Chemical Composition in the IRAS 16562–3959 High-mass Star-forming Region

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Abstract

We have analyzed the Atacama Large Millimeter/submillimeter Array cycle 2 data of band 6 toward the G345.4938+01.4677 massive young protostellar object (G345.5+1.47 MYSO) in the IRAS 16562–3959 high-mass star-forming region with an angular resolution of ∼0′′3, corresponding to ∼760 au. We spatially resolve the central region, which consists of three prominent molecular emission cores. A hypercompact H II region (Core A) and two molecule-rich cores (Core B and Core C) are identified using the moment zero images of the H30α line and a CH3OH line, respectively. Various oxygen-bearing complex organic molecules, such as (CH3)2CO and CH3OCHO, have been detected toward the positions of Core B and Core C, while nitrogen-bearing species, CH3CN, HCN, and its 13C isotopologues, have been detected toward all of the cores. We discuss the formation mechanisms of H2CO by comparing the spatial distribution of C18O with that of H2CO. The 33SO emission, on the other hand, shows a ring-like structure surrounding Core A, and it peaks on the outer edge of the H30α emission region. These results imply that SO is enhanced in a shock produced by the expanding motion of the ionized region.

Unified Astronomy Thesaurus concepts: Astrochemistry (75); Interstellar molecules (849); Massive stars (732)

1. Introduction

Complex organic molecules (COMs), consisting of more than six atoms and rich in hydrogen, are abundant in the compact (∼0.1 pc) dense and hot gas (n ≥ 107 cm−3, T ∼ 100 K) around massive young protostars (Herbst & van Dishoeck 2009). Their chemistry is known as hot core chemistry. Development of radio observational facilities has enabled detailed investigation of this chemistry toward high-mass star-forming regions (Tercero et al. 2018; Bonfand et al. 2019; Gieser et al. 2019; Pagani et al. 2019). Well-studied Galactic hot cores are Sagittarius B2 (e.g., Bonfand et al. 2017, 2019) and the Orion region (e.g., Friedel & Widicus Weaver 2012; Widicus Weaver & Friedel 2012; Feng et al. 2015). Outside the Galaxy, oxygen-bearing COMs (e.g., methanol, methyl formate, and dimethyl ether) have been detected from hot cores in the Large and Small Magellanic Clouds (Sewilo et al. 2019).

Hot core chemistry processes are far from being settled, and detailed observational data from a variety of sources is still needed. For example, the levels of deuterium fractionation of COMs in Sgr B2 are lower than that predicted by chemical modeling (Belloche et al. 2016), and there is still no definitive explanation for the different spatial distributions of the nitrogen-bearing COMs and oxygen-bearing COMs in the Orion region (Feng et al. 2015). The chemical diversity found around massive young stellar objects (MYSOs) suggests two distinctive types of sources: carbon-chain-poor/COMs-rich sources and carbon-chain-rich/COMs-poor sources (Taniguchi et al. 2017, 2018a, 2018b). In addition, a possible relation between interstellar COMs and prebiotic molecules have been suggested by the detection in Sgr B2 of isopropyl cyanide (Belloche et al. 2014). The detection of this branched alkyl molecule suggests a possible link with amino acids found in meteorites due to their key side chain structure.

The G345.5+1.47 MYSO (Mottram et al. 2007) is located in the center of the IRAS 16562–3959 high-mass star-forming region (Skrutskie et al. 2006). The distance and bolometric luminosity (Lbol) are 2.4 kpc and 154,400 L⊙ (Lumsden et al. 2013), respectively. In the IRAS 16562–3959 high-mass star-forming region, 18 continuum cores have been detected in Atacama Large Millimeter/submillimeter Array (ALMA) band 3 (Guzmán et al. 2014). They also detected various sulfur-bearing species such as SO, SO2, CS, and OCS, and velocity gradients in the first moment maps of the first two. A hot molecular outflow driven by an ionized jet has been detected at the G345.5+1.47 MYSO (Guzmán et al. 2011). Cesaroni et al. (2017) investigated whether a circumstellar rotating disk around the G345.5+1.47 MYSO exists by analyzing the CH3CN (12 − 11), 13CH3CN (13 − 12), and SiO (5 − 4) rotational transitions using ALMA. Although such disks are ubiquitous in low-mass YSOs, they could not identify it around this high-mass YSO. Guzmán et al. (2018) showed the spatial distributions of several molecules toward the IRAS 16562–3959 by using the ALMA band 3 observations. In this region, Guzmán et al. (2018) suggested the presence of different chemically evolutionary stages, and thus it is crucial to investigate its chemical properties in detail. However, an angular resolution of 1″7 was not enough to spatially resolve the central G345.5+1.47 MYSO (Guzmán et al. 2018). It is still unclear whether chemical properties of hot cores in the same region are similar to each other or not, and, if they are different, whether the difference relates to the local physical conditions or not.

In this paper, we present ALMA band 6 data toward the G345.5+1.47 MYSO with a higher spatial resolution of ∼0″3 (∼760 au). In Section 2, details about the archival data and reduction procedures are described. The continuum image, moment zero images of several molecular emission lines, and spectra toward three cores that we identify in this paper are presented in Sections 3.1–3.3, respectively. Analytical methods
and results of the spectra are described in Section 3.4. We compare the chemical composition between the two main cores detected in Section 4.1. We discuss relationships of spatial distributions between C$^{18}$O and H$_2$CO, and between $^{33}$SO and H$^{30}$α in Sections 4.2 and 4.3, respectively. In Section 5, we summarize the main conclusions of this paper.

### 2. Data and Reduction Procedure

We present archival data from cycle 2 data, band 6 (project ID: 2013.1.00489.S, PI: Riccardo Cesaroni). Observational details are given by Cesaroni et al. (2017). Table 1 summarizes the frequency band and resolution of each spectral window. The spectral window with the widest frequency coverage was used for a continuum observation. The field of view and largest angular scale of the 12 m array observations are $\sim 26''$ and $\sim 4''/''$, respectively. The coordinate of the center of the target source is $(\alpha_{2000}, \delta_{2000}) = (16^h59^m41^s61, -40^\circ03'43''3'')$. The angular resolutions are approximately $0''/32 \times 0''/25$, corresponding to 768 au $\times$ 600 au at the source distance of 2.4 kpc.

We conducted data reduction and imaging using the Common Astronomy Software Application (CASA v 4.3.1; McMullin et al. 2007) on the pipeline-calibrated visibilities. The data cubes were imaged with the TCLEAN task within CASA. Natural weighting was applied. Velocity resolutions for each spectral window and the noise levels attained are given in Table 1. Continuum images were obtained from the data cubes using the IMCONTSUB task. The rms noise level of the continuum image is 1.6 mJy beam$^{-1}$.

### 3. Results and Analyses

#### 3.1. Continuum Image and the H$_2$ Column Density of Identified Cores

Figure 1 shows the continuum image made from the widest spectral window (216.961–218.834 GHz, Table 1). The angular resolution is $0''/32 \times 0''/25$. The strongest continuum peak associates with the G345.5+1.47 MYSO, which is indicated as Core A in Figure 1. Another continuum peak corresponds to Core C, which we will identify later in this subsection. A small continuum peak, labeled as D in Figure 1, is detected at the north position from Core A, and a weak continuum emission has been detected at the Core B position.

We define the position of the hypercompact (HC) H II region and that of prominent molecular emission based on the H$^{30}$α and CH$_3$OH ($4_{2,3} - 3_{1,2}$ E) moment zero maps. These positions are shown in the continuum map (Figure 1) and in the moment zero maps of the H$^{30}$α and of the methanol transition shown in Figure 2. Core A corresponds to the HCH II region, and Cores B and C correspond to the strongest rich molecular cores identified in IRAS 16562–3959 by Cesaroni et al. (2017) and by Guzmán et al. (2018). Table 2 lists general properties of these cores based on 2D Gaussian fittings to the moment zero maps.

We derived the H$_2$ column density, $N_{\text{H}_2}$, at each core using the following formula (Kauffmann et al. 2008):

$$N_{\text{H}_2} = 2.02 \times 10^{20} (\text{e}^{1.439(\lambda/\text{mm})^{-1}(T/10\text{ K})^{-1}} - 1) \times \left(\frac{\nu}{0.01 \text{ cm}^2 \text{ g}^{-1}}\right)^{-1} \left(\frac{F_{\nu}^{\text{beam}}}{\text{mJy beam}^{-1}}\right) \left(\frac{\theta_{\text{HPBW}}}{10''}\right)^{-2} \left(\frac{\lambda}{\text{mm}}\right)^3,$$

(1)

where

$$\kappa_{\nu} = 0.1 \left(\frac{\nu}{1 \text{ THz}}\right)^{\beta}.$$

(2)

The symbols of $\lambda$, $T$, $\kappa_{\nu}$, $F_{\nu}^{\text{beam}}$, and $\theta_{\text{HPBW}}$ in Equation (1) are the wavelength, temperature, dust opacity, flux of dust continuum emission, and half power beamwidth, respectively. The continuum data wavelength is approximately 1.37 mm. The flux values at each core are summarized in Table 2. These fluxes are beam-averaged values with beam sizes of $0''/3$ for Core A and $0''/5$ for the others, respectively. We corrected the continuum emission toward Core A by subtracting the free–free continuum emission calculated from the H$^{30}$α spectra in Figure A1 as we describe in Appendix A. We subtracted this free–free component from the continuum flux and derived the dust continuum emission. H$^{30}$α emission toward Core B and Core C was not detected. The dust opacity at the 1.37 mm ($\kappa_{\nu}$) is calculated using Equation (2) (Planck Collaboration et al. 2011) with $\beta = 1.6$ (Sadavoy et al. 2013). The dust temperature ($T$) is assumed to be 100 K, because COMs have been detected toward all of the cores as shown in Section 3.2. If we change the temperature between 50 and 200 K, the derived $N_{\text{H}_2}$ values

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**Table 1**

| Frequency (GHz) | Frequency Resolution (kHz) | Velocity Resolution (km s$^{-1}$) | 1σ noise (mJy beam$^{-1}$) |
|-----------------|-----------------------------|---------------------------------|-----------------------------|
| 216.976–218.849| 1953.1                      | 3.0                             | 1.1                         |
| 219.533–219.767| 488.3                      | 0.8                             | 1.5                         |
| 220.533–220.767| 488.3                      | 0.8                             | 2.0                         |
| 231.803–232.037| 488.3                      | 0.8                             | 2.1                         |

**Note.**

$^a$ Obtained from Cesaroni et al. (2017).
change by a factor of $\sim 2$. The derived $N_{\text{H}_2}$ values are summarized in Table 2.

### 3.2. Moment Zero Images

We made moment zero images of each molecular line integrating the whole velocity range where emission is detected. Figure 3 shows the spatial distributions of (a) C$^{18}$O (2 – 1), (b) H$_2$CO (3$_{2,2}$ – 2$_{2,1}$), (c) DCN (3 – 2), and (d) $^{33}$SO (6$_5$ – 5$_4$). Their spatial distributions, except for $^{33}$SO, are relatively extended compared to those of COMs (Figures 4 and 5). The red crosses indicate positions of Cores A to C (Figure 2 and Table 2). Table 3 summarizes species, transition, rest frequency, excitation energy, and peak intensity of each moment zero image analyzed in this work.

The spatial distributions of C$^{18}$O and H$_2$CO show arc-like structures with strong peaks at Core B. There is also weaker emission associated with Core C. In Section 4.2, we discuss the formation mechanisms of H$_2$CO by comparing between the spatial distributions of C$^{18}$O and H$_2$CO.

The DCN spatial distribution (panel (c) of Figure 3) is different from the above two species. A strong peak is located at Core B and a filamentary structure can be seen at the northeastern region, corresponding to the northeast outflow cavity wall (NEC-wall) in Guzmán et al. (2018). Other emission regions are located nearby and to the west of Core C.

Panel (d) of Figure 3 shows a close-up moment zero image of $^{33}$SO (6$_5$ – 5$_4$) emission at G345.5+1.47. One $^{33}$SO peak is associated with Core B, and other peaks are located near Core A. The $^{33}$SO emission seems to surround Core A. We discuss the $^{33}$SO spatial distribution around Core A in detail in Section 4.3.

Figures 4 and 5 show moment zero maps of various molecular emission lines’ more compact morphology. The information of lines and peak intensities for each panel is listed in Table 3. Most of the molecular emissions are associated with both Cores B and C as shown in Figures 4 and 5.

Figure 4 shows the spatial distributions of COMs in panels (a)–(e) and H30$\alpha$ in panel (f). The CH$_3$OH (4$_{2,2}$ – 3$_{1,1}$) line in panel (a) shows more extended spatial distribution than the CH$_3$OH (20$_{1,19}$ – 19$-$20$_{0,20}$) line in panel (b). This is caused by their different upper energy levels; $E_u/k = 44.5$ K for panel (a) and 508.4 K for panel (b), respectively (Table 3).

The CH$_3$CN (12 – 11, $K = 3$) line comes from Cores A, B, and C, while the lines of oxygen-bearing COMs mainly come from Core B and Core C (Figure 4). The upper energy level of the CH$_3$CN line of panel (c) is 133.2 K, which is an intermediate value compared to those of panels (a) and (b). Therefore, the different spatial distributions between CH$_3$OH and CH$_3$CN are not brought by the different upper energy level of the lines. The different morphologies between CH$_3$OH (4$_{2,2}$ – 3$_{1,1}$) and the CH$_3$CN line seem to reflect different origins. As indicated in Figure 6, the CH$_3$OH (4$_{2,2}$ – 3$_{1,1}$) line has been detected at Core A, although there is no emission peak at Core A (panel (a) of Figure 4). Since low excitation energy lines of CH$_3$OH trace shock regions (e.g., Taniguchi et al. 2020), the CH$_3$OH line around Core A is possibly originated in a shock region. Shock regions are induced by several star formation phenomena, such as jets and molecular outflows. Guzmán et al. (2011) identified the SE–NW molecular outflow and the central knot of the jet/outflow system is consistent with the Core A position (Guzmán et al. 2010). Alternatively, the CH$_3$OH line may trace a remnant gas scattered by the HCHII region. The CH$_3$CN emission, on the
the moment zero image of the CH3OH line by the 2D Gaussian fitting. Core B and Core C are identified by the 2D Gaussian fitting of the moment zero image of the CH3OH (4.23 - 3.12 E) line.

**Notes.** Core A is identified based on the moment zero map of the H30 line by the 2D Gaussian fitting. Core B and Core C are identified by the 2D Gaussian fitting of the moment zero image of the CH3OH (4.23 - 3.12 E) line.

- **a** Obtained by the Gaussian fitting of the J = 12 - 11, K = 4 line of CH3CN.
- **b** Continuum fluxes with beam sizes of 0.03 for Core A and 0.05 for the others, respectively.
- **c** Errors were derived by changes in assumed temperatures between 50 and 200 K.

### 3.3. Spectra toward the Three Cores

Figures 6 and 7 show spectra of the 217.0–218.6 GHz and 219.56–219.76 GHz bands toward Cores A, B, and C, respectively. The bottom three panels are a zoom of the top three. We identified lines using the CASSIS software with the Cologne Database for Molecular Spectroscopy (CDMS; Müller et al. 2005) and the Jet Propulsion Laboratory (JPL) catalog (Pickett et al. 1998). Since the velocity resolution of the final spectra of Figure 6 is low (3 km s\(^{-1}\)), some lines could not be identified without ambiguity. At the position of Core C, the 13SO line is detected as a spururious-like line (Figure 6). Such a spurarious-like feature is considered to be brought by very low-velocity resolution (3 km s\(^{-1}\)). We confirm that it does not affect other regions. We then neglect the position of Core C in its moment zero image. We did not apply Gaussian fitting for detected lines due to the low-velocity resolution. Table 4 summarizes species, transition, rest frequency, and excitation energy of detected lines at each core position.

Core B is the most line-rich position, where various oxygen-bearing COMs, e.g., CH2OCH3 and CH3OCHO, have been detected. Furthermore, vibrational-excited lines of H2CO, whose upper energy levels are extremely high (E\(_u\)/k ∼ 775 K), have been detected.

As shown later, the excitation temperature of CH3CN is derived to be above 200 K at Core C. Furthermore, the abundances of COMs are high. For example, the CH3OH abundance is around 10\(^{-6}\) (Figure 9). This abundance can be reproduced only after the temperature reaches above 200 K (Taniuchi et al. 2019). These results suggest active hot core chemistry at Core C. Guzmán et al. (2018) also concluded that Core C is associated with a second hot molecular core within IRAS 16562–3959, linked to an MYSO less massive than
In summary, all of these results imply that a very young star is embedded at Core C.

3.4. Analyses

We analyzed spectra at the three cores using the CASSIS software (Caux et al. 2011). In the analyses presented here, we have used the local thermodynamic equilibrium (LTE) model available in the CASSIS spectrum analyzer by assuming lines are optically thin. The rotational diagram fittings of CH$_3$CN do not show any systematic shifts as shown in Figure 8. Thus, the assumption of the optically thin regime seems to be reasonable in our case.

Except for CH$_3$CN, only one or a few lines with similar excitation energies have been detected for each species. We then applied the Markov Chain Monte Carlo (MCMC) method, which is an interactive process that goes through all of the parameters with a random walk and heads into the solutions space, and $\chi^2$ minimization gives the final solution.

We derive the excitation temperatures and column densities of CH$_3$CN using its $K$–ladder lines of the $J = 12 – 11$ transition. Left panels of Figure 8 show spectra of the eight $K$–ladder lines of the $J = 12 – 11$ transition ($K = 0 – 7$) toward the three cores. The lines from right to left correspond to from $K = 0$ to $K = 7$. We fitted the spectra with a Gaussian profile. We cannot fit the $K = 7$ line toward Core A, and we omitted it from the fitting.

Right panels of Figure 8 show the rotational diagram using the Gaussian fitting results of the left panels. The derived column densities and excitation temperatures are summarized in Table 5. The column densities and excitation temperatures are $(1.0 \pm 0.1) \times 10^{16}$ cm$^{-2}$ and $279 \pm 57$ K; $(1.4 \pm 0.2) \times 10^{16}$ cm$^{-2}$ and $420 \pm 117$ K; and $(1.3 \pm 0.2) \times 10^{15}$ cm$^{-2}$ and

G345.5+1.47. In summary, all of these results imply that a very young star is embedded at Core C.
213 ± 25 K at Cores A, B, and C, respectively. Although we assumed that the CH$_3$CN lines are optically thin, we cannot rule out the optically thick case due to the scatter. The plots for the first three $K$-ladder lines ($K = 0 - 2$) are coincident with each other within their errors, but the plots for the $K = 0$ line may be slightly lower than the other two plots. If the lines are optically thick, the derived rotational temperature should be overestimated (Beltrán et al. 2011; Furuya et al. 2011).

We derived the column densities and excitation temperatures of other species using the MCMC method and the LTE model in the CASSIS software. We considered the following two cases:

1. assume excitation temperatures between 50 and 200 K, and

2. assume a range of temperatures around the excitation temperatures derived by the CH$_3$CN fitting.

We assume the excitation temperature range of the first case taking the typical temperature at the hot core of 100 K into consideration. For the second case, we tested the following temperature ranges: 220–340 K for Core A, 250–540 K for Core B, and 185–240 K for Core C, respectively.

We fixed source sizes, or size of the emitting region, to 0$''$.3 for Core A and 0$''$.5 for Core B and Core C, respectively (Table 2). Because the cores appear to be resolved, we assume a filling factor of unity. The line width (FWHM) was treated as a free parameter, constrained between 1 and 10 km s$^{-1}$. The line widths derived by the fitting are $\sim$2–4 km s$^{-1}$ for Core A and Core B, and $\sim$3–5 km s$^{-1}$ for Core C, respectively. Derived line widths agree well with those of typical hot cores.

Figure 4. Moment zero images. The contour levels are 20%, 40%, 60%, and 80% of their peak intensities. The full transitions and peak intensities of each panel are summarized in Table 3. The white ellipse at the left bottom indicates the angular resolution of approximately 0$''$32 × 0$''$25. Red crosses indicate positions of Cores A, B, and C. The color scales are adjusted from rms noise levels to the peak intensities for each panel.
Table 6 summarizes the derived column densities and excitation temperatures of the detected species except for CH$_3$CN toward each core. “Case 1” and “Case 2” represent the different assumed excitation temperature ranges, as described above. The excitation temperatures of H$_2$CO and CH$_3$OH are consistent within their standard deviation errors in all cases.

Figure 5. Moment zero images. The contour levels are 20%, 40%, 60%, and 80% of their peak intensities. The transitions and peak intensities of each panel are summarized in Table 3. The white ellipse at the left bottom indicates the angular resolution of approximately 0"32 × 0"25. Red crosses indicate positions of Cores A, B, and C. The color scales are adjusted from rms noise levels to the peak intensities for each panel.
Other oxygen-bearing COMs (CH$_3$OCHO, CH$_3$OCH$_3$, and (CH$_3)_2$CO) have similar excitation temperatures, except for (CH$_3)_2$CO assuming Case 1 toward Core C. Although there is a large uncertainty of the CH$_3$CN excitation temperature at Core B, the excitation temperatures of all the species are coincident with each other at each core in Case 2. We will discuss comparisons of the chemical compositions between Cores B and C in Section 4.1 with the results of Case 2.

### 4. Discussions

#### 4.1. Comparison of the Chemical Composition between Core B and Core C

We derived fractional abundances, $X$(molecules) = $N$(molecules)/$N_{H_2}$, of each species toward Cores B and C, and compare them as shown in Figure 9. We took the errors from both $N$(molecules) and $N_{H_2}$ into consideration.

The observed H$_2$CO and CH$_3$OH abundances at Cores B and C can be reproduced after their thermal desorption from dust grains (Figure B1 in Appendix B and Figure 6 of Taniguchi et al. 2019). The thermal desorption of H$_2$CO and CH$_3$OH occurs at $\sim$50 K and $\sim$100 K, respectively. Abundances of other COMs ($\sim$10$^{-8}$–$10^{-7}$) are reproduced in a hot core model with temperature above 100 K (Garrod 2013). These results suggest hot core chemistry is taking place at both Core B and Core C.

All of the species have larger fractional abundances at Core B compared to Core C. While the fractional abundances of CH$_3$OH and H$_2$CO at Core B are higher than those at Core C by a factor of $\approx$100, the differences in fractional abundances of other species are around one order of magnitude. Methanol (CH$_3$OH) is important for formation of oxygen-bearing COMs (Oberg et al. 2009). Hence, oxygen-bearing COMs except for H$_2$CO and CH$_3$OH are expected to be formed later than H$_2$CO and CH$_3$OH. These results suggest that Core B is more chemically rich or a more evolved hot core with enough time for molecules to sublimate from dust grains and newly form in the hot gas.
4.2. Formation Mechanisms of H$_2$CO

Most COMs are generally abundant in hot core regions with temperatures above 100 K where ice mantles sublime. As shown in Figures 3 and 4, the spatial distribution of H$_2$CO is different from distributions of other oxygen-bearing COMs; the distribution of H$_2$CO shows an arc-like structure with a strong peak at Core B, while other COMs are concentrated at Core B and Core C. Such different spatial distributions may suggest that the main formation mechanism of H$_2$CO is different from those of other COMs.

Figure 6. Spectra in the frequency range of 217.0–218.4 GHz toward the three cores. The bottom three panels are a zoom of the top three.
In this subsection, we discuss possible main formation mechanisms of H$_2$CO.

According to Taniguchi et al. (2019), the formation mechanisms of H$_2$CO are highly sensitive to the physical evolution of the cores. Based on this, we can clearly distinguish three major formation processes of H$_2$CO (Figure B1 in Appendix B):

1. formation in the gas-phase through the reaction CH$_3$ + O → H$_2$CO + H, active in cold starless core phase when $T \approx 10$ K and $n_H \approx 10^4$–$10^7$ cm$^{-3}$;

2. nonthermal desorption of H$_2$CO ice formed through the successive hydrogenation of CO ice (ice–H + ice–CO → ice–HCO, ice–HCO + ice–H → ice–H$_2$CO) active in the lukewarm stage when $10$ K < $T$ < $25$ K and $n_H \approx 10^7$ cm$^{-3}$;

3. thermal evaporation of H$_2$CO ice, active in hot core stage when $T > 50$ K and $n_H \approx 10^7$ cm$^{-3}$.

Figure 10 shows the spatial distributions of C$^{18}$O (color) and H$_2$CO (white contours). Their spatial distributions show a similar structure: an arc-like extended structure and a strong peak at Core B. The extended structure seems to suggest that heating sources are not necessary for formation of the gas-phase H$_2$CO. This means that either gas-phase formation or nonthermal desorption is important for H$_2$CO. The similar spatial distributions of C$^{18}$O and H$_2$CO support the grain-surface formation and nonthermal desorption. Still, this does
not mean that gas-phase formation is irrelevant for H$_2$CO. To distinguish the two reactions, we need further observations, e.g., O1 distribution.

The H$_2$CO abundance with respect to H$_2$ at Core B is derived to be around $10^{-5}$ (Figure 9). This abundance can be reproduced only after thermal evaporation of H$_2$CO (Figure B1) with temperatures above 50 K. Since many COMs have been detected at Core B, the dust temperature is expected to be above 100 K. Thus, the thermal evaporation seems to work efficiently at this position.

4.3. Spatial Distribution of $^{33}$SO Emission around Core A

Guzmán et al. (2014) showed the spatial distributions of sulfur-bearing species, SO, SO$_2$, CS, and OCS, with an angular resolution of $2''\times1''$. They found that the emission lines of these species come from a molecular core with a size of around 3000 au at the G345.5+1.47 MYSO. Guzmán et al. (2014) suggested that the observed SO emission and morphology at Core B can be understood qualitatively using the predictions of hot gaseous phase chemical models (e.g., van der Tak et al. 2003). Panel (d) of Figure 3 shows a ring-like
distribution of $^{33}$SO around Core A. Such a structure has been found for the first time in this source owing to the high spatial resolution. In this subsection, we discuss this $^{33}$SO structure.

Figure 11 shows the spatial distributions of $^{33}$SO (color) and H$_3^0\alpha$ (magenta contours) emissions. The strong emission peaks of $^{33}$SO are located at the outer edge of H$_3^0\alpha$ emission. There are two possible scenarios for such a ring-like structure around the HCH II region; one is molecular destruction by the UV radiation from the central star, and the other is the gas-phase formation of SO at this position. If such a ring-like structure has been formed by molecular destruction by the UV radiation from the central star, other molecules are expected to show similar structures. However, we do not find ring-like structures in moment zero images of other molecules (Figures 4 and 5). This implies that the destruction did not produce the ring-like structure of $^{33}$SO emission by the UV radiation from the central star.

Sulfur monoxide (SO) is considered to be a shock tracer. At Core A, shocks can be produced by a molecular outflow and an expanding motion of the HCH II region. However, the morphology of the $^{33}$SO emission does not match the orientation of the molecular outflow nor the jet reported by Guzmán et al. (2011). Hence, the molecular outflow does not seem to be an origin of the $^{33}$SO emission feature. In summary, $^{33}$SO is expected to be enhanced in shock regions produced by an interaction between a thick cloud and an expanding motion of the HCH II region. In shock regions, SO is considered to be formed by the following reactions (Espplugues et al. 2014):

$$O_2 + S \rightarrow SO + O,$$  

(3)

| Position | $N$ (cm$^{-2}$) | $T_{ex}$ (K) |
|----------|----------------|--------------|
| Core A   | $(1.0 \pm 0.1) \times 10^{16}$ | $279 \pm 57$ |
| Core B   | $(1.4 \pm 0.2) \times 10^{16}$ | $420 \pm 117$ |
| Core C   | $(1.3 \pm 0.2) \times 10^{15}$ | $213 \pm 25$ |

Note. Errors represent the standard deviation.
Table 6
Derived Column Densities and Excitation Temperature

| Species         | Core A                  | Core B              | Core C              |
|-----------------|-------------------------|---------------------|---------------------|
|                 | $N$ (cm$^{-2}$)          | $T_{ex}$ (K)        | $N$ (cm$^{-2}$)      | $T_{ex}$ (K)        | $N$ (cm$^{-2}$)      | $T_{ex}$ (K)        |
| CH$_3$OH        | $(4.3 \pm 2.3) \times 10^{19}$ | 98 ± 14         | $(3.8 \pm 0.6) \times 10^{19}$ | 169 ± 20        | $(4.4 \pm 4.8) \times 10^{18}$ | 58 ± 4        |
| HC$_3$N         | $(1.6 \pm 0.7) \times 10^{17}$ | 135 ± 50         | $(1.1 \pm 0.4) \times 10^{18}$ | 99 ± 28         | $(1.4 \pm 0.8) \times 10^{18}$ | 60 ± 9         |
| HC$_3^{13}$CN   | $(3.1 \pm 0.7) \times 10^{14}$ | 130 ± 37         | $(6.9 \pm 1.4) \times 10^{14}$ | 103 ± 30        | $(6.1 \pm 1.9) \times 10^{13}$ | 76 ± 19        |
| HCC$^{13}$CN    | $(2.4 \pm 0.6) \times 10^{14}$ | 130 ± 38         | $(4.8 \pm 0.9) \times 10^{14}$ | 111 ± 23        | $(1.3 \pm 0.3) \times 10^{14}$ | 92 ± 32        |
| H$_2$CO         | $(1.4 \pm 0.7) \times 10^{7}$ | 96 ± 37          | $(8.0 \pm 6.3) \times 10^{9}$ | 140 ± 16        | $(6.2 \pm 3.4) \times 10^{6}$ | 59 ± 6         |
| CH$_3$OCHO      | ...                     | ...               | $(8.3 \pm 1.0) \times 10^{16}$ | 60 ± 6         | $(3.2 \pm 0.7) \times 10^{16}$ | 79 ± 18        |
| CH$_3$OCH$_3$   | ...                     | ...               | $(4.0 \pm 0.5) \times 10^{17}$ | 64 ± 5         | $(2.1 \pm 0.9) \times 10^{17}$ | 62 ± 11        |
| (CH$_3$)$_2$CO  | ...                     | ...               | $(8.3 \pm 1.0) \times 10^{15}$ | 66 ± 8         | $(7.2 \pm 2.1) \times 10^{15}$ | 122 ± 24       |
| HNCO            | ...                     | ...               | $(7.0 \pm 3.6) \times 10^{16}$ | 82 ± 14        | $(6.5 \pm 1.1) \times 10^{15}$ | 134 ± 17       |

Notes.

a Assume that excitation temperatures are between 50 and 200 K.

b Use the excitation temperatures derived by the CH$_3$CN fitting.

Figure 9. Comparison of chemical compositions between Cores B and C. The black, blue, and green lines indicate $X$(Core B)=$X$(Core C), $X$(Core B) = 10 $X$(Core C), and $X$(Core B) = 100 $X$(Core C), respectively.

and

$$\text{OH} + \text{S} \rightarrow \text{SO} + \text{H.} \tag{4}$$

Esplugues et al. (2014) suggested that reaction (3) is efficient just after the shock passes and the temperature is still high ($T \geq 1000$ K), while reaction (4) becomes more efficient in cool gas regions. According to the Kinetic Database for Astrochemistry (KIDA: http://kida.astrophy.u-bordeaux.fr/), the $\alpha$ values for the reaction rate coefficients, defined as $k = \alpha(T/300)^{2/3} \exp(-\gamma/T)$ cm$^3$ s$^{-1}$, are $2.1 \times 10^{-12}$ and $6.6 \times 10^{-11}$ for reactions (3) and (4), respectively. The $\gamma$ values for both of the reactions are reported as zero (Vidal et al. 2017).

Therefore, the reaction (4) is expected to proceed faster than the reaction (3), and could be a main formation pathway of SO around the observed HCH II region.

5. Conclusion

We have analyzed the ALMA cycle 2 data toward the IRAS 16562-3959 high-mass star-forming region. We spatially resolve the central bright sources into a binary system, a HCH II region and a younger molecule-rich core. We identified molecular emission cores using the moment zero images of the H30α line and a CH$_3$OH line, which we name Cores A, B, and C. We have detected several oxygen-bearing COMs, CH$_3$CN, and HC$_3$N and derived their column densities and excitation temperatures at three cores. While oxygen-bearing COMs have been detected toward Cores B and C, CH$_3$CN, HC$_3$N, and HNCO are located in all of the cores.

We compare the chemical composition between Core B and Core C. The fractional abundances at Core B are higher than those at Core C by around one order of magnitude, while the fractional abundances of CH$_3$OH and H$_2$CO at Core B are higher by a factor of $\approx 100$. These results seem to imply that Core B is a more evolved hot core, where enough time has elapsed for molecules to sublimate from dust grains and new molecules to form in the hot gas.

We investigate the main formation mechanism of H$_2$CO toward this high-mass star-forming region by a comparison of the spatial distributions between H$_2$CO and C$^{18}$O. Their extended arc-like structure suggests that gas-phase reaction...
and/or a grain-surface reaction followed by nonthermal evaporation are likely formation routes of the gas-phase H$_2$CO. The enhancement of the gas-phase H$_2$CO at Core B also indicates efficient thermal evaporation of H$_2$CO.

The spatial distribution of $^{33}$SO around Core A shows a unique structure distributing at the outer edge of the H$_3^0$ $\alpha$ emission region. These results seem to indicate that $^{33}$SO is enhanced in a shock region produced by an expanding motion of the HCH II region.

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Facility: Atacama Large Millimeter/submillimeter Array (ALMA).

Software: Common Astronomy Software Applications package (CASA; McMullin et al. 2007), CASSIS (Caux et al. 2011).

Appendix A
H$_3^{30}$$\alpha$ Spectra toward Core A

Figure A1 shows a spectra of the H$_3^{30}$$\alpha$ line (231.9009 GHz) toward Core A. A Gaussian fitting to the line is shown with a red line in Figure A1. The peak intensity and FWHM were derived to be 46.7 ± 0.3 K (1$\sigma$) and 49.5 ± 0.3 km s$^{-1}$, respectively.

Under LTE conditions, the line optical depth of the recombination line is given by $\tau_L = \phi(\nu)$, where $\tau_L$ is defined in Equation (B5) in Guzmán et al. (2014) and $\phi(\nu)$ is the line profile. Dividing $\tau_L$ by the free–free opacity $\tau_{ff}$ (e.g., Wilson et al. 2013, Section 10.6) we obtain the line to continuum equivalent width. For the H$_3^{30}$$\alpha$ transition and assuming $T_e = 7000$ K, this width is 104.044 MHz or 134.504 km s$^{-1}$.

Therefore, assuming optically thin conditions and considering that the line is well fitted by a Gaussian (which means we
can ignore to a first approximation pressure and opacity broadening), the line peak to continuum ratio for a $49.5 \pm 0.3 \text{ km s}^{-1}$ width $\text{H}_3\alpha$ line is

$$\frac{134.504 \text{ km s}^{-1}}{\sqrt{\pi} / \log(16) 49.5 \text{ km s}^{-1}} = 2.55.$$  

Therefore, the expected free–free contribution to the continuum is $46.7 K / 2.55 = 18.3 K$.

### Appendix B

#### Model Results of H$_2$CO

We investigate main formation pathways of H$_2$CO using the results of Taniguchi et al. (2019) with the Nautilus (Ruaud et al. 2016). The details of this model were described in Taniguchi et al. (2019). The gas density ($n_H$) increases from $10^4$ to $10^7 \text{ cm}^{-3}$. In order to investigate the temperature dependence in detail, we use results of the three-phase (gas, dust surface, and bulk of ice mantle) and slow warm-up ($1 \times 10^6$ yr) model.

Figure B1 represents the time evolution of H$_2$CO from a starless core to the hot core phase through the warm-up phase. The upper panel of Figure B1 shows the time evolution of gas-phase H$_2$CO abundance together with the temperature profile. The lower panel shows the production rates of the main formation pathways of H$_2$CO together with the temperature profile.

During the low-temperature (10 K) starless core stage, the gas-phase reaction between CH$_3$ and an oxygen atom (O) is the main formation route of H$_2$CO. After the gas density reaches $10^7 \text{ cm}^{-3}$ and the temperature starts to increase, the following reaction contributes to the gas-phase H$_2$CO formation:

$$\text{ice-H} + \text{ice-HCO} \rightarrow \text{HCO} + \text{H}_2\text{CO}.$$  

This reaction efficiently works before the temperature reaches 25 K. After the temperature rises above $\sim 50$ K, the thermal evaporation of H$_2$CO, which is formed by successive hydrogenation reactions of CO molecules on dust surfaces, is the most efficient route.

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**Figure A1.** Spectra of H$3$\(\alpha\) toward Core A. Red line indicates the result of a Gaussian fitting.

**Figure B1.** Time dependences of the gas-phase H$_2$CO abundance (upper panel) and fractions of its main formation pathway (lower panel). Black lines indicate the time dependence of the temperature.
