Molecular-cloud-scale Chemical Composition. III. Constraints of Average Physical Properties through Chemical Models

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Abstract

It is important to understand the origin of molecular line intensities and chemical composition at the molecular-cloud scale in Galactic sources because it serves as a benchmark to compare with the chemical compositions of extragalactic sources. Recent observations of 3-mm spectra averaged over a 10 pc scale show similar spectral patterns among sources for molecular lines HCN, HCO+, CCH, HNC, HNCO, c-C3H2, CS, SO, N2H+, and CN. To constrain the average physical properties emitting such spectral patterns, we model molecular spectra using a time-dependent gas-grain chemical model followed by a radiative transfer calculation. We use a grid of physical parameters such as the density \( n = 3 \times 10^2 - 3 \times 10^4 \text{ cm}^{-3} \), temperature \( T = 10 - 30 \text{ K} \), visual extinction \( A_V = 2, 4, 10 \text{ mag} \), cosmic-ray ionization rate \( \zeta = 10^{-17} - 10^{-16} \text{ s}^{-1} \), and sulfur elemental abundance \( S/\text{H} = 8 \times 10^{-8} - 8 \times 10^{-7} \). A comparison with observations indicates that spectra are well reproduced with a relatively low density of \( n = (1-3) \times 10^3 \text{ cm}^{-3} \), \( T = 10 \text{ K} \), \( \zeta = 10^{-17} \text{ s}^{-1} \), and a short chemistry timescale of \( 10^5 \text{ yr} \). This short chemistry timescale may indicate that molecular clouds are constantly affected by turbulence, and exposed to low-density, low-A\(_V\) regions that “refresh” the chemical clock by UV radiation. The relatively low density obtained is orders of magnitude lower than the commonly quoted critical density in the optically thin case. This range of density is consistent with results from recent observational analysis of molecular-cloud-scale mapping.

Key words: astrochemistry – ISM: clouds – ISM: molecules

1. Introduction

The composition of multiple molecular species sensitively reflects the physical conditions and ages in molecular clouds. Their evolution along the stages of star formation has been studied in many prestellar and protostellar cores (e.g., Herbst & van Dishoeck 2009; Caselli & Ceccarelli 2012; Yamamoto 2017). In addition to the age of a molecular cloud, surrounding environments such as UV radiation, cosmic rays, X-rays, or shocks can change the chemical composition (see Harada 2018 and references therein). Most astrochemical studies on Galactic sources have so far focused on sub-pc regions in the star-forming regions, and we have limited knowledge on how the molecular emission of various molecular species is distributed in the 10 pc scale molecular cloud. Such large-scale observations can reveal various stages of chemical evolution, while the chemistry is more evolved in star-forming regions. Recent high-capability interferometers such as the Atacama Large Millimeter/submillimeter Array (ALMA) have accelerated the development of astrochemical studies in external galaxies. In those observations, a readily available angular resolution (~0′′5) corresponds to a linear scale of 10 pc at 4 Mpc distance, and hence it is important to understand the chemistry in Galactic molecular clouds with known physical environments at the 10 pc scale. To resolve this lack of a “benchmark,” there have recently been several studies observing Galactic molecular could complexes in the parsec to the 10 pc scale: W49 in the 1 mm band (Nagy et al. 2015), the Orion B Molecular Cloud (Pety et al. 2017; Shimajiri et al. 2017), Orion A (Kaufmann et al. 2017), W51 (Watanabe et al. 2017), W3(OH) (Nishimura et al. 2017), and Aquila and Ophiuchus (Shimajiri et al. 2017) in the 3 mm band.

Astrochemistry in some external galaxies can be significantly different from that in the Milky Way, and the chemistry can be used as probes of their activity. They may be going through violent stages of active galactic nuclei (AGNs) or starbursts. Even with single-dish telescopes with a ~1 kpc beam, variation in chemical composition has been found between different types of galaxies such as starburst galaxies versus AGN-host galaxies (Aladro et al. 2015; Nakajima et al. 2018), luminous infrared galaxies (Costagliola et al. 2011), and low-metallicity galaxies (Nishimura et al. 2016). With ALMA, multi-species observations have been conducted for AGN-containing galaxies (Takano et al. 2014; Viti et al. 2014; Martin et al. 2015; Nakajima et al. 2015), starburst galaxies (Meier et al. 2015), and a galaxy merger (Ueda et al. 2017; Qi&Harada et al. 2018) with a resolution at the 10 pc or 100 pc scale. A relatively quiescent spiral arm region in M51 was also studied by Watanabe et al. (2014). Spatial variation in chemical composition can also be studied within individual galaxies in regions of galactic centers, bars, and spiral arms. To
study those galaxies, a benchmark in a quiescent region at the 10 pc scale is important.

Results from large-scale Galactic astrochemical observations in spiral arm regions by Watanabe et al. (2017) and Nishimura et al. (2017) as well as observations in an extragalactic spiral-arm region of M51 (Watanabe et al. 2014) indicate that there is very little variation in spectral pattern among different star-forming clouds when averaged at the 10 pc scale, within a factor of a few for most of the detected species. These similar molecular intensity patterns indicate that the average physical properties in those molecular clouds are also similar. This similarity leads us to ask: what are the physical conditions contributing most to this spectral pattern? All those regions are located in spiral arms and are free of extreme starbursts, X-ray sources, or metallicity. With an understanding of such typical physical conditions of relatively quiescent regions at the molecular-cloud scale, we are able to highlight regions with extreme physical conditions such as higher star formation rate, influence of AGNs, or varied metallicities.

In this paper, we attempt to constrain such physical properties that lead to similar spectra among sources by comparing chemical modeling, the spectra of the Galactic molecular cloud W51 observed at the 10 pc scale, and the spectra of the extragalactic molecular cloud M51 at the 100 pc scale. We use a grid of parameters to obtain chemical abundances of molecular clouds using a gas-grain chemical model. From the chemical abundances, we also simulate emission intensities by solving radiative transfer, and the observed spectra are compared with the simulated spectra. Although grid-model calculations for a wide range of physical parameters have been explored in the extragalactic context (e.g., Bayet et al. 2009, 2011; Viti 2017), we here focus on a detailed analysis in the smaller physical parameter space that is relevant to molecular-cloud-scale observations of Galactic star-forming regions. This paper is organized as follows. Section 2 explains the chemical model and parameters that we use. Parameters for the radiative transfer code are also discussed in this section. In Section 3, we present chemical abundances and simulated spectra, and those results are discussed in Section 4. Finally, we summarize our results in Section 5.

2. Model

2.1. Chemical Models

We use a time-dependent, gas-grain model based on Nautilus (Hersant et al. 2009; Semenov et al. 2010). This is a two-phase model of the gas phase and the ice phase, without the distinction between the ice surface layers and the bulk of the ice. The reaction network contains 1574 species with 122,496 reactions. The gas-phase network that we use is based on KIDA\(^\text{11}\) with the implementation of deuterated species by U. Hincelin et al. (2014, private communication; see also Coutens et al. 2014; Furuya et al. 2015) although we do not discuss results for deuterated species. The grain-surface network refers to that in Garrod & Herbst (2006). The gas phase and grain-surface chemistry are connected via adsorption and desorption. In addition to thermal desorption, we include non-thermal desorption by UV photons (e.g., Öberg et al. 2007) and cosmic rays (Hasegawa & Herbst 1993). Reactive desorption is also included (Garrod et al. 2007) with the ratio of the surface-molecule bond-frequency to the frequency at which energy is lost to the grain surface being \(a = 10^{-4} - 0.01\), depending on reactions. We use the elemental abundances commonly used in chemical modeling of dark clouds (“low-metal abundances” in Wakelam & Herbst 2008) although we also use two enhanced values for sulfur (Table 1). We run our models with three different values of sulfur abundances because it is uncertain how much sulfur is depleted on grains at the 10 pc scale due to less sulfur depletion in photon-dominated regions (Goicoechea et al. 2006), and there is variation in the degree of depletion from diffuse to dense clouds (Fuente et al. 2018). The initial condition for each element is fully molecular for H, atomic for N, O, and He, and ionic for the rest of the elements. We employ a so-called “pseudo-time-dependent” approach, where physical conditions are kept constant while the time evolution of the chemistry is calculated using rate equations. A more realistic picture is where a molecular cloud evolves from a diffuse to a dense medium (e.g., Bergin et al. 2004; Furuya et al. 2015). Nonetheless, a pseudo-time-dependent approach has historically shown good agreement with observations of dark clouds. We run chemical models using a grid of physical parameters shown in Table 2. We use five values of molecular hydrogen density \(n_{\text{H}_2}\), three values of the gas temperature, three values of the visual extinction, and two values of the cosmic-ray ionization rate. We choose these density and temperature values referring to those derived from the non-local thermodynamic equilibrium analysis of the multi-line H2CO observations toward the spiral arm region of M51 with the 0.7–1 kpc beam (Y. Nishimura et al. 2018, in preparation). In our chemical model, we set the gas and dust temperatures to be equal. Although these H2CO observations of M51 show the best-fit densities around \(3 \times 10^{-3} - 3 \times 10^4 \text{ cm}^{-3}\), we expand our parameter space to \(3 \times 10^2 \text{ cm}^{-3}\) following the

| Element | X/H |
|---------|-----|
| He      | 0.14|
| N       | 2.14(−5) |
| O       | 1.76(−4) |
| C       | 7.3(−5) |
| S       | 8.0(−8), 2.5(−7), 8.0(−7) |
| Si      | 8.0(−9) |
| Fe      | 3.0(−9) |
| Na      | 2.0(−9) |
| Mg      | 7.0(−9) |
| P       | 2.0(−10) |
| Cl      | 1.0(−9) |

Note. \(a(−b)\) stands for \(a \times 10^b\).

| Parameter | Value |
|-----------|-------|
| \(n_{\text{H}_2}\) | Molecular hydrogen density |
| \(T_{\text{gas}}(=T_{\text{dust}})\) | Gas and dust temperature |
| \(A_v\) | Visual extinction |
| \(\zeta\) | Cosmic-ray ionization rate |

Note. The interstellar radiation field \(G_0 = 1\) was used for all the models.

\(^{11}\) http://kida.obs.uj-bordeaux.fr
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Table 3

| Species   | Transition | Frequency (GHz) |
|-----------|------------|-----------------|
| C₃H₂      | 2₁,₂ − 1₀,₁ | 85.33889        |
| CCH       | N = 1 − 0, J = 5/2 − 3/2 | 87.31690        |
| CCH       | N = 1 − 0, J = 3/2 − 3/2 | 87.40199        |
| HNCO      | 4₀,₄ − 3₀,₃ | 87.92524        |
| HCN       | 1 − 0      | 88.63160        |
| HCO⁺      | 1 − 0      | 89.18840        |
| HNC       | 1 − 0      | 90.66357        |
| N₂H⁺      | 1 − 0      | 93.17370        |
| CH₃OH     | 2₀ − 1₀, A⁺ | 96.74137        |
| CS        | 2 − 1      | 97.98095        |
| SO        | N_J = 2₁ − 1₂ | 99.29987        |
| HNCO      | 5₀,₅ − 4₀,₄ | 109.90576       |
| CN        | N = 1 − 0, J = 1/2 − 1/2 | 113.16867       |
| CN        | N = 1 − 0, J = 3/2 − 1/2 | 113.49492       |
| CO        | 1 − 0      | 115.27120       |
| CI        | 3P₁−₂P₀     | 492.16065       |

results of Kauffmann et al. (2017) and Pety et al. (2017). Since we consider three values for the elemental abundance of sulfur (S/H), we run a total of 270 models. Fractional abundances at times t = 10⁷ and 10⁶ yr are used for the radiative transfer calculation. In total 540 simulated spectra are produced.

2.2. Radiative Transfer

In order to calculate molecular intensities expected for each set of physical parameters, we run a publicly available non-local thermodynamic equilibrium radiative transfer code RADEX (van der Tak et al. 2007). Input parameters of RADEX are: N—the column density of the species for which emission intensity is calculated, Δν—the line width, T_gas—the gas temperature, T_bg—the background temperature, and n_H₂—the H₂ density. We assume a fixed value of N_H₂ = 10²² cm⁻² since the chemical model only calculates fractional abundances, i.e., abundance ratios of certain species over total hydrogen abundance. This column density is not necessarily consistent with the visual extinction because both observations and simulations suggest molecular clouds have filamentary and clumpy structures within (André et al. 2010; Inoue & Fukui 2013; Inutsuka et al. 2015). This total column density corresponds to 0.1–10 pc in the density range that we use. For the line width, we use the value of 10 km s⁻¹ for simplicity. This value is somewhat smaller than the line width commonly observed at 10 pc scale molecular clouds. Although we conduct our analysis with integrated intensities only, the line width may change the optical depth of the molecular lines. Therefore, we repeated our analysis assuming N_H₂ = 10²¹ cm⁻², and confirmed that the results do not change significantly for lower optical depths. We use the cosmic microwave background temperature as the background temperature T_bg = 2.73 K. Table 3 lists the transitions that we model for our analysis. For CO(J = 1 − 0) and CI(3P₁−₂P₀), the modeled intensities are only used to calculate CI/CO intensity ratios.

3. Results

3.1. Fractional Abundances

Here we discuss how fractional abundances vary with input physical parameters and the sulfur elemental abundances. All the fractional abundances that are shown here are in the gas phase.

3.1.1. Dependence on Density

The change in density mainly affects the chemical time; it becomes shorter with increasing density. Figure 1 shows fractional abundances in models with T = 10 K, ζ = 1 × 10⁻¹⁷ s⁻¹, A_V = 10 mag, S/H = 8 × 10⁻⁸, and densities of n_H₂ = 3 × 10⁹ cm⁻³, 1 × 10⁹ cm⁻³, 3 × 10⁸ cm⁻³, 1 × 10⁷ cm⁻³, and 3 × 10⁶ cm⁻³. Figure 1 shows that the peak abundance does not depend on the gas density, except for isocyanic acid (HNCO); this is produced by a series of surface reactions

\[ \text{CN(s) + O(s)} \rightarrow \text{OCN(s)} \]  \hspace{1cm} (1)

\[ \text{OCN(s) + H(s)} \rightarrow \text{HNCO,} \]  \hspace{1cm} (2)

where “(s)” indicates species in the form of ice, and which are destroyed by an ion-neutral reaction with He⁺. Since the ionization fraction is lower in higher-density environments, such reactions with He⁺ are slower for higher density in comparison with other reactions. At low visual extinction, A_V = 2 mag, photodissociation competes with molecular formation in lower-density conditions. At a lower density of n = 3 × 10⁶ cm⁻³, the effect of UV photons is more prominent for lower densities. At a lower density of n = 3 × 10⁷ cm⁻³, the UV photons dissociate these molecules. For SO, destruction via the reaction with C⁺ is also efficient, and the products of this reaction are S⁺ + CO, S + CO²⁺, and O + CS⁺ with the same branching ratios. At a lower density of n = 3 × 10⁶ cm⁻³, the effect of UV photons is stronger. Although fractional abundances of CN and CCH are enhanced at A_V = 2 mag at time t ~ 10⁵ yr when n_H₂ = 3 × 10⁹ cm⁻³, they are not enhanced when n = 3 × 10⁷ cm⁻³ (Figure 4). These effects of UV photons become less obvious in the case of higher density n_H₂ = 3 × 10⁴ cm⁻³, and the differences in fractional abundances between the cases of A_V = 2 mag and A_V = 4 mag become less compared with the case of n_H₂ = 3 × 10⁹ cm⁻³ (Figure 5). For all densities, there is little difference.

12 Rates of photodissociation or photoionization have the form d[A] / dt ∝ −G0[A]exp(−γA) where [X] is the number density per unit volume of species X and γ is a constant usually having values of 2–3. On the other hand, rates of two-body reactions A + B → C + D scale as d[C]/dt ∝ [A][B]. Since the two-body reactions have terms squared of densities while photodissociation or photoionization reactions have terms proportional to the density, photon-related reactions are more prominent at lower densities.
between cases of $A_V = 4\,\text{mag}$ and $A_V = 10\,\text{mag}$ because photodissociation or photoionization reactions are already ineffective at $A_V = 4\,\text{mag}$.

3.1.3. Dependence on Temperature

While gas-phase reactions in general do not show a strong temperature dependence between 10 and 30 K, such a
temperature change alters the thermal desorption rate from the ice phase into the gas phase. Two species with strong dependence on temperature are CH$_3$OH and HNCO. Figure 6 shows fractional abundances at $n_{\text{H}_2} = 1 \times 10^4$ cm$^{-3}$, $\zeta = 1 \times 10^{-17}$ s$^{-1}$, $A_V = 10$ mag, and $S/H = 8 \times 10^{-8}$. Fractional abundances of CH$_3$OH decrease with increasing temperature; the formation of CH$_3$OH on the grain surface is severely hindered by the fast evaporation of atomic hydrogen at high
temperatures, which leaves very little time for H to react with CO. This temperature dependence of CH$_3$OH was already discussed in Acharyya & Herbst (2015). On the other hand, fractional abundances of HNCO are highest at $T = 20$ K. At $T = 30$ K, the peak fractional abundance is by a factor of a few higher than that at $T = 10$ K and is reached at a later time. Although HNCO is also formed on grains, the fractional abundances of HNCO do not decrease at $T = 20$–$30$ K because OCN is made efficiently on...
grains from CN ice under such relatively warm conditions. At $T = 10$ K, the main destruction route of CN is through H atoms on grains to form HCN. However, at $T \gtrsim 20$ K, the destruction route via H is much slower, and the main destruction route of CN becomes that through O atoms to produce OCN. Although the H atoms on grains become less abundant by orders of magnitude at higher temperatures, the efficient formation of HNCO on grains is still effective.

Figure 4. Fractional abundances of analyzed species with varying $A_V$ at $n_{H_2} = 3 \times 10^2$ cm$^{-3}$, $T_{\text{gas}} = T_{\text{dust}} = 10$ K, $\zeta = 1 \times 10^{-17}$ s$^{-1}$, and $S/H = 8 \times 10^{-8}$. 

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3.1.4. Dependence on Cosmic-Ray Ionization Rate

Cosmic rays cause ionization reactions of atoms or molecules, and photodissociation of molecules by secondary UV photons.

Figure 7 shows fractional abundances in models with $n_{\text{H}_2} = 1 \times 10^4 \text{ cm}^{-3}$, $T = 10 \text{ K}$, $A_V = 10 \text{ mag}$, and $S/H = 8 \times 10^{-8}$ for $\zeta = 10^{-17}$ and $10^{-16} \text{ s}^{-1}$. An order of magnitude enhancement of
cosmic-ray ionization rate results in the variation of fractional abundances of most species less than a factor of a few. Species with a relatively strong dependence on the cosmic-ray ionization rate are N$_2$H$^+$, HCO$^+$, CS, SO, and HNCO. N$_2$H$^+$ and HCO$^+$ are produced via the reaction

$$\text{H}_3^+ + \text{N}_2 \rightarrow \text{H}_2 + \text{N}_2\text{H}^+, \quad (3)$$
and destroyed via recombination with an electron or the reaction
\[ \text{N}_2\text{H}^+ + \text{CO} \rightarrow \text{N}_2 + \text{HCO}^+. \]  

Since the \( \text{H}_3^+ \) fractional abundance increases with a higher cosmic-ray ionization rate, \( \text{N}_2\text{H}^+ \) also increases. The higher cosmic-ray ionization rate increases the fractional abundance of these species.
of SO; it is made via a reaction with OH, while OH is formed via ion–molecule reactions and subsequent dissociative recombination. Thus, SO increases with the higher ionization rate. Since HNCO is destroyed by He$^+$ or H$^+$, increased ionization fraction decreases the HNCO fractional abundance.

Figure 8. Fractional abundances of analyzed species with varying S/H at $n_{\text{H}_2} = 3 \times 10^3$ cm$^{-3}$, $T_{\text{gas}} = T_{\text{dust}} = 30$ K, $A_V = 2$ mag, and $\zeta = 1 \times 10^{-16}$ s$^{-1}$.
3.1.5. Dependence on Elemental Sulfur Abundance

The abundance of S-bearing species varies almost proportionally to the elemental abundance of sulfur. Varying S/H also affects the ionic molecules because $S^+$ can take up the charge from other ions. Our results show that this influence on ionized species is minor in most cases, causing a decrease of molecular ions such as $HCO^+$ and $N_2H^+$. Figure 8 shows fractional abundances in a model where the effect of S/H on $HCO^+$ and $N_2H^+$ is largest ($n_{H_2} = 3 \times 10^4 \text{ cm}^{-3}$, $T_{\text{gas}} = T_{\text{dust}} = 30 \text{ K}$, $A_V = 2 \text{ mag}$, and $\zeta = 1 \times 10^{-17} \text{ s}^{-1}$).

3.2. Simulated Spectra

Next, we present some of the simulated spectra from the radiative transfer calculation. While larger fractional abundances (equivalently column densities) increase the emission intensities in general, these intensities also depend on the optical depths and the excitation conditions. Molecules such as CH$_3$OH, CCH, c-C$_3$H$_2$, and HNCO stay optically thin in all of our calculations. On the other hand, the optical depths of $^{12}$CO, CN, HCN, HNC, HCO$^+$, $N_2H^+$, CS, and SO vary from an optically thin regime to $\tau \gtrsim 10$ depending on the models. Notes on the optical depth and the effect of physical conditions on the excitation conditions are included in the Appendix.

In order to measure how well each model fits the observation, we calculate the correlation function of modeled spectra with the observed spectra of the spiral-arm region in an external galaxy, M51 (Watanabe et al. 2014), and a star-forming cloud in our W51 (Watanabe et al. 2017). The correlation coefficient is calculated as

$$ r = \frac{\sum_i (I_i^{\text{cal}} - \bar{I}^{\text{cal}})(I_i^{\text{obs}} - \bar{I}^{\text{obs}})}{\sqrt{\sum_i (I_i^{\text{cal}} - \bar{I}^{\text{cal}})^2 \sum_i (I_i^{\text{obs}} - \bar{I}^{\text{obs}})^2}} $$(5)
where $I_{\text{mod}}^{i}$ is the modeled intensity and $I_{\text{obs}}^{i}$ is the observed intensity for species $i$. We use the correlation coefficient because we aim to analyze the spectral pattern, not the absolute quantities of the intensities. For W51, we omit CN ($N = 1 - 0$, $J = 1/2 - 1/2$) from our analysis because the observed intensity seems to have a significant error. Figure 9 shows two examples of simulated spectra, one with a moderate fit with the observed spectra, and the other with a large discrepancy. The observed spectra in W51 and M51 used for the comparison in our analysis are shown in Figure 10.

A quantitative comparison between models and observations for each species is made in Figures 11 (comparison with W51) and 12 (comparison with M51). Here we choose the fiducial model from one of the highest $r$ with the parameters $n = 3 \times 10^{3} \text{ cm}^{-3}$, $T = 20 \text{ K}$, $\zeta = 1 \times 10^{-17} \text{ s}^{-1}$, $A_V = 2 \text{ mag}$, $S/H = 8 \times 10^{-8}$, and $t = 10^{2} \text{ yr}$. For other panels, only the physical parameters that are different from those of the fiducial model are shown. A correlation coefficient for each model is shown at the right bottom of each panel.

From the Einstein A coefficients, CN ($N = 1 - 0$, $J = 1/2 - 1/2$) is expected to have a weaker velocity-integrated intensity than CN ($N = 1 - 0$, $J = 3/2 - 1/2$). However, the observed value of the CN ($N = 1 - 0$, $J = 1/2 - 1/2$) integrated intensity is higher than that of CN ($N = 1 - 0$, $J = 3/2 - 1/2$) in W51. We investigated the reason for this trend, and concluded that the baseline subtraction of CN ($N = 1 - 0$, $J = 1/2 - 1/2$) may not have been correct because the original data suffered from a distorted baseline.

Figure 11. Observed intensities (abscissa) of W51, and modeled intensities (ordinate) with parameters shown above each panel. The fiducial model shown in panel (a) has physical parameters of $n = 3 \times 10^{3} \text{ cm}^{-3}$, $T = 20 \text{ K}$, $\zeta = 1 \times 10^{-17} \text{ s}^{-1}$, $A_V = 2 \text{ mag}$, $S/H = 8 \times 10^{-8}$, and $t = 10^{2} \text{ yr}$. For other panels, only the physical parameters that are different from those of the fiducial model are shown.
it is in the high-density cases. If we take the intensities at a later time ($t = 10^6$ yr) than the fiducial case, then the intensities of HCO$^+$ and N$_2$H$^+$ become higher. Changes in both intensities can be accounted for from higher abundances (panels (e)). For the high-density cases, the emission intensities of HCO$^+$ become overproduced in the model. When the density is lower, the CCH and CN intensities increase (panels (f)). On the other hand, higher densities enhance the intensities of HCO$^+$, N$_2$H$^+$, and SO (panels (g)). Higher temperatures do not affect most species, except for CH$_3$OH and HNCO (panels (h)). The intensity of CH$_3$OH is underproduced in all cases. This underproduction of gas-phase CH$_3$OH may result from the turbulence or shock that causes the increase of methanol abundance in observations of molecular clouds. If the intensity of CH$_3$OH is enhanced through a mechanism that we did not include, our results would not be reasonable if this deviation of CH$_3$OH from the observations affected the correlation coefficients significantly. Therefore, we also calculated correlation coefficients without CH$_3$OH, and confirmed that the correlation coefficients with and without CH$_3$OH only change by at most 0.05, and on average by 0.01–0.02. Furthermore, the change caused by excluding CH$_3$OH affects most models in a similar way, and the discussion of constraints in the physical conditions in the following sections is essentially unchanged whether we calculate the correlation coefficients with or without CH$_3$OH. Our analysis includes methanol in the derivation of the correlation coefficients.

4. Discussion

4.1. Constraints on Physical Conditions

4.1.1. Constraints from W51

Figure 13 shows correlation coefficients for sets of the physical parameters for W51. There are four regions in the parameter space that have relatively high correlation...
coefficients ($r \gtrsim 0.7$), and those regions are indicated as gray rectangles. The first region is $n = 3 \times 10^3$ cm$^{-3}$, $A_V = 2$ mag with $S/H = (0.8-2.5) \times 10^{-7}$, $t = 10^5$ yr and $\zeta = 10^{-17}$ s$^{-1}$ (parameter space region R1). The second region is $n = 1 \times 10^3$ cm$^{-3}$, $A_V = 2$ mag, $\zeta = 10^{-17}$ s$^{-1}$ and $t = 10^6$ yr (R2).

The third region indicated as R3 has parameters of $n = 3 \times 10^3$ cm$^{-3}$, $A_V = 2$ mag with $S/H = (2.5-8) \times 10^{-7}$, and the last region, R4, has physical parameters of $n = 3 \times 10^3$ cm$^{-3}$, $A_V = 2$ mag with $S/H = 8 \times 10^{-7}$, $t = 10^5$ yr and $\zeta = 10^{-16}$ s$^{-1}$. We choose those

Figure 13. Correlation coefficients between modeled emission intensities and observed intensities of W51. Sets of parameters with moderate agreement are shown as gray rectangles.
regions because they have high correlation coefficients for a relatively large volume in the parameter space. Although some sets of physical parameters show high correlation coefficients, we do not consider them to be likely conditions if the correlation coefficients are low in almost all of their neighboring locations in the parameter space.

### 4.1.2. Constraints from M51

For the case of M51, regions similar to R1, R2, and R3 in W51 also have relatively good agreement, and they are marked as R′1, R′2, and R′3. However, compared with R1 and R3, R′1 and R′3 tend to have higher densities. For example, R′1 in Figure 14 has a higher density range of $n = (3–10) \times 10^3$ cm$^{-3}$ compared with...
R1 ($n = (1–3) \times 10^3 \text{ cm}^{-3}$). The temperature range is also slightly narrower in R1 than in R1 ($T = 10–30 \text{ K}$ in R1 while $T = 10–20 \text{ K}$ in R1). Likewise, R3 has agreement with $n = (1–3) \times 10^3 \text{ cm}^{-3}$ instead $n = 3 \times 10^2 \text{ cm}^{-3}$ in R3. Another difference between R3 and R3' is the range of sulfur elemental abundance, which is lower in R3' ($S/H = (0.8–2.5) \times 10^{-7}$).

In addition to regions R1’–3, which are similar to R1–3, there is a parameter space region R4’ where the agreement is relatively high for the case of M51 (Figure 14). Physical parameters of R4’ are $n = 3 \times 10^4 \text{ cm}^{-3}$, $A_V = 4–10$, and $t = 10^6 \text{ yr}$. However, we argue that they are unlikely to represent the real physical conditions. Despite some differences, spectra from M51 and W51...
Figure 16. Correlation coefficients between modeled emission in the two-component model and observed intensities in W51. For the two-component model, the emission intensity of each model is added to the fiducial model with varying fractions from 0% to 100%, and the maximum correlation coefficient among various fractions is shown for each model.
are similar, and the correlation coefficient between the spectra of M51 and W51 shows a relatively high value of 0.83. Therefore, the true physical parameters in those observations should be close to each other. This means that physical parameters that show high correlation coefficients for both sources are more likely solutions. If this is the case, R'4 can be excluded from the likely physical parameters.

![Figure 17. Same as Figure 16, but for M51.](image-url)
parameters. There is another reason to exclude R′4 from the plausible parameter space; the high correlation with the observations in R′4 is likely caused by the non-physical behavior of the chemical model. As discussed in Garrod et al. (2007), at late times, CO and CH3OH can be converted to CH4 due to cosmic-ray-induced photodissociation of CH3OH into CH3. Methane can be efficiently formed from CH3 on the grain surface. With time, methane can be converted into other hydrocarbons. However, such behavior at late times is not well understood, and has not been observed in the astrophysical environment. In our modeled results, CH4 is indeed overproduced at 10 K within the physical conditions of R′4, and becomes more abundant than CO ice. Observationally, CH4 is seen to be less abundant than CO ice (Öberg et al. 2011). On the other hand, for the case of 30 K, CH4 is not the most abundant form of ice; CH4 is volatile, and the majority is in the gas-phase. Instead of CH4, CO2 and C2H6 take over as abundant forms of ice. Abundant C2H6 still leads to a similar effect as abundant CH4.

4.1.3. Constraints from Absolute Intensities

In above discussion, we compare the spectral pattern of models and observations, but not the brightness temperature itself. This is because high-density clouds are likely to have low volume-filling factors in molecular-cloud-averaged spectra. Since the gas with higher density gives a higher intensity for a given column density, it is possible for models to be consistent with observations even if the modeled intensities are higher than observed values. However, we can exclude some models if they underproduce intensities even when the maximum possible total column densities are used for radiative transfer calculations. For this reason, we argue that molecular emission from \( n = 3 \times 10^2 \) cm\(^{-3} \) is not the dominant contributor to our observed spectra. Since our observation of W51 covers a 50 pc region, the maximum possible total column density from gas with \( n = 3 \times 10^2 \) cm\(^{-3} \) is \( N_{\text{HI2}} \sim 5 \times 10^{22} \) cm\(^{-3} \). When we run models with this total column density, the emission predicted from most models fails to produce high enough intensities equivalent to the observed values for the case of \( n = 3 \times 10^2 \) cm\(^{-3} \). A few lines in limited models do produce as much intensities as the observed ones, but those models do not show low correlation coefficients when we compare their spectral pattern with the observed one.

4.1.4. Constraints from CI/CO Intensity Ratios

From constraints obtained from W51, M51, and the absolute intensity argument above, we have sets of physical parameters with moderate agreement with observations. In order to impose another constraint, we also simulated the intensities of CO(J = 1 – 0) and CI(J\(^{3}P_{1} – 3P_{0})\). The simulated CI/CO intensity ratios are shown in Figure 15. Although CI/CO ratios toward our target areas of W51 and M51 are not reported, CI/CO ratios in molecular clouds are generally known to be 0.05–0.1 (Ikeda et al. 2002; Kamegai et al. 2003). This CI/CO ratio is observationally found to be relatively constant in various regions of molecular clouds. Thus, we compare this ratio with our model. Parameters that have moderate agreement with observations from constraints obtained above are also shown as gray rectangles with solid or dotted lines. If we add another constraint of a factor of 4 within this range \( 0.0125 < \text{CI/CO} < 0.4 \), most cases at \( t = 10^5 \) yr are excluded.

From all the constraints from Sections 4.1.1–4.1.4, we conclude that sets of physical parameters that likely represent conditions in observations are regions shown as solid gray rectangles in Figure 15. Those sets of parameters are \( n = 3 \times 10^3 \) cm\(^{-3} \), \( A_{\nu} = 2 \) mag, \( \zeta = 10^{-17} \) s\(^{-1} \), \( S/H = (0.8–2.5) \times 10^{-8} \), and \( t = 10^5 \) yr, or \( n = (1–3) \times 10^3 \) cm\(^{-3} \), \( A_{\nu} = 4–10 \) mag, \( \zeta = 10^{-17} \) s\(^{-1} \), \( S/H = (0.8–2.5) \times 10^{-8} \), and \( t = 10^5 \) yr.

4.2. Density Constraints

The range of densities constrained by our model is \( n = (1–3) \times 10^3 \) cm\(^{-3} \), which is much lower than the critical densities of most of the species in the optically thin case (see Table 3 of Nishimura et al. 2017 for values of critical densities). This range of densities is still reasonable in the optically thick case. The critical density considering the optical depth by Tielens (2005) is lower by a factor of 50 at \( \tau = 10 \) compared with the optically thin case due to radiation trapping. The optical depth in our models varies as discussed in the Appendix, and there are cases where it is as high as 10 or more. Shirley (2015) calculated
the effective critical density in the optically thick case. If the
column densities of the species are \( N = 10^{14} \, \text{cm}^{-2} \), similar values
to those in our models, HCO\(^+\) and HCN have effective critical
densities of \( 10^3 \) and \( 8 \times 10^2 \, \text{cm}^{-3} \), respectively.

Kauffmann et al. (2017) derived the mean density of gas in
their Orion A observations. In this analysis, they assumed a
power-law density distribution of the filament, and made a fit to
the dust column density. As a result, they concluded that mean
density of line-emitting gas is \( 870 \, \text{cm}^{-3} \) for most molecules
\(^{12}\text{CO}, \, ^{13}\text{CO}, \, \text{C}\(^{18}\text{O}, \, \text{CN}, \, \text{CCH}, \, \text{and HCN}\),
while \( \text{N}_2\text{H}^+ \) is emitting from gas with the density \( n \sim 4000 \, \text{cm}^{-3} \).
Although we used the averaged spectra in the larger observed area for
our analysis, our results show a similar range of density to
that suggested by Kauffmann et al. (2017). Pety et al. (2017)
also derived similar values of densities in their Orion B
observations; in their regions sub-divided by \( A_V \), lines of most
species are emitted from regions with mean densities of \( n = 890 \, \text{cm}^{-3} \) and \( n = 2700 \, \text{cm}^{-3} \) except for \( \text{CH}_3\text{OH}, \, \text{H}^{13}\text{CO}^+, \, \text{and N}_2\text{H}^+ \), whose emission also comes from higher-density
regions of \( n = 7500 \, \text{cm}^{-3} \). Both Kauffmann et al. (2017) and
Pety et al. (2017) observed a smaller area than Watanabe et al.
(2017) did for W51, yet, their derived densities are equivalent
to our best-fit densities. Our results provide further evidence
that low-density gas can generate high enough luminosity for
species that are conventionally thought as “dense-gas tracers.”

4.3. Remarks on Visual Extinction

In our model analysis (Section 4.1), there are two different
ranges of \( A_V \): \( A_V = 2 \, \text{mag} \) in R1 and \( A = 4–10 \, \text{mag} \) in R2. In
our observed area, there are variations of density, temperature,
and visual extinction. For the case of density, components with relatively low density are the main contributors to the average molecular emission as discussed above. However, a relatively good fit over various values of $A_V$ suggests that the contribution from various values of $A_V$ may be comparable. Therefore, multi-component models with different values of $A_V$ may give a better fit to observations.

Having good agreement over a wide range of visual extinction also seems to be reasonable when we consider other observational data. Pety et al. (2017) reported that 3, 51, 40, and 8% of the CO-traced gas mass is distributed in regions with $1 < A_V$ (mag) < 2, 2 < $A_V$ (mag) < 6, 6 < $A_V$ (mag) < 15, and $15 < A_V$ (mag) < 222, respectively, while the ratios are 8%, 38%, 36%, and 20% when the mass is traced by dust. The interstellar radiation field $G_0$ in their observations has a wide range of values of 4–28,000, with the mean values of individual regions ranging from 30 to 72. Note that we used $G_0 = 1$ in our model, and $A_V = 2$ mag in our model corresponds to the chemistry with $A_V = 3.1–4.1$ mag for the above-mentioned mean radiation field of $G_0 = 30–72$ (assuming $\gamma = 2–3$; see footnote 2 in Section 3.1). Similarly, the chemistry in $A_V = 4$ mag in $G_0 = 1$ corresponds to $A_V = 5.1–6.1$ mag when $G_0 = 30–72$. Kauffmann et al. (2017) reported $A_V$ of 6.1 mag for most species and $A_V$ of 16 mag for N$_2$H$^+$ although they did not list the range of $G_0$.

Figure 20. Same as Figure 19, but for other species.
analyzed the effect of electron excitation, and concluded that strongly irradiated regions. Goldsmith & Kauffmann (2004) used in the model of 1 timescale is much shorter than the lifetime of molecular clouds (10^6–10^7 yr; e.g., Hartmann et al. 2001; Tassis & Mouschovias 2004). The freefall time of clouds at the densities n = (1–3) × 10^3 cm^{-3} is (0.6–1) × 10^9 yr, which is still longer than our chemistry time. On the other hand, the turbulent crossing time \( t_{\text{cross}} \approx \frac{R}{v_{\text{turb}}} \), where R is the length and \( v_{\text{turb}} \) is the turbulent velocity. The total column density that we used in the model \( (N = 10^{22} \text{ cm}^{-2}) \) corresponds to a source size of 1–3 pc for \( n = (1–3) \times 10^3 \text{ cm}^{-3} \), but the actual geometry of the source is likely to be filamentary with a width of \( R \approx 0.1 \text{ pc} \). For \( R = 1 \text{ pc} \), \( v_{\text{turb}} = 1.1 \text{ km s}^{-1} \) assuming the object follows Larson’s law (Larson 1981), which gives \( t_{\text{cross}} = 10^3 \text{ yr} \). If \( R = 0.1 \text{ pc} \), Larson’s law gives \( v_{\text{turb}} = 0.45 \text{ km s}^{-1} \), which means the crossing is 2.2 × 10^4 yr. This is equivalent to, in order of magnitude, our derived chemistry time. If such turbulence occurs, the molecular medium may be constantly exposed to a low-density environment with a high flux of UV photons to dissociate molecules. If \( G_0 = 30 \), \( A_V \ll 1 \) and the rate coefficient is a typical value of \( k = 10^{-10} \text{ cm}^3 \text{ mol}^{-1} \text{s}^{-1} \), photodissociation can easily occur in a very short timescale of 10 yr. This photodissociation can bring the chemistry close to the initial condition of the atomic/ionic state, and set the chemistry clock back to zero. It should be noted that our models were run with the pseudo-time-dependent approach, and the actual age of the molecular cloud may by longer than our derived chemistry timescale.

4.4. Implication of Timescale

The simulated spectra and the CI/CO ratio suggest that a chemistry time of 10^3 yr is preferred in our model. This timescale is much shorter than the lifetime of molecular clouds (10^6–10^7 yr; e.g., Hartmann et al. 2001; Tassis & Mouschovias 2004). The freefall time of clouds at the densities \( n = (1–3) \times 10^3 \text{ cm}^{-3} \) is (0.6–1) × 10^9 yr, which is still longer than our chemistry time. On the other hand, the turbulent crossing time \( t_{\text{cross}} \approx \frac{R}{v_{\text{turb}}} \), where R is the length and \( v_{\text{turb}} \) is the turbulent velocity. The total column density that we used in the model \( (N = 10^{22} \text{ cm}^{-2}) \) corresponds to a source size of 1–3 pc for \( n = (1–3) \times 10^3 \text{ cm}^{-3} \), but the actual geometry of the source is likely to be filamentary with a width of \( R \approx 0.1 \text{ pc} \). For \( R = 1 \text{ pc} \), \( v_{\text{turb}} = 1.1 \text{ km s}^{-1} \) assuming the object follows Larson’s law (Larson 1981), which gives \( t_{\text{cross}} = 10^3 \text{ yr} \). If \( R = 0.1 \text{ pc} \), Larson’s law gives \( v_{\text{turb}} = 0.45 \text{ km s}^{-1} \), which means the crossing is 2.2 × 10^4 yr. This is equivalent to, in order of magnitude, our derived chemistry time. If such turbulence occurs, the molecular medium may be constantly exposed to a low-density environment with a high flux of UV photons to dissociate molecules. If \( G_0 = 30 \), \( A_V \ll 1 \) and the rate coefficient is a typical value of \( k = 10^{-10} \text{ cm}^3 \text{ mol}^{-1} \text{s}^{-1} \), photodissociation can easily occur in a very short timescale of 10 yr. This photodissociation can bring the chemistry close to the initial condition of the atomic/ionic state, and set the chemistry clock back to zero. It should be noted that our models were run with the pseudo-time-dependent approach, and the actual age of the molecular cloud may by longer than our derived chemistry timescale.

4.5. Excitation with Electrons

In regions with high electron fractions, collisional excitation with electrons can be important in addition to excitation with H2 or H. This electron excitation was in fact brought up as a possible mechanism of enhancing HCN emission intensities in strongly irradiated regions. Goldsmith & Kauffmann (2017) analyzed the effect of electron excitation, and concluded that this excitation mechanism may be significant when \( X(e^-) \gtrsim 10^{-5} \) and \( n \lesssim 10^{2.5} \text{ cm}^{-3} \) for the case of HCN. In our chemical model, there are some conditions where electron excitation becomes important. The highest electron fraction is \( X(e^-) \approx 2.9 \times 10^{-5} \) when \( n = 3 \times 10^2 \text{ cm}^{-3} \), \( A_V = 2 \text{ mag} \) and \( \zeta = 10^{-16} \text{ s}^{-1} \). When \( n = 1 \times 10^3 \text{ cm}^{-3} \), there are still cases where the electron fraction is high enough for collisions with electrons to be significant \( (X(e^-) \approx 1.6 \times 10^{-5}) \). For the higher density of \( n = 3 \times 10^3 \text{ cm}^{-3} \), \( X(e^-) \lesssim 2 \times 10^{-6} \) even with a set of parameters to cause the highest ionization fraction \( (A_V = 2 \text{ mag}, \zeta = 10^{-16} \text{ s}^{-1}, \text{ and } S/H = 8 \times 10^{-7}) \), and the electron excitation gives only a minor contribution to the emission. Unfortunately, the collisional cross sections with electrons are not available for all species, which are needed for the comparison of the spectra. For this reason, we do not consider electron excitation here, but the results for the low-density cases need to be taken with caution.

4.6. Two-component Model

In Section 4.3, we argued that the molecular emission likely comes from multiple components. To test this claim, we examine whether the superposition of two components provides a better fit than the single-component model. We found that better agreement with observations is achieved for M51, but not significantly for W51. To create two-component spectra, we added modeled spectra of each model to that of the fiducial model with varying fraction of 0%–100% in 1% increments. Then, we calculated the correlation coefficients between the observations and modeled spectra. The maximum value of correlation coefficients among models of varying contributions from the fiducial model is kept for each model. Those values are shown in Figures 16 (W51) and 17 (M51). In those figures, only the physical parameters of the additional components are shown. From the way we construct the two-component models, the minimum values of correlation coefficients in the two-component model are those of the fiducial model. The improvement from using two-component models is not significant for the case of W51. The highest
improvement is made by combining the model with higher S/H with the fiducial model, not necessarily those with different physical parameters. There are still several cases where the high-density \( n = 3 \times 10^4 \text{ cm}^{-3} \) and late-time \( (t = 10^6 \text{ yr}) \) model gives better correlation coefficients than fiducial model alone. On the other hand, for the case of M51, the correlation coefficients improve by more than 0.1 when additional components of high-density \( (n = (1-3) \times 10^5 \text{ cm}^{-3}) \) models are combined with the fiducial model. Among these, high correlation coefficients are achieved at low \( A_V \) of 2 mag and \( t = 10^5 \text{ yr} \), or at higher \( A_V = 4-10 \text{ mag} \) and \( t = 10^6 \text{ yr} \).

The use of a two-component model also alleviates the disagreement in SO/CS ratio in some models. Observed ratios of SO/CS are 0.13 in M51 and 0.23 in W51. However, this ratio is underproduced by a few orders of magnitude in most models that have high correlation coefficients in single-component models, as shown in Figures 11 and 12. In two-component models, there are a few that reproduce the observed SO/CS ratios within a factor of a few while having high overall correlation coefficients.

5. Summary

In this paper, we modeled the emission intensities of molecular species commonly observed in the 3 mm band using a grid of physical parameters. We conducted molecular abundance calculations using the gas-grain time-dependent chemical model followed by radiative transfer calculations. Our results are compared with observations taken at a scale of a few tens of parsecs in W51 and M51.

Below we list our main findings.

1. Variation of emission intensities with physical parameters can be mostly explained by abundance variations. The dependence of modeled intensities on physical parameters and comparison with observed spectral pattern are summarized as follows.
   (a) When \( A_V = 2 \text{ mag} \) at higher densities, \( N_2H^+ \) is formed in a shorter time, and its intensity increases.
   (b) The emission intensities of HCO\(^+\) and \( N_2H^+ \) increase with higher cosmic-ray ionization rate.
   (c) \( N_2H^+ \) and HCO\(^-\) intensities are higher at \( t = 10^6 \text{ yr} \) than at \( t = 10^5 \text{ yr} \).
   (d) With higher visual extinction, emission intensities of CN and CCH become weaker while those of HCO\(^+\), \( N_2H^+ \) and HNC increase.
   (e) The emission intensities of sulfur-bearing molecules CS and SO increase with the higher elemental abundance of sulfur. The higher sulfur abundance overproduce CS intensities, while SO is overproduced in some high-density, late-time models when compared with observed spectral pattern.
   (f) Our models do not reproduce enough intensities of CH\(_3\)OH in all cases. This underproduction suggests that CH\(_3\)OH may be enhanced by a mechanism that is not included in our model such as sputtering through shocks or turbulence.

2. Our comparison of models with the observations of W51 and M51 suggests physical conditions of \( n = (1-3) \times 10^4 \text{ cm}^{-3} \), \( A_V \geq 4 \text{ mag} \), \( \zeta = 10^{-17} \text{ s}^{-1} \), \( t = 10^5 \text{ yr} \) or \( n = 3 \times 10^5 \text{ cm}^{-3} \), \( A_V = 2 \text{ mag} \), \( \zeta = 10^{-17} \text{ s}^{-1} \), \( t = 10^5 \text{ yr} \), and \( S/H = (0.8-2.5) \times 10^{-7} \).

3. The derived values of density are lower than the critical densities of most species in the optically thin case, but are similar to observationally determined values in the Orion A and Orion B clouds (Kauffmann et al. 2017; Pety et al. 2017). Our results provide more supporting evidence that enough emission can come from relatively low-density regions.

4. The short timescale derived in our analysis \( (t = 10^5 \text{ yr}) \) is consistent with the turbulent mixing timescale that allows exposing the medium to UV photons, which refreshes the chemistry clock.

5. Better correlation with observations of M51 is achieved using two-component models, i.e., summation of the spectral pattern of some of high-density models with that of the fiducial model for the case of M51. For the case of W51, improvement of the correlation is not significant. Such use of two-component models can also alleviate the discrepancy between observation and models for the sulfur-bearing molecules CS and SO.

The observed spectral pattern and the derived physical conditions from the model serve as a benchmark of the chemistry in a relatively quiescent molecular cloud. In future studies of regions with more extreme physical conditions, the differences from this benchmark can be examined.

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Software: RADEX (van der Tak et al. 2007), Nautilus (Hersant et al. 2009; Semenov et al. 2010).

Appendix

Notes on the Excitation Conditions

To highlight the dependence of excitation on emission intensity, we plot the ratio of molecular emission over the column density ratio \( I(X)/N(X) \) with respect to the lowest-excitation case (Figure 18). It is a simple measure to examine how modeled intensities are dependent on either abundances or physical conditions (i.e., \( n \) and \( T \)). In Figure 18 (left), we compare the density variation of \( I(X)/N(X) \) normalized to the \( I(X)/N(X) \) in the case of \( n = 3 \times 10^2 \text{ cm}^{-3} \) with other parameters being \( A = 2 \text{ mag} \), \( \zeta = 10^{-17} \text{ s}^{-1} \), \( S/H = 8 \times 10^{-8} \), and \( T = 10 \text{ K} \). Figure 18 (right) compares the variation in temperature, and values of \( I(X)/N(X) \) are normalized to the case of \( T = 10 \text{ K} \) with \( A = 2 \text{ mag} \), \( \zeta = 10^{-17} \text{ s}^{-1} \), \( S/H = 8 \times 10^{-8} \), and \( n = 3 \times 10^4 \text{ cm}^{-3} \). Note that the above cases are only examples because the emission intensities are dependent on the optical depth, and dependence of intensity on density and temperature may vary for other cases. The dependence on density is large for species other than CO and CI. On the other hand, ratios between the intensities of those species that we used for our analysis only vary by at most a factor of 3–4 when we vary \( n = 3 \times 10^2-3 \times 10^4 \text{ cm}^{-3} \). Similarly, an increase in temperature gives higher intensities for all species, but the variation between them is kept within a factor of a few.
In our model calculations, there are transitions with large optical depth ($\tau \gg 1$) in some conditions while there are transitions that are optically thin in all cases. Figures 19–21 show the optical depth in our model calculations for transitions that have cases with $\tau \gtrsim 1$. Note that Figures 19–21 only use the color scale range of $10^{-1}–10$ to show whether the condition is optically thin or thick.

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