resolution at 500 m wavelength (36 .4). We then regridded the convolved data from each band to achieve a common pixel size (approximately 1/3 of the angular resolution, following Nyquist sampling criteria, i.e., 12) and alignment, recalculating the flux for each pixel during this process.

Following the procedure of Yuan et al. [42], we employed the Starlink software's Clump Identification (CUPID)–findback algorithm to iteratively construct foreground and background flux maps for the G 011.0970–0.1093 molecular cloud observation region. The algorithm works as follows: first, each input pixel is replaced by the minimum value among its surrounding pixels. Then, each pixel value is replaced by the maximum value within a box (2 .5 × 2 .5) centered on that pixel. Finally, for each pixel in these preliminarily processed data, we take the average value within a box (2 .5 × 2 .5) centered on that pixel for further processing. Since APEX is ground-based, any uniform astronomical signal on spatial scales larger than 2 .5 is filtered out along with atmospheric radiation [28]. Therefore, we used the same box size (2 .5 × 2 .5) in all three steps to obtain preliminary foreground and background flux estimation maps (see the CUPID–findback algorithm description for detailed procedures). During iteration, the foreground and background flux estimation maps generated from the previous processing step serve as input for the next iteration; this iterative pro-

cess is repeated 10 times to obtain the final foreground and background flux maps to be subtracted.

After smoothing multi-band dust continuum data to uniform spatial resolution, regridding to common pixel sizes, and subtracting foreground and background fluxes, we fitted each band's frequency optical depth τ using the following modified blackbody model:

S = Ωb B (T)(1 − e−τ) (1)

where S is the flux density at frequency , Ωb is the beam solid angle, and B (T) represents the Planck equation. The H2 column density can then be obtained through:

NH2 = Rgd τ / (H2 mH) (2)

where Rgd is the gas-to-dust mass ratio, typically taken as 150 [43]; H2 is the mean molecular weight, typically 2.8 [44]; mH is the hydrogen atom mass, taken as 1.67 × 10−24 g; and is the assumed dust opacity, with 230GHz = 0.899 cm2 g−1 [45]. Assuming a dust emissivity index $\beta = 1.8$, we performed fitting using the Levenberg-Marquardt algorithm Lmfit (Lmfit: Non-Linear Least-Square Minimization and Curve-Fitting for Python) to obtain the physical environment maps shown in [Figure 4: see original paper]. From subfigures (a)–(b), we see: NH2 ranges from 1022–1023 cm−2 (with uncertainty 10% per pixel), Tdust spans 10–20 K (with uncertainty 5% per pixel), and both are consistent with the spatial distribution of 870 m continuum radiation. Particularly, at the 70 m faint and 870 m peak (PC18O), the center is colder and denser than the envelope edge, showing a trend of decreasing Tdust and increasing NH2 from center to edge. At the 70 m bright and 870 m peak (PDCO+), the region is warmer and denser than the envelope edge, also showing a decreasing trend from center to edge. This suggests that heating in PC18O is dominated by external radiation, while PDCO+ may already host protostellar heating sources.

3.3.2 Gas Temperature NH3 molecules in cold (T < 20 K) and dense (nH > 104 cm−3) environments may not be depleted like other molecules (e.g., CO) [9, 14, 16], and both (J;K) = (1;1) and (2;2) inversion transitions can be effectively excited in the 10–100 K temperature range [35, 48–52]. In Feng et al.'s [6] study of other sources in the MIAO sample, fitting of these two lines' hyperfine structures (using the HfS package [53]) demonstrated their effectiveness as high-precision (uncertainty 1 K) temperature probes in such environments. For the G 011.0970−0.1093 molecular cloud observation region, we used the same method to obtain a gas temperature map: for each pixel, we performed hyperfine structure fitting to obtain excitation temperature (Tex) maps for each line, then summed the components of both lines to derive column density (Np-NH3) through a rotation diagram. Notably, the observed NH3 lines are para isomers, so the fitted Np-NH3 represents only part of the total NH3 column density (see discussion in Section 3.4). Because GBT observations have an angular resolution of 34 .7, consistent with the unified continuum resolution, the temperature

map here is not smoothed.

[Figure 4: see original paper] The physical structure of the tail of G 011.0970–0.1093 molecular cloud. Subfigures (a) and (b) show the H2 column density (NH2) map and dust temperature (Tdust) map, obtained from SED fitting to multi-wavelength continuum, both with an angular resolution of 36 .4. Subfigures (c) and (d) show the gas temperature (Tkin(p-NH3)) map and para-NH3 column density (Np-NH3) map, derived from rotation diagram fitting of the two inversion transition lines, both with an angular resolution of 34 .7. Black contours in each subfigure indicate the continuum emission observed by APEX at 870 m [28], starting from 5σ (σ = 5.6 MJy sr−1) and increasing in steps of 5σ, with an angular resolution of 18 .2. The 870 m continuum peaks are marked with gray 'x' symbols, while PDCO+ and PC18O markers are placed here. Only regions with S/N > 3 at 870 m are shown in each subfigure, with the angular resolution of each parameter indicated by the black circle in the top right corner.

Overall, at comparable angular resolution (dust at 36 .4, gas at 34 .7), the difference between gas temperature Tkin and dust temperature Tdust is <20% pixel by pixel, allowing us to reasonably assume thermal coupling between dust and gas at parsec scales.

3.4 Molecular Deuteration and Gaseous CO Depletion

Given that the gas temperature Tkin and dust temperature Tdust differ by <20% pixel by pixel, we can reasonably assume dust-gas coupling at parsec scales. Therefore, the paired clumps studied in this work are defined as regions of one beam size (36 .4) at the 870 m peak, which enhances signal-to-noise ratios for molecular lines and increases the credibility of comparative analysis.

We calculated the deuterium fraction and gaseous CO depletion for five molecules in the 70 m bright and dark clump pair at the terminus of G 011.0970–0.1093, following the validated assumptions of Feng et al. [6, 24] after comparing multiple methods. That is, we assume target spectral lines are optically thin, have a beam filling factor of 1, are in Local Thermal Equilibrium (LTE), and have excitation temperatures similar to dust temperatures at an angular resolution of 36 .4 to derive column densities for all target molecules except NH3.

Under these assumptions, for different molecules X, the column density can be calculated as:

NT = (3kBQ(Tex) / 8π3 2S) eEu/kBTex TB(v)dv (4)

where kB is the Boltzmann constant; Q(Tex) is the partition function, obtained by interpolating from molecular spectroscopy databases (JPL or CDMS); and S can also be obtained from JPL or CDMS databases; TB(v)dv is the integrated intensity of the molecular line (obtained by integrating over the range shown in [Figure 2: see original paper] except for NH3). lists the average column

densities for each molecule in a beam-sized (36 .4) region centered on PDCO+ and PC18O.

Column densities of molecules towards the 70 m bright and dark clumps pair in G 011.0970–0.109

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By comparing hydrogenated and deuterated isotopologue column density maps, we obtained the deuterium fraction maps for five molecular groups and the gaseous CO depletion map, shown in [Figure 5: see original paper], where subfigures (a)–(e) show the deuterium fraction maps for each molecule. For N2H+, the deuterium fraction is calculated as:

fD(N2H+) = N(N2D+) / N(N2H+) (5)

For molecules other than N2H+ that contain 13C, such as HCN, the calculation is as follows: based on statistical results from Giannetti et al. [54], we assume the 12C/13C isotope ratio in our target follows the variation with Galactocentric distance (RGC = 4.9 kpc [24]): 12C/13C = 6.1RGC(kpc) + 14.3, and this ratio does not vary within the molecular cloud. We also assume the isotopologue abundance ratio equals the isotope ratio [6, 24]. Taking HCN as an example:

fD(HCN) = N(DCN) / N(H13CN) × R12C/13C (6)

Notably, N2H+ column density calculations can correct for optical depth of hyperfine components through fitting of resolvable hyperfine structures. For NH3, we use the optically thin 13C J = 1–0 line to estimate column density and derive its deuterium fraction. As mentioned in Section 3.3.2, NH3 exists in ortho and para states with different ortho-to-para ratios (OPR). Assuming OPR follows statistical results of 3 and 1 for ortho and para respectively [55−56], we can convert para-NH3 column density to total (ortho+para) NH3 column density to derive the expected NH2D abundance.

In molecular cloud environments without gaseous CO depletion, the 16O/18O isotope ratio also varies with Galactocentric distance [57−58]. Therefore, the depletion rate of gaseous C18O can be expressed as the ratio between expected gaseous C18O column density and observed column density, shown in Figure 5: see original paper:

fD(C18O) = NE(C18O) / NO(C18O) (9)

where NE(C18O) is the expected column density and NO(C18O) is the observed column density.

Meanwhile, using the column density ratio method, we can also obtain the gaseous CO depletion map. In molecular cloud environments without gaseous CO depletion, Giannetti et al. [54] provide statistical results for the expected abundance ratio of C18O relative to H13CO+:

[Figure 5: see original paper] The relative abundance ratio maps between the deuterated and hydrogenated species and the CO depletion map. In subfigures

(a) to (e), pixels with integrated intensities <3σ (see for sigma rms for each line) are masked out. In subfigure (f) only the region with 870 m continuum emission >3σ is shown. Black contours in each subfigure represent the continuum emission observed by APEX at 870 m [28], starting from 5σ (σ = 5.6 MJy sr−1) and increasing in steps of 5σ, with an angular resolution of 18 .2. The 870 m continuum peaks are marked with gray 'x' symbols, while PDCO+ and PC18O markers are placed here. The angular resolution for each parameter is 36 .4, indicated by the black circle in the top right corner of each subfigure.

From the deuterium fraction and gaseous CO depletion rate (Figure 5: see original paper and (f)), and the physical properties, gaseous CO depletion, and differential molecular deuteration () of the 70 m bright and dark clump pair at the molecular cloud terminus, we find:

The average deuterium fraction of DCO+ in the PDCO+ region (clump) is 2.3 times that in the PC18O region, and the gaseous CO depletion rate is 33% higher in the PDCO+-dominated clump than in the PC18O-dominated clump.

Physical properties, depletion, and differential deuterium fraction of various molecules towards the 70 m bright and dark clumps pair in G 011.0970–0.1093

[The table content is preserved exactly as in the original]

Although the effective mapping area (pixels with S/N > 3) for four other molecular deuterium fractions is relatively small in our observations, the statistical results across the entire map remain meaningful. For DCO+ (1–0), despite effective mapping pixels comprising only 16% of total image pixels, the spatial distribution similarity between DCO+ and C18O (Figure 5: see original paper and (d)) is still evident. Specifically, the deuterium fraction in the PC18O-dominated clump is about an order of magnitude higher than in the PDCO+-dominated clump (see Figure 5: see original paper–(e)). The deuterium fraction of N2H+ in the PDCO+-dominated clump (0.7%) is higher than in other molecules (except DCO+), consistent with observations by Caselli et al. [9] and simulations by Albertsson et al. [59].

The isomeric pair HCN/HNC shows completely different deuteration enhancement behaviors (see Figure 5: see original paper–(c) and). HNC deuteration is particularly enhanced in the PC18O-dominated clump at 1.4%, about 17% higher than in the PDCO+-dominated clump. However, HCN shows the opposite trend, with deuteration in the PDCO+-dominated clump being 17% higher than in the PC18O-dominated clump. In terms of integrated line intensities, the HNC (1–0) to H13CN (1–0) ratio is 1.5 and 1.2 in the PC18O and PDCO+ clumps respectively, while the HCN (1–0) to H13CN (1–0) ratio is 0.6 and 1.2 in the PC18O and PDCO+ clumps respectively. While past observations have noted intensity differences between HCN/HNC ground-state transitions and attributed them to different formation activation energies [54, 60−62], the observationally opposite deuteration trends for this isomeric pair have only been noted in Feng et al.'s [6] pilot imaging study of G 28.34+0.06 and some recent point-source observations [63]. The "control mapping" observations of all MIAO

sample sources, including G 011.0970–0.1093, indicate that these differential deuteration trends have universality.

The average deuterium fraction of NH3 across the entire map is 0.5%, consistent with previous studies [55, 64]. However, NH2D is affected by standing waves in observations (see [Figure 2: see original paper]), resulting in relatively large uncertainties in its deuterium fraction calculation (20%). Even considering uncertainties, Figure 5: see original paper still shows no significant variation in NH3 deuteration across the map (except for edge noise-induced fluctuations), consistent with Feng et al.'s [6] conclusion from the pilot study source G 28.34+0.06 that NH3 deuteration is insensitive to temperature changes of 14–22 K.

The differential deuteration among these five molecular groups may be related to their gas-dust reaction pathways. For example, DCO+ can be formed both in gas phase and on dust surfaces, while N2D+ is formed only in gas phase.

4 Correlation Discussion

Although the numerical values of gas and dust temperatures, H2 column densities, and molecular column densities calculated in Sections 3.3 and 3.4 have relative errors due to uncertainties in physical quantities such as Rgd and , the gradients in temperature, H2 column density, and molecular deuteration shown in [Figure 4: see original paper] and [Figure 5: see original paper] are not caused by errors but represent intrinsic properties. Since the external environmental conditions where these gradients appear can be considered consistent (neighboring clumps within the same molecular cloud), the spatial variations of these physical quantities directly reflect the physical-chemical processes of central star formation. To quantify possible correlations among the spatial distributions of these five parameters, we extracted values from pixels with S/N $>$ 3 in each parameter map at a unified angular resolution (36 .4), generating four sets of bivariate Gaussian kernel density plots (see [Figure 6: see original paper]). Density contours in [Figure 6: see original paper] are colored red and blue according to whether they were extracted from PDCO+- or PC18O-dominated regions, with corresponding Spearman correlation coefficients ( ) indicated in matching colored text [65]. Additionally, the overall Spearman correlation coefficient (all) for the entire region is shown in black. To quantify possible correlations between parameter pairs, we follow Feng et al.'s [24] classification: $| | \geq 0.5$ indicates strong correlation or strong anti-correlation; $0.3 \leq | | < 0.5$ indicates moderate correlation or moderate anti-correlation; $0.1 \leq | | < 0.3$ indicates weak correlation or weak anti-correlation; $| | < 0.1$ indicates no correlation. From [Figure 6: see original paper], we summarize the following interesting patterns:

In subfigure (a), the PC18O-dominated clump shows a strong spatial anti-correlation between Tdust and NH2 (= –0.75), indicating that in relatively denser regions, temperatures are relatively lower, and external contributions likely dominate heating of the gas and dust in this region. In contrast, the PDCO+-dominated clump shows weak spatial positive correlation (= 0.19),

suggesting an increasing trend from envelope to center, indicating that internal heating sources may already exist within the clump, possibly from protostellar core radiation.

Subfigure (b) shows that in specific regions, the relative abundance ratio of gaseous DCO+ to C18O in the relatively warm PDCO+-dominated clump (16–18 K) is about 4 times higher than in the relatively cold PC18O-dominated clump (11–16 K).

According to subfigure (c), for the PDCO+-dominated clump, the parameters DCO+ deuteration and C18O depletion show strong positive correlation in both PDCO+-dominated (= 0.92) and PC18O-dominated (= 0.64) clumps. Theoretically, H13CO+ (1–0) has a higher critical density (ncrit = 9.3 × 105 cm−3 at T = 10–20 K). In the PDCO+-dominated clump, these parameters show even stronger positive correlation (= 0.92) in relatively denser regions. This stronger positive correlation (> 0.70) exists not only in this source but also in other MIAO sample sources such as G 28.34+0.06, G 15.22–0.43, and G 14.49–0.13 [6, 24].

In subfigure (d), the entire observation region shows strong positive correlation (= 0.78), while the PDCO+-dominated clump shows even stronger positive correlation (= 0.83). These correlations can be understood as resulting from the comprehensive efficiency of the chemical reaction network: HCO+ formation involves CO chemistry (e.g., H3+ + CO → H2 + HCO+), while DCO+ deuteration can occur through multiple pathways including CO deuteration (e.g., H2D+ + CO → H2 + DCO+), D2H+ + CO → HCO+ + D2, and HCO+ + D → DCO+ + H [66–69].

[Figure 6: see original paper] Bivariate Gaussian kernel density plots depicting relationships between various variables. Data in each subplot are smoothed to a consistent angular resolution (36 .4) and extracted from pixel grids, with contours drawn using bivariate Gaussian kernel density estimation. Regions dominated by PDCO+ and PC18O are highlighted in red and blue respectively, with Spearman correlation coefficients ( ) indicated in corresponding colors. The overall Spearman correlation coefficient (all) is shown in black. Pixel data where the 870 m continuum radiation is $<3\sigma$, or where the integrated intensity of DCO+(1–0) $<3\sigma$, are masked.

5 Conclusions

To quantitatively characterize the physical-chemical environment of extremely early-stage high-mass star-forming regions, we initiated the MIAO survey program. This paper focuses on a pair of neighboring clumps at the terminus of filamentary molecular cloud G 011.0970–0.1093 that both peak at 870 m continuum but appear bright and faint respectively at 70 m continuum. Through analysis of deuteration in five molecular groups and parsec-scale gaseous CO depletion at an angular resolution of 36 .4 (corresponding to a spatial scale resolution of 0.5 pc), we find that this target source shares consistent physical-

chemical characteristics with the MIAO pilot study source G 28.34+0.06, suggesting that differential molecular deuteration in relatively cold environments and the strong positive correlation between gaseous CO depletion and DCO+ deuteration at parsec scales may be universal:

1. After subtracting foreground and background emission, SED fitting of multi-wavelength dust continuum data indicates that the temperature and density of the 70 m bright region decrease from the clump center (17 K, 3.5 × 1022 cm−2) to the envelope edge, suggesting that protostar formation may have already begun within the clump. Conversely, the center of the 70 m dark clump is colder (11 K) and denser (5.0 × 1022 cm−2) than its periphery, with a strong anti-correlation between H2 column density and dust temperature, indicating that heating of this clump may be dominated by external interstellar radiation.

2. The gas kinetic temperature map derived from NH3 and the dust temperature map differ by <20% pixel by pixel, allowing reasonable assumption of thermal coupling between dust and gas. The integrated intensity distributions of C18O (2–1) and DCO+ (1–0) show clear spatial offsets. Under conditions of optically thin lines, beam filling factor of 1, LTE, and consistent isotopologue abundance ratios with isotope ratios based on Galactic elemental abundance statistics, the molecular column density and relative abundance maps derived through 12C/13C and 16O/18O conversion indicate: the deuterium fraction of DCO+ reaches as high as 7 in the cold, dense PC18O-dominated clump, about 2.3 times higher than in the warmer PDCO+-dominated clump. Gaseous CO depletion and DCO+ deuteration show strong positive correlation in spatial distribution (= 0.92) at parsec scales. The deuterium fractions of the five molecular groups differ significantly.

3. The integrated intensity distributions of DCO+ (1–0) and DNC (1–0) coincide with the 70 m dark region, where the deuteration fraction (1.4% for DNC, 0.7% for DCO+) is 30%–150% higher than in the 70 m bright region, indicating these molecules are more easily deuterated in cold environments. In contrast, the integrated intensities of N2D+ (1–0) and NH2D (11,10s–10,10a) highly coincide with the 70 m bright region, where the deuteration fraction (0.5% for NH3) is 17% higher than in the 70 m dark region, suggesting these molecules may be more easily deuterated in warm environments (14–20 K). NH3 shows no significant deuteration enhancement at 14–20 K. These differential deuteration characteristics may be related to the gas-dust formation pathways of these molecules.

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References

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Note: Figure translations are in progress. See original paper for figures.