

# Carbon-Chain Chemistry around Massive Young Stellar Objects – Revealing the Origins of Chemical Diversity –

Kotomi Taniguchi,<sup>1</sup> Kei E. I. Tanaka,<sup>2,3</sup> & Masao Saito<sup>3,4</sup>

<sup>1</sup>*Department of Physics, Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima-ku, Tokyo 171-8588, Japan*

<sup>2</sup>*Center for Astrophysics and Space Astronomy, University of Colorado Boulder, Boulder, CO 80309*

<sup>3</sup>*National Astronomical Observatory of Japan, 2-21-1 Osawa, Mitaka-shi, Tokyo 181-8588*

<sup>4</sup>*Department of Astronomical Science, School of Physical Science, SOKENDAI (The Graduate University for Advanced Studies), 2-21-1 Osawa, Mitaka-shi, Tokyo 181-8588, Japan  
kotomi.taniguchi@gakushuin.ac.jp*

## Abstract

Recent radio astronomical observations have found chemical diversity around massive young stellar objects (MYSOs). Such chemical diversity is likely related to the variety of environments and/or processes during the starless core phase or the later protostellar phase. Hence, it is important for the understanding of the formation processes of massive stars to investigate the characteristics and origins of the chemical diversity around MYSOs. High angular-resolution ( $\lesssim 1000$  mas) and high velocity-resolution ( $\sim 0.2$  km s<sup>-1</sup>) observations of unsaturated carbon-chain species and saturated complex organic molecules (COMs) by the next generation Very Large Array (ngVLA) will draw their spatial distributions of abundance and excitation condition, kinematics of envelopes and inner hot gas, and the heritage of the chemical composition from envelopes to disk structures around MYSOs. Such observations will shed light on puzzles about complex chemistry around MYSOs.

**Key words:** Astrochemistry — ISM: molecules — stars: massive

## 1. Introduction

### 1.1. The diversity of carbon chemistry around massive young stellar objects

Approximately 200 molecules have been detected in the interstellar medium and circumstellar shells so far. The chemical composition is a useful tool to investigate star formation processes, and evolutionary stages and physical conditions in star-forming regions (e.g., ?; ?). Hence, it is important to reveal relationships between the chemical composition and physics in star-forming regions. Notable, carbon is one of the essential elements in the universe, as it is the pivotal element of organic molecules including prebiotic molecules.

Saturated complex organic molecules (COMs) have been found to be abundant around massive young stellar objects (MYSOs), namely hot core chemistry (e.g., ?). A similar chemical character was found around low-mass young stellar objects (YSOs) and named hot corinos. These COMs are mainly formed on dust surface during the cold starless and lukewarm protostellar phases (e.g., ?).

Another type of molecules containing carbon abundantly is unsaturated carbon-chain species. Their chemistry has been studied in detail in low-mass star-forming regions. Carbon-chain molecules are known as early-type species; they are abundant in young starless cores, and their abundances decrease in star-forming cores (e.g., ?; ?). Carbon-chain molecules are efficiently formed by ion-molecule reactions or exothermic neutral-neutral reactions without reaction barriers involving C<sup>+</sup> and/or C in the cold gas in starless cores ( $\sim 10$  K).

In contrast to the classic carbon-chain chemistry in cold starless cores, it was found that carbon-chain molecules are anew

formed around low-mass YSOs from CH<sub>4</sub> sublimated from ice mantles at the warm temperatures around 25 K. This carbon-chain formation around low-mass YSOs was named “warm carbon-chain chemistry” (WCCC; ?). In WCCC sources, COMs are relatively deficient compared to those in hot corino sources, and it was suggested that there is chemical diversity around low-mass YSOs.

On the other hand, the carbon-chain chemistry in high-mass star-forming regions has been revealed only fairly recently (e.g., ?; ?; ?; ?; ?). It was found that HC<sub>5</sub>N, the second shortest member of the cyanopolyne family (HC<sub>2n+1</sub>N), is abundant in hot cores and/or warm envelopes of their target MYSOs (?; ?). Cyanopolyynes are one of the unsaturated carbon-chain series. In addition, ? found chemical diversity around MYSOs; COM-poor cores are surrounded by carbon-chain-rich envelopes, while COM-rich cores, namely hot cores, are encompassed with CH<sub>3</sub>OH-rich envelopes. A subsequent study with the Nobeyama 45-m radio telescope (?) reported the CCH/HC<sub>5</sub>N column density ratios around MYSOs of  $\sim 15$ , which is significantly lower than the ratio around the L1527 low-mass WCCC source ( $\sim 625$ ). These results indicate that carbon-chain molecules around MYSOs at least partially exist in higher temperature regions than those around low-mass WCCC sources.

In order to investigate the formation mechanisms of cyanopolyynes around MYSOs, chemical network simulations have been conducted (?). The models unveiled a new intriguing path of the cyanopolyne chemistry in the warm and hot gas phases. Cyanopolyynes first form in the warm gas (25–100 K), but most of them are once absorbed and stored in ice mantles of dust grains. Later, as the temperature increases to the ice sublimation temperature of 100 K, the cyanopolyynes

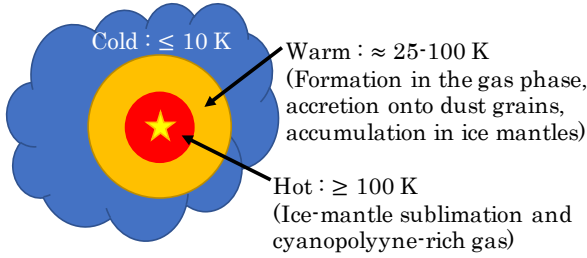


Fig. 1. A schematic view of HCCC (?).

are released and show their gas-phase peak abundances. Fig.?? shows a schematic view of this cyanopolyynes chemistry around MYSOs. We call the carbon-chain chemistry around MYSOs “hot carbon-chain chemistry (HCCC)” in this document.

In summary, carbon-chain molecules are formed anew around MYSOs, and there is the chemical diversity around MYSOs.

### 1.2. Possible factors producing the chemical diversity around MYSOs

The chemical diversity should be related to the variety of environments and/or formation processes when starless cores form and after YSOs are born. If we consider a condition with identical elemental abundances, there are three possible factors producing the chemical diversity; (1) formation and destruction mechanisms of each molecule, (2) different amounts of illumination from the interstellar radiation field (ISRF; ?) or cosmic-ray ionization, and (3) different heating timescale (?). In order to disentangle these factors observationally, it is necessary to carry out high spatial-resolution and high velocity-resolution observations of both carbon-chain molecules and COMs toward MYSOs. The next generation VLA (ngVLA) will be a particularly ideal observational facility, because it will enable us to study the above factors.

## 2. Observations of carbon-chain molecules and COMs around MYSOs with the ngVLA

### 2.1. General observational strategy

In order to investigate the characteristics of the chemical diversity around MYSOs, it is essential to reveal spatial distributions of molecular abundance and excitation condition of both carbon-chain species and COMs around MYSOs. Such observations will be useful for the investigation of the effects of formation and destruction mechanisms of each species on the chemical diversity. It is generally known that carbon-chain molecules are formed in the gas phase, whereas COMs are formed mainly on dust surfaces. Some COMs could be formed in the gas phase (e.g., ?). Hence, the spatial distributions of abundance and excitation condition are expected to be different among species with different formation/destruction mechanisms. Comparisons of their spatial distributions among different types of species in various MYSOs could provide information about the carbon-chain chemistry around MYSOs, or the HCCC mechanism (?).

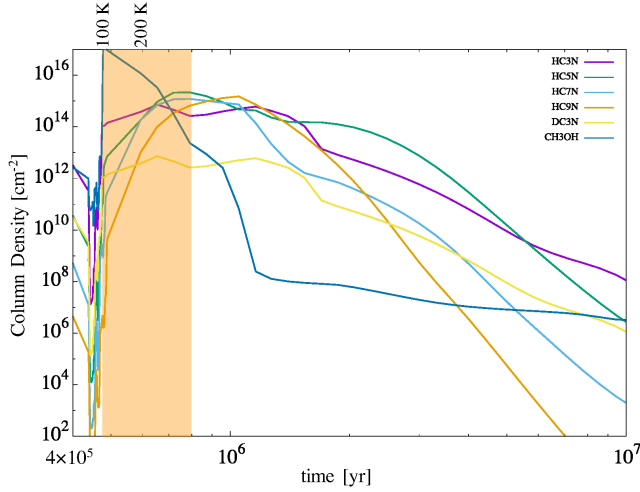
Observations with the ngVLA will answer the effect of the

different heating timescale. The heating timescale ( $t_h$ ) depends not only on spectral type of the central star but also on the infall velocity ( $V_{\text{infall}}$ ) and the size of the warm region ( $R_{\text{warm}}$ ) (?). Here, “warm” means temperatures around 25 – 100 K (see Fig.??). It can be considered that  $t_h$  is proportional to  $\frac{R_{\text{warm}}}{V_{\text{infall}}}$  (?). The ngVLA is expected to draw the gas motion, i.e.,  $V_{\text{infall}}$ , even in dense regions where it is opaque in ALMA observations. The ngVLA will also cover the  $\text{NH}_3$  lines at the 23 GHz band, a useful temperature probe. We can derive spatial distributions of the gas kinetic temperature using the  $\text{NH}_3$  data. Combining these results, we can evaluate how long materials pass in warm regions when they accrete onto the central hot regions. By this means, we will assess the effects of the heating timescale on the chemical diversity. Furthermore, observations of the magnetic field will be related to this study, because the magnetic field controls the infalling motion (?; ?).

One good target source as a carbon-chain-rich source is the G28.28–0.36 MYSO. The  $\text{HC}_5\text{N}/\text{CH}_3\text{OH}$  ratio toward G28.28–0.36 is higher than the other MYSOs by one order of magnitude (?). A unique characteristic of this source is that the cosmic-ray ionization does not seem to work efficiently compared to other MYSOs and carbon-chain species are formed by bottom-up mechanisms (?). This feature enables us to investigate temperature dependences of formation and destruction mechanisms of carbon-chain species and COMs and confirm the HCCC mechanism.

Cyanopolyynes ( $\text{HC}_{2n+1}\text{N}$ ) are good candidates as target carbon-chain molecules. For assessment of the effects of the ISRF on the chemical diversity, it is necessary to carry out observations of carbon-chain species and COMs toward several MYSOs located inside and outside of the same giant molecular clouds (GMCs) or clusters. If the ISRF is important for the chemical diversity around MYSOs, as suggested by ?, it is expected that MYSOs located outside of GMCs are rich in carbon-chain species. However, we need to distinguish whether carbon-chain molecules are formed by the HCCC mechanism or by the bottom-up formation involving  $\text{C}/\text{C}^+$  produced in photodominated regions (PDRs) in order to confirm the chemical diversity. It is necessary to confirm that carbon-chain molecules are formed by the HCCC mechanism in order to claim the chemical diversity around MYSOs. Although CCH traces PDRs, long cyanopolyynes, such as  $\text{HC}_7\text{N}$  and  $\text{HC}_9\text{N}$ , are probably not enhanced in PDRs (?). Hence, we will be able to distinguish whether carbon-chain species are enhanced by the HCCC mechanism or not with observations of long cyanopolyynes. As shown later, the ngVLA can cover many lines of long cyanopolyynes. For example, rotational lines of  $\text{HC}_9\text{N}$  from  $J = 36 - 35$  ( $E_{\text{up}} = 18.5$  K) to  $J = 86 - 85$  ( $E_{\text{up}} = 104.3$  K) are covered by the ngVLA Bands 4 and 5.

In order to achieve these science goals, we need high angular-resolution and high velocity-resolution observations. Because the typical size of hot core is  $\approx 0.1$  pc with the distance of 2–5 kpc, a required angular resolution is estimated at  $< 1000$  mas. The velocity resolution of  $\sim 0.2 \text{ km s}^{-1}$  is needed to investigate gas kinematics of envelopes and cores around MYSOs.



**Fig. 2.** Estimations column densities of cyanopolynes and  $\text{CH}_3\text{OH}$  based on hot core models with the fast warm-up period ( $5 \times 10^4$  yr) model (?). The orange covered range is used for determining column densities.

## 2.2. Feasibility of observations with the ngVLA

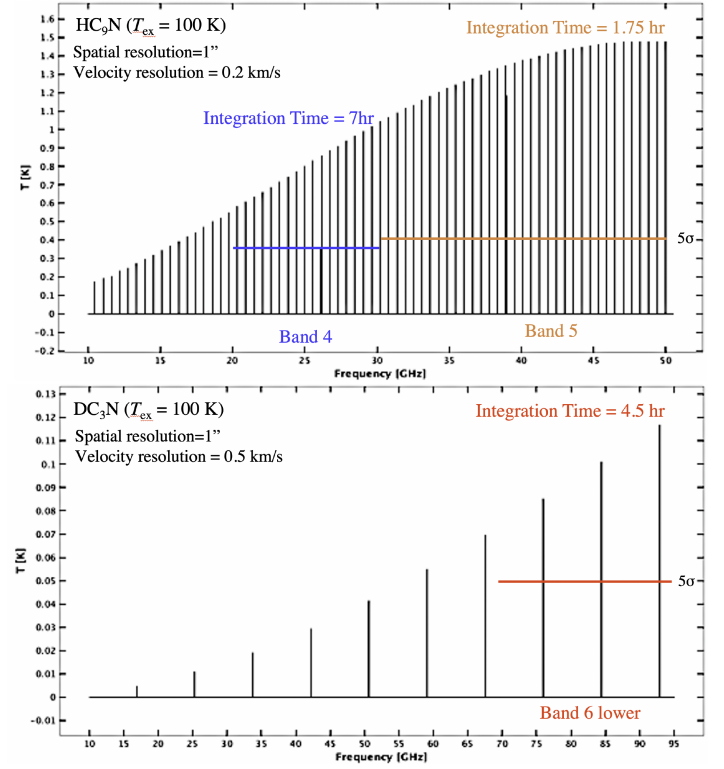
We study the feasibility of observations of carbon-chain molecules around MYSOs with the ngVLA. Regarding COMs, other authors have already studied (?). Thus, we evaluate the observability of only cyanopolynes here.

In addition to the main isotopologues of cyanopolynes, we investigate the rare isotopologues. Since the deuterium fractionation is an important factor to investigate evolutionary stages and conditions of star-forming cores, we investigate the deuterium species. The deuterium factor of  $\text{HC}_3\text{N}$  may provide a hint of star-formation history from before cores form to after protostars are born (?; ?).

Our procedures for estimations of line intensities are as follows. We derived the column densities of molecules using the results of chemical network simulations by ?, assuming that the  $\text{H}_2$  column density is  $10^{22} \text{ cm}^{-2}$ . Since we are interested in cyanopolynes in hot regions ( $T > 100 \text{ K}$ ), we determined the column densities by the time average while the temperature is 100 – 200 K (orange covered range in Fig.??). We assumed that the  $\text{HC}_3\text{N}/\text{DC}_3\text{N}$  is 100. The column densities of  $\text{HC}_9\text{N}$  and  $\text{DC}_3\text{N}$  are derived to be  $5.9 \times 10^{13} \text{ cm}^{-2}$  and  $1.9 \times 10^{12} \text{ cm}^{-2}$ , respectively.

Using the CASSIS<sup>1</sup> software, we estimated line intensities of rotational lines of  $\text{HC}_9\text{N}$  and  $\text{DC}_3\text{N}$  with the above column densities and a fixed excitation temperature (100 K) and a fixed line width (FWHM;  $2.0 \text{ km s}^{-1}$ ). The results are shown in Fig.?. We also indicate the  $5\sigma$  limits of observations by the ngVLA with setups and integration times shown in the figure. As seen in the upper panel of Fig.?, the  $\text{HC}_9\text{N}$  lines can be easily detected in Band 4 and Band 5.

Regarding  $\text{DC}_3\text{N}$ , we assumed that observations with the velocity resolution of  $0.5 \text{ km s}^{-1}$  instead of  $0.2 \text{ km s}^{-1}$ , because its detection is only a matter. In Band 6 lower, three lines ( $J = 9 - 8$ ;  $E_{\text{up}} = 18.2 \text{ K}$ ,  $J = 10 - 9$ ;  $E_{\text{up}} = 22.3 \text{ K}$ ,



**Fig. 3.** Estimations of line intensities for  $\text{HC}_9\text{N}$  (upper panel) and  $\text{DC}_3\text{N}$  (lower panel).

$J = 11 - 10$ ;  $E_{\text{up}} = 26.7 \text{ K}$ ) are expected to be detected by observations with an integration time of 4.5 hours. Moreover, rotational lines of  $\text{HC}_5\text{N}$  (from  $J = 27 - 26$ ;  $E_{\text{up}} = 48.3 \text{ K}$  to  $J = 35 - 34$ ;  $E_{\text{up}} = 80.5 \text{ K}$ ) and  $\text{HC}_7\text{N}$  (from  $J = 63 - 62$ ;  $E_{\text{up}} = 109.1 \text{ K}$  to  $J = 84 - 83$ ;  $E_{\text{up}} = 193.3 \text{ K}$ ) lie in this frequency band, and most of them can be expected to detect simultaneously within the short observing time. Therefore, we can trace the deuterium fractionation and warm and hot gas simultaneously with the ngVLA. Such observations will be benefit for studying evolutionary stage and environments in hot core regions.

Observations with the ngVLA toward hot cores will provide us a new insight into the chemistry of both carbon-chain species and COMs (see also ?). Using radio astronomical facilities which are available currently or in the near future, we can prepare for future observations with the ngVLA. For instance, survey observations of carbon-chain molecules and COMs in the 7 mm band toward MYSOs will provide us good target source lists. The ngVLA will boost up studies about characteristics of the chemical diversity around MYSOs.

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