Chemical Diversity in Young Protoplanetary Disk

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Abstract

Planets are a common product of the star formation process and there is an incredible variety of planetary systems in the Galaxy that are significantly different from the Solar System. Recent observations reveal diversity even in chemical nature: various complex organic molecules are found to be abundant in protoplanetary-disk forming regions, whose compositions are significantly different depending on sources. Our Solar system thus may not be a common type in the Universe, suggesting rarity of our existence. Understanding the initial chemical diversity among protoplanetary-disk is one of the key step to know the rarity or similarity. There could be two ways: statistical survey of chemical composition in embedded protoplanetary-disks and high-resolution observations that reveals detailed distribution of molecules in representative sources. In both cases, the biggest concern is dust opacity reducing the line intensities at submillimeter wavelengths. Centimeter-wave observations with ngVLA allow us to overcome the difficulty.

Key words: Astrochemistry – ISM: molecules – Stars: formation – Stars: protostars – Protoplanetary disks –

1. Introduction

In the past two decades, it is clearly demonstrated that envelopes as well as protostellar disks around solar-type protostars have significant chemical diversity: some sources harbor various saturated complex organic molecules (COMs), so called hot corinos (Cazaux et al. 2003; Lefloch et al. 2018; Oya et al. 2016), whereas some others harbor unsaturated species instead, so called Warm Carbon-Chain Chemistry (WCCC) sources (Sakai et al. 2008; Yoshida et al. 2019; Sakai et al. 2014a). The chemical diversity would originate from the evolution of the physical environment, such as the timescale of the starless core phase (Sakai and Yamamoto 2013; Higuchi et al. 2018). Sources showing both types of molecules may support this scenario (Oya et al. 2017; Imai et al. 2018). Some theoretical studies have also investigated the origin of such chemical diversity (Aikawa et al. 2020; Kalvans 2021), suggesting that the environment plays a significant role in the production of carbon-chain molecules. Chemical evolution during formation of protoplanetary disk is, therefore, one of the most important targets to be explored, because it directly determines the initial chemical compositions of disks, where planets form.

While millimeter/submillimeter wave observations with ALMA have showed detailed chemical compositions of early-stage protostellar disks, the dust opacity sometimes prevents us from characterizing the molecular properties. High dust opacity reduces the intensity of molecular emission, resulting considerable underestimation of molecular abundances. Thus, it is difficult to determine whether nondetections of COM emission are due to high dust opacity or lack of COMs. NGC 1333 IRAS 4A1, a Class 0 protostar, is the most demonstrative case. Known as a system showing hot corino chemistry (Bottinelli et al. 2004), NGC 1333 IRAS 4A turns out to be a binary system, which consists of two Class 0 protostars, A1 and A2. Both protostars drive powerful molecular outflows (Santangelo et al. 2015), while only 4A2 shows emission of COMs (Persson et al. 2012; Taquet et al. 2015; López-Sepulcre et al. 2017; Sahu et al. 2019). Centimeter wave observation with VLA have made a breakthrough on this problem. De Simone et al. (2020) detected and mapped the CH_3OH emission at 25 GHz band (K-Band) in 4A1, which has a stronger dust continuum emission and no emission of COMs at higher frequencies. They clearly demonstrated that dust blocks molecular emissions in 4A1 at millimeter/submillimeter wavelengths, whereas dust becomes optically thin at centimeter wavelengths allowing us to characterize the chemistry of 4A1. We expect similar situation in other protostellar sources that lead to underestimation of chemical abundance or nondetections.

2. Chemical Diversity Seen in Millimeter/Submillimeter Observations

In order to understand the chemical diversity, Yang et al. (2021) surveyed 50 young stellar object located in Perseus molecular cloud complex ($d \sim 300$ pc) by ALMA (the Perseus ALMA Chemistry Survey: PEACHES). Such survey of COMs toward large sample of solar-type protostars, has never been done before. With a spatial resolution of 100 au in radius, rotational transitions of methanol (CH_3OH), acetonitrile (CH_3CN), methyl formate (CH_3OCHO), and dimethyl ether (CH_3OCH_3) were observed at ~250 GHz. The survey shows that 58% of the sources harbor CH_3OH with 42% of the sources exhibiting no sign of organic molecules. Figure 1 shows examples of the distribution of CH_3OH ($5_{14} - 4_{13}$, $E_u = 49.66$ K) and CH_3OCHO ($24_{0/1,24} - 23_{0/1,23}$, $E_u = 158.23$ K) lines.

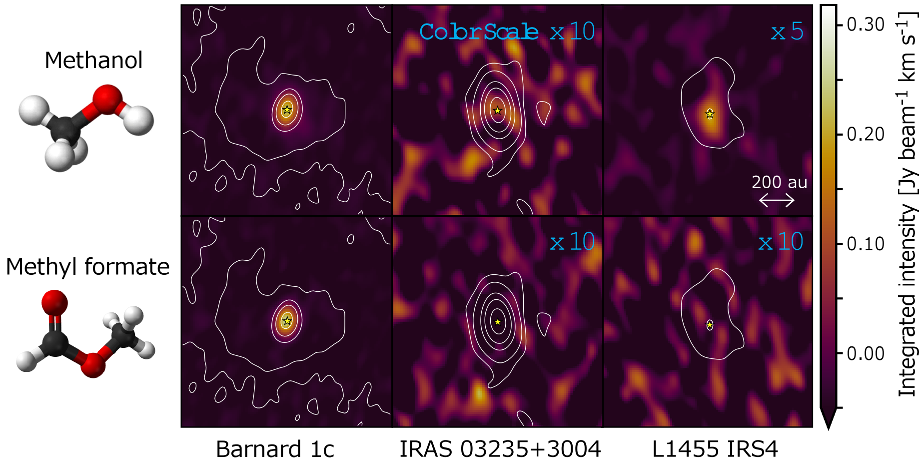

Fig. 1. Distribution of molecular gas around the protostars. Three typical cases are selected from the 50 sources. Color shows intensities of molecular emission, whereas contours show the thermal emission from dust.

Because the brightness temperature of the 1 mm dust continuum emission is higher toward Barnard 1c, the nondetection of the lines in IRAS 03235+3004 could be understood by the poorness of the COMs rather than high dust opacity. Whereas IRAS 03235+3004 has a brighter continuum indicative of more materials than that of L1455 IRS4, only L1455 IRS4 shows emission of COMs, suggesting that the appearance of organic molecules is irrelevant to the total amount of material (Fig. 1). CH_3OH and CH_3OCHO are some of the most frequently detected molecules in the PEACHES survey, found in 54% and 30% of the sample, respectively. By modeling the spectra, they further derived the excitation temperature of CH_3OH and CH_3OCHO ranging from 120–360 K and 80–330 K, respectively. Their finding is consistent with the hypothesis that COMs are evaporated from dust grains in the hot region near the protostar.

The derived column densities of CH_3OH and CH_3CN show huge variance, more than two orders of magnitude (Fig.2a). Same variance persists after correcting the total gas/dust amount in each source (Fig.2b). Sources without COMs emission have a wide range of continuum intensities. Physical conditions, such as luminosity and temperature, are also found to be irrelevant to the chemical abundances. Therefore, the actual chemical diversity, which could be caused by the difference in local environmental history of individual target, may be the primary cause for such variance.

On the other hand, relative ratios between COMs are similar in most of the sources. In particular, CH_3OH and CH_3CN column densities are tightly correlated with a correlation coefficient of 0.87 (Fig.2). The column densities of CH_3OCHO and CH_3OCH_3 also correlate with CH_3OH with lower values of the correlation coefficient, 0.76 and 0.48, respectively. Correlation between the parent molecule and daughter molecule can naturally occur because of the direct relation in their formation pathways. However, the tight correlation between oxygen-bearing COMs and nitrogen-bearing COMs is not easily understood. CH_3OH is known to be formed on grains by hydrogenation of CO (Watanabe et al. 2003), whereas the formation mechanism of CH_3CN, which involves both gas-phase and grain surface processes, is not well understood yet. The almost perfect correlation found in the PEACHES survey gives strong constraints on this problem. However, more detailed comparison in distributions and excitation conditions are required to reveal the origin of the correlation.

Judging from the extremely beautiful correlation between abundances of CH_3OH and CH_3CN (Fig.2), it seems likely that the dust opacity plays an insignificant role on the relation between the two species. However, the sources without any molecular emission toward the continuum peak may suffer from the opacity problem, leading to apparent absence of COM emission. Furthermore, the dust opacity may affect the derivation of column densities of all COMs, which can not been recognized in the apparent correlation if at all. The large variety of COMs abundances could be affected by high dust opacity, especially in the sources with strong continuum emission. To unambiguously characterize the chemistry in disk-forming regions, we need to address this opacity issue. Centimeter wave observations of COMs with ngVLA will solve this problem easily because of the low optical depth of dust at ngVLA frequencies. Thus, we will directly measure the abundance of COMs without impedance.

3. Observations with ngVLA

In ngVLA Band 4 (20.5–34 GHz), there is a number of important molecular lines. We can observe the Q-branch lines of CH_3OH simultaneously. Furthermore, inversion transitions of NH_3, a fundamental nitrogen-bearing species, can be observed in the same frequency range (Fig.3). This coincidence enables us to constrain the properties of CH_3OH, kinetic temperature and column density, at almost the same observing condition such as beam sizes and weather conditions. Apart from the Band 4, ngVLA can observe important H_2CO lines in Band 3 ($2_{11}-2_{12}$) and 6 ($1_{01}-0_{00}$). If we assume an ortho-para-ratio of H_2CO, those combination of lines tells us the H_2 density of the region. Because larger molecules tend to emit lines at lower frequencies due to smaller rotational constant B, ngVLA will probe the inventory of long carbon-chain molecules as well as large COMs. Together with au-scale resolution at nearby star-forming regions, ngVLA will map the chemical composition

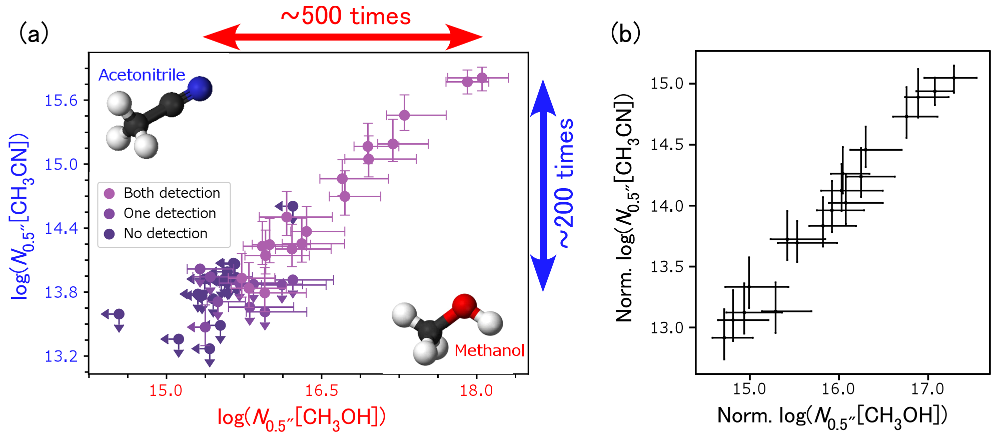

Fig. 2. (a) Direct comparison between column densities of methanol (x-axis) and acetonitrile (y-axis) in logarithmic scale. They have a wide range of values, more than two orders of magnitude. (b) Comparison of the column densities of methanol and acetonitrile after the normalization by the brightness of the dust emission. Even after the normalization, the data still show tight correlation between the abundances of two molecules across more than two orders of magnitude.

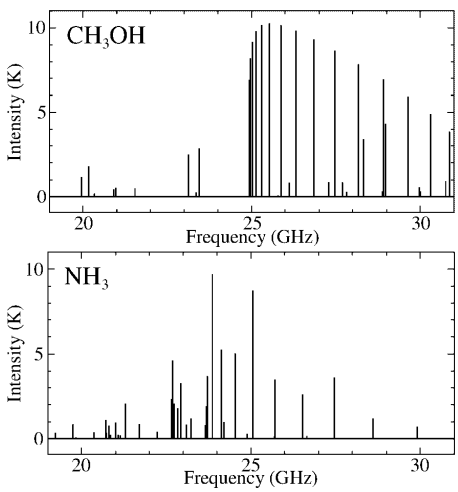

Fig. 3. Spectral lines of CH_3OH and NH_3 observable in ngVLA Band 4 (20.5-34 GHz)

in young disks, which are still growing around embedded protostar and host sites of planet formation. Here we present two science cases for ngVLA proposal.

3.1. *Example 1: Chemical Survey*

In the ALMA bands, high dust opacity poses a critical issue on chemistry surveys. As demonstrated by De Simone et al. (2020), the observation of one of the most abundant COMs, CH_3OH, takes 10s of hour per source with VLA, making surveys of large sample of protostars infeasible. With ngVLA, we can survey COMs and other complex molecules towards a few 10s of sources, such as samples in the PEACHES survey, with an rms of 10 K at 0.3″ beam (0.44 mJy/beam at 24 GHz) and 0.5 km/s velocity resolution. An hour per source is required to give an approximate exposure time for such survey. Chemical compositions of growing disks around Class 0 protostars determine the initial chemical condition of protoplanetary disks. Thus, measuring the initial chemical composition is extremely important to understand the chemical evolution in protoplanetary disks and eventually in planetary systems.

3.2. *Example 2: Detailed chemical view along disk-substructure formation*

The second science case is deep integration observation toward several representative young disks. Around the infant disks, materials are still accreting onto the disk, keeping the disk geometrically thicker. Inside such young disk, dust growth as well as disk substructure formation occur. Recent observations show substructures in young disks around Class 0 protostars (Sheehan & Eisner 2018; Segura-Cox et al. 2020; Oya et al. 2020). The edge-on disk of L1527, a Class I protostar, shows warped structure as well as ring-like structure (Sakai et al. 2019; Nakatani et al. 2020; Ohashi et al. 2021). These substructures and dynamics can affect the distribution of molecules and regulate the chemical evolution in disk. Thus, mapping the distribution of chemical composition in those substructures, such as rings and gaps, is important to study the initial chemical condition of planet formation, which may cause or may be caused by those substructure formation. Furthermore, in the millimeter/submillimeter band, we could only obtain chemical composition of the disk surface, while centimeter-wave observations directly probe the disk midplane. With ngVLA, we will have necessary spatial resolution (au scale) at low frequency to characterize the young and potentially planet-forming disks. If such substructures are observed by multiple-transition lines at ~10 au resolution (0.07″), where the substructures are detected, it enable us to measure the temperature and density in substructures. Towards edge-on sources, we can obtain layered structure of chemistry, which has only be done in models.

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