HCN TO HCO⁺ MILLIMETER LINE DIAGNOSTICS OF AGN MOLECULAR TORI. I.
RADIATIVE TRANSFER MODELING

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Abstract
We explore millimeter line diagnostics of an obscuring molecular torus modeled by a hydrodynamic simulation with three-dimensional non–local thermodynamic equilibrium radiative transfer calculations. Based on the results of a high-resolution hydrodynamic simulation of the molecular torus around an active galactic nucleus, we calculate the intensities of the HCN and HCO⁺ rotational lines as two representative high-density tracers. Three-dimensional radiative transfer calculations shed light on a complicated excitation state in the inhomogeneous torus, even though a spatially uniform chemical structure is assumed. We find that similar transition coefficients for the HCN and HCO⁺ rotational lines lead to a natural concordance of the level population distributions of these molecules and a line ratio \( R_{\text{HCN}/\text{HCO}^+} \leq 1 \) for the same molecular abundance value over 2 orders of magnitude. Our results suggest that HCN must be much more abundant than HCO⁺ \( (\gamma_{\text{HCN}} \gtrsim 10\gamma_{\text{HCO}^+}) \) in order to obtain the high ratio \( R_{\text{HCN}/\text{HCO}^+} \sim 2 \) observed in some nearby galaxies. There is a remarkable dispersion in the relation between integrated intensity and column density, indicative of possible shortcomings of the HCN\((1−0)\) and HCO⁺\((1−0)\) lines as high-density tracers. The internal structures of inhomogeneous molecular tori down to subparsec scales in external galaxies will be revealed by the forthcoming Atacama Large Millimeter/submillimeter Array. Three-dimensional radiative transfer calculations of molecular lines with a high-resolution hydrodynamic simulation prove to be a powerful tool to provide a physical basis for molecular-line diagnostics of the central regions of external galaxies.

Subject headings: galaxies: active — galaxies: ISM — ISM: molecules — radiative transfer — radio lines: galaxies

1. INTRODUCTION

Molecular gas at the center of an active galaxy is a subject of crucial importance for observational and theoretical studies of galaxy formation. Various kinds of molecular lines such as \(^{12}\text{CO}, \, \text{HCN}, \, \text{H}^{13}\text{CO}^+, \) and CS have been detected in the central regions of a number of nearby Seyfert galaxies (Aalto et al. 1995; Curran et al. 2000; Usero et al. 2004; Kohno 2005) and luminous and ultra-luminous infrared galaxies (LIRGs and ULIRGs; Gao & Solomon 2004b; Nakanishi et al. 2005; Papadopoulos 2007; Graciá-Carpio et al. 2007). Highly sensitive millimeter telescopes have enabled an increasing number of observations of high-density tracer lines such as HCN or \(^{12}\text{CO}^+, \) aiming at examination of the density structure of the central regions of external galaxies (Curran et al. 2000; Gao & Solomon 2004a; Graciá-Carpio et al. 2006). Imaging observations of nearby galaxies show complex structures in molecular gas in the galactic centers (radius \( R \lesssim 1 \) kpc), such as compact cores and outer rings (NGC 1068 [Planas et al. 1991; Jackson et al. 1993; Schinnerer et al. 2000; Usero et al. 2004]; M51 [Kohno et al. 1996; Scoville et al. 1998; Matsushita et al. 2004]; for reviews of recent results see Kohno 2005; García-Burillo et al. 2007; Kohno et al. 2007). The similar profiles of the CO and HCN lines, the optical thicknesses of which are suggested to differ, support a small volume filling factor of high-density molecular gas (mist model; Solomon et al. 1987). Nguyen-Q-Rieu et al. (1992) concluded from the observation of 15 external galaxies that molecular gas in the central region is composed of numerous clumps smaller than the observational beam size of the IRAM 30 m telescope (\( \Delta \theta_{\text{HPBW}} = 26'' \)).

Zooming into a smaller scale, the unified model of active galactic nuclei (AGNs) postulates a compact, obscuring dusty molecular torus around the central engine (e.g., Antonucci & Miller 1985; hereafter we refer to the molecular gas at the central region \( R \lesssim 100 \) pc of an active galaxy as a “molecular torus”). Current observations have failed to resolve the small, dense regions within compact molecular tori of radius \( \leq 100 \) pc. The dynamical and thermal properties of the putative molecular torus, its structure, and its origin remain ambiguous.

High-resolution hydrodynamic simulations predict a highly inhomogeneous structure inside the molecular torus, which is characterized by clumps and filaments on a subparsec to parsec scale (Wada & Norman 2001, 2002; Wada & Tomisaka 2005). In such an inhomogeneous gas, the energy level population should also be complicated, and interpretation of molecular line emissions requires detailed and careful modeling and calculations. For example, a numerical simulation of \(^{12}\text{CO} \) rotational lines by Wada & Tomisaka (2005) demonstrated a large scatter of the “X-factor,” a conversion constant between the \(^{12}\text{CO} \) luminosity and molecular hydrogen column density in an inhomogeneous torus. Inhomogeneous density and temperature structures are not the only factors that generate the intricate excitation conditions. There are increasing numbers of arguments concerning the effects of peculiar chemical evolution due to X-ray and UV radiation from the central AGN and the accompanying nuclear starburst (Kohno et al. 2001, 2007; Kohno 2005; Imanishi et al. 2004, 2006; Imanishi & Nakanishi 2006; Aalto et al. 2007; Meijerink et al. 2007; for a recent review see García-Burillo et al. 2007 and references therein). The observed line intensity is the consequence of the complex
coupling of various factors, such as hydrodynamic and thermal structures and chemical abundance distribution. Furthermore, the line intensity of high-density tracers, such as HCN, may not necessarily represent the local density (Graciá-Carpio et al. 2006, 2007; Papadopoulos 2007).

In this article we study the role of high-density tracers with the combination of a high-resolution hydrodynamic simulation of an inhomogeneous molecular torus and three-dimensional radiative transfer calculations without the assumption of local thermodynamic equilibrium (non-LTE). We calculate the rotational lines of HCN and H$^{12}$CO$^+$ (hereafter we omit the isotope number 12) and thoroughly examine the excitation status inside the inhomogeneous molecular torus. As the first step, we pursue the nonlinear response of the non-LTE level population in a uniform chemical abundance torus. Chemical evolution in the torus will be discussed separately in a subsequent article.

It should be noted that our calculations can present a direct prediction of the intensity distribution of high-density tracer lines. Our radiative transfer results are able to be directly compared with observational data. They can provide not only valuable suggestions concerning the role of high-density tracers (such as HCN and HCO$^+$ lines) in current observations, but also the theoretical basis for line diagnostics of the thermal and chemical structure of a molecular torus. A compact and inhomogeneous molecular torus at the center of a galaxy will be an interesting target for future observational instruments, such as the Atacama Large Millimeter/submillimeter Array (ALMA). Three-dimensional simulations of a radiation field with high-resolution hydrodynamics will be an important tool for deriving astrophysical properties from the current and forthcoming high-quality observational data.

The organization of this article is as follows: In § 2 we describe the methods of the hydrodynamical and radiative transfer calculations. We display our results for the excitation conditions, the intensity and line-ratio distributions, and the relation to the torus structure in § 3. We briefly discuss the possible effect of chemical evolution on the line ratio of HCN and HCO$^+$ and show implications for future observations with ALMA in § 4, and summarize our article in § 5.

2. MODELS AND EQUATIONS

2.1. Hydrodynamic Model of an AGN Molecular Torus

We first performed hydrodynamic modeling and simulations of the interstellar medium (ISM) around a supermassive black hole (SMBH) following Wada & Tomisaka (2005). An ordinary set of hydrodynamic equations was solved with AUSM (the advection upstream splitting method; Liou & Steffen 1993). We simulated a $64^2 \times 32$ pc$^3$ region with $256^2 \times 128$ uniform Cartesian grid points. We employed model A in Wada & Tomisaka (2005), in which the molecular torus evolves in a steady gravitational potential composed of a SMBH of $M_{\text{BH}} = 10^8 M_\odot$ at the center of the galaxy and a galactic dark halo. These potential fields are described as $\Phi_{\text{ext}} = -(27/4)^{1/2} v_c^2 / (r^2 + a^2)^{1/2}$ for the latter and $\Phi_{\text{SMBH}} = -GM_{\text{BH}} / (r^2 + b^2)^{1/2}$ for the former. We took values for the maximum circular velocity $v_c$ of 100 km s$^{-1}$ and for the core radius $a$ of 10 pc for the gravitational potential of the galactic dark halo $\Phi_{\text{ext}}$, and a value for the core radius $b$ of 1 pc for the SMBH potential $\Phi_{\text{SMBH}}$. The thermal evolution of the torus was calculated with an empirical formula of a cooling function of solar metallicity ($Z = 1 Z_\odot$), photoelectric heating by strong UV background radiation ($G_\odot = 10$ in Habing units), and heating by supernova explosions within the torus. The parameters that determine the cooling and heating rates, $Z$ and $G_\odot$, are not expected to significantly affect the thermal structure of the turbulent multiphase medium in the torus, since they are determined not only by cooling/heating rates but also by dynamical processes and energy feedback from star formation (Wada & Norman 2001; Wada et al. 2002). The torus model assumes a nuclear starburst, which induces an average supernova explosion rate of $\sim 0.36$ yr$^{-1}$. In this model, supernova explosions take place randomly in the disk plane. The dynamical evolution of supernova blast waves in a differentially rotating inhomogeneous torus was explicitly calculated in the simulation, as well as the thermal evolution due to radiative cooling.

The structures of density and temperature and the geometry of the torus are determined by the balance of external gravitational forces (originating from $\Phi_{\text{ext}}$ and $\Phi_{\text{SMBH}}$), self-gravity of the gas, turbulent energy dissipation due to radiative cooling, and feedback from supernova explosions. Wada & Tomisaka (2005) showed that the molecular torus model is globally quasi-steady over a timescale of $\sim 10^8$ yr, although local gravitational instability develops into a significantly inhomogeneous and clumpy internal structure. In our radiative transfer calculations, we use density, temperature, and velocity structures taken from a snapshot of the hydrodynamic simulation results. Strong heating by supernova explosions generates a hot ($T \approx 10^6$ K) and tenuous ($n < 1$ cm$^{-3}$) atmosphere above the dense torus (Wada & Norman 2001, 2002). In the hot atmosphere, neither HCN nor HCO$^+$ molecules are expected. Therefore, we remove the hot atmosphere from the hydrodynamic simulation results as an input to the radiative transfer calculations. The threshold temperature for removing the hot atmosphere is assumed to be $T_{\text{th}} = 10^4$ K, after comparing with preliminary radiative transfer calculations with lower $T_{\text{th}} = 400$ K. We found little difference in these results, and then confidently chose $T_{\text{th}} = 10^4$ K. Thus, the temperature range of the input data is $20$ K $\leq T \leq 1000$ K, and the maximum density reaches as high as $n_{\text{H}_2} \approx 2 \times 10^6$ cm$^{-3}$.

2.2. Radiative Transfer Calculations

We then calculate the HCN and HCO$^+$ molecular line intensities using the results of the hydrodynamic simulations. The input hydrodynamic data are appropriately smoothed from the original high-resolution results ($256^2 \times 128$) to $64^2 \times 32$ grid data. The three-dimensional non-LTE radiative transfer scheme used by Wada & Tomisaka (2005) for CO rotational lines is adopted. We calculate the non-LTE population distribution simultaneously with ray tracing along randomly sampled rays toward the outer boundary from each cell (for details, see Hogerheijde & van der Tak 2000).

The non-LTE level population $n_J$ of energy level $J$ (where $J$ is the rotational quantum number) is calculated by solving the statistical equilibrium rate equation,

$$n_J \sum_{J' \neq J} R_{JJ'} = \sum_{J' \neq J} (n_{J'} R_{J'J}) \quad (1)$$

$$R_{JJ'} = \begin{cases} A_{JJ'} + B_{JJ'} J' + C_{JJ'}, & J > J', \\ B_{JJ'} J + C_{JJ'}, & J < J', \end{cases} \quad (2)$$

where $A_{JJ'}$ and $B_{JJ'}$ represent the Einstein coefficients from energy level $J$ to $J'$, and $C_{JJ'}$ is the collisional transition rate per unit time. In equation (1) the left-hand side is the outgoing rate from the level $J$ under consideration, and the right-hand side is the incoming transition rate to level $J$. The average intensity $I_v$ is calculated from the specific intensity $I_v$,

$$\bar{I} \equiv \frac{1}{4\pi} \int_0^\infty I_v \phi (\nu) d\nu d\Omega, \quad (3)$$
where $\phi(\nu)$ is the normalized absorption coefficient profile (see below). The collisional transition rate $C_{ij}$ is described as

$$C_{ij} = \sum_{X} \gamma_{ij} n_X,$$

(4)

where $n_X$ represents the number density of collision partners and $\gamma_{ij}$ is the corresponding collisional excitation (or de-excitation) coefficient. In this paper we replace $n_X$ by the number density of molecular hydrogen $n_H$.

We calculate the specific intensities $I_\nu$ by solving the equation of radiative transfer,

$$\frac{dI_\nu}{d\tau} = -I_\nu + S_\nu,$$

(5)

where $S_\nu$ denotes the source function. Radiatively induced transition rates are calculated from $\bar{J}$, which is obtained by averaging the specific intensities over the sampling rays coming to each grid cell based on the Monte Carlo method. Rate equations (1) and (2) and transfer equation (5) are iteratively solved until both the level population and radiation field converge self-consistently. The convergence speed is improved by using a version of accelerated lambda iteration (Hogerheijde & van der Tak 2000) that is optimized for our scalar-parallel computer. At the outer boundary we impose the condition that the radiation field be identical to the cosmic microwave background (CMB) radiation.

As for the transition coefficients ($A_{ij}$, $B_{ij}$, and $\gamma_{ij}$), we use the database at Leiden University (Schöier et al. 2005). In order to obtain accurate level population distributions, we solve the rate equation for $0 \leq J \leq J_{\text{max}}$ with a maximum energy level $J_{\text{max}} = 10$ for both the HCN and HCO$^+$ lines. The number of sampling rays for $\bar{J}$ ranges from ~300 to ~900 for each grid point to achieve a convergence level $|\Delta n_j/n_j| \lesssim 10^{-6}$ for all $J$-levels ($\Delta n_j = n_j - n_j^0$ is defined as the maximum of the difference between $n_J$ of the $i$th and $(i-1)$th iterations on the same grid). For low energy levels ($J \lesssim 7$), the degree of convergence progressively improves to $|\Delta n_j/n_j| \lesssim 10^{-10}$.

The model torus has a supersonic turbulent velocity field with a large dispersion $\Delta v \approx 50$ km s$^{-1}$, in comparison with the thermal velocity 0.2 km s$^{-1} \lesssim c_s \lesssim 6.4$ km s$^{-1}$. This turbulent velocity influences the degree of “overlapping” of the lines, which accounts for the optical thickness. We assume microturbulence in the absorption coefficient profile $\phi(\nu)$,

$$\phi(\nu) d\nu = \frac{1}{\Delta \nu \sqrt{\pi}} \exp \left[ -\frac{(\nu - \nu_0)^2}{(\Delta \nu)^2} \right] d\nu,$$

(6)

$$\int^{+\infty}_{-\infty} \phi(\nu) d\nu = 1,$$

(7)

where $\nu_0$ is the line center frequency measured in the rest frame of each fluid element and $\Delta \nu \equiv (\nu_0/c) \sigma_{\text{turb}}$ is the effective Doppler width described by $\sigma_{\text{turb}}$, the velocity of the microturbulence. The velocity structure of the torus is reflected via the profile $\phi(\nu)$ in equation (6). In order to determine a reasonable value for $\sigma_{\text{turb}}$, we survey the parameter space ranging over 1 km s$^{-1} \lesssim \sigma_{\text{turb}} \lesssim 50$ km s$^{-1}$. After confirming the convergence stability of the solution over a wide range of parameters, 10 km s$^{-1} \lesssim \sigma_{\text{turb}} \lesssim 50$ km s$^{-1}$, we choose the value of $\sigma_{\text{turb}} = 20$ km s$^{-1}$ in the following calculations.

The non-LTE population calculation starts with a solution of the rate equation (2) in the optically thin limit with only background radiation $\bar{J} = B_\nu(T_{\text{CMB}})$ [where $B_\nu(T)$ denotes the Planck function] throughout the torus. We examine the effects of the initial guess of the population distribution on the final solution by starting with an alternative initial condition. For this opposite extreme alternative, we select a Boltzmann level distribution with the local kinetic temperature of each grid cell for a starting point. We confirm that these two initial conditions result in the same solution within errors of order $|\Delta n_j/n_j| \lesssim 10^{-5}$. The convergence speed of the radiative transfer calculation is about 2–3 times faster for the optically thin initial condition than for the LTE for both the HCN and HCO$^+$ lines. We conclude that both initial conditions give correct solutions, and then we adopt the optically thin initial condition in our radiative calculations because of its faster convergence to the final solution.

In order to focus on the effects of the structure of the inhomogeneous torus on the excitation conditions and emergent line intensities, we assume spatially uniform abundances of the emitting molecules (HCN and HCO$^+$). The fractional abundance $y \equiv n_{\text{mol}}/n_H$ is assumed to be $10^{-11} \lesssim y \lesssim 10^{-7}$. For the same reason we ignore the radiative pumping by continuum emission from the AGN and/or nuclear starbursts. The nonuniform abundance distribution due to AGNs and nuclear starbursts will be discussed separately in Paper II (M. Yamada et al., in preparation).

3. RESULTS

3.1. Intensity Distribution

Figure 1 (left) displays the integrated intensity distribution of the HCN(1–0) line of a face-on torus. In this panel we adopt the fiducial value of $y_{\text{HCN}} = 2 \times 10^{-9}$ for the molecular abundance. The panel exhibits a significantly inhomogeneous intensity distribution which reflects the highly inhomogeneous structure inside the torus (see Figs. 1 and 2 of Wada & Tomisaka [2005] for the density structure). Since level population is independent of viewing angle, we use the face-on data in the following analysis unless otherwise stated.

Figure 1 (right) displays the line-ratio distribution of HCN(1–0) and HCO$^+(1–0)$,

$$R_{\text{HCN}}(1–0)/\text{HCO}^+(1–0) \equiv \frac{\int T_{\text{A}}(\text{HCN}) d\nu}{\int T_{\text{B}}(\text{HCO}^+) d\nu} = R_{\text{HCN}/\text{HCO}^+}$$

($T_{\text{B}}$ is the brightness temperature) for the same molecular abundance $y_{\text{HCN}} = y_{\text{HCO}^+} = 2 \times 10^{-9}$.

The panel shows that in spite of the significant inhomogeneity of the intensity distributions, the line ratio is restricted to a narrow range from ~0.2 to ~1.2 (the probability distribution function of $R_{\text{HCN}/\text{HCO}^+}$ has a sharp peak around the median, ~0.6). The similarity of the HCN(1–0) and HCO$^+(1–0)$ intensities arises from the almost identical values of the rotational constant $B$ and permanent electric dipole moment $\mu_e$ for these molecules, which determine the energy levels and the Einstein $A$- and $B$-coefficients for pure rotational transitions (see Table 1). The coefficients in Table 1 are calculated by the equations

$$E_J = BhJ(J + 1),$$

(8)

$$B_{J,J+1} = \frac{32}{3} \pi^4 \mu_e^2 \frac{1}{h^2 c^2} \frac{J}{2J + 1},$$

(9)

$$A_{J,J+1} = \frac{16}{3} \frac{h}{c^2} B^3 J^3 B_{J,J+1},$$

(10)

where $E_J$ is the energy measured from the ground state, $h$ is the Planck constant, and $c$ is the velocity of light. Besides these coefficients, the critical density for LTE distribution, $n_{\text{crit}} \equiv A_{J,J}/\gamma_J$, 1 LAMDA: http://www.strw.leidenuniv.nl/~moldata/.
is different between HCN and HCO\(^+\) molecules. However, the amount of gas mass with density larger than the critical density of HCN(1–0) \(n_{\text{crit}} \sim 10^6 \text{ cm}^{-3}\) is \(\sim 3.6 \times 10^5 \text{ M}_\odot\), and the amount larger than the critical density of HCO\(^+\)(1–0) \(n_{\text{crit}} \sim 10^5 \text{ cm}^{-3}\) is \(\sim 1.3 \times 10^6 \text{ M}_\odot\), which agree within a factor of order unity. In the optically thin limit, the line ratio straightforwardly traces the mass ratio, which becomes about unity in our simulation. In our calculations the average optical thickness over the entire field of view is at most \(\langle \tau_0 \rangle = 2\) (see § 3.2 below), and thus the dependence of the line ratio on the critical density is weak.

The overall tendency \(R_{\text{HCN/HCO}^+} \approx O(1)\) does not depend on the molecular abundance \(y\). In Figure 2 we present the integrated intensities averaged over the field of view \((64 \times 64 \text{ pc}^2)\) as a function of \(y\) for both the HCN(1–0) and HCO\(^+\)(1–0) lines. Figure 2 shows that \(\langle I \rangle_{\text{HCN(1–0)}}(y) / \langle I \rangle_{\text{HCO}^+(1–0)}(y)\) for over 2 orders of magnitude of \(y\). This inequality \(\langle I \rangle_{\text{HCN(1–0)}}(y) / \langle I \rangle_{\text{HCO}^+(1–0)}(y) < 1\) implies that in order to obtain the high ratio \(R_{\text{HCN/HCO}^+} \sim 2\) observed in some nearby galaxies (e.g., NGC 1068; Usero et al. 2004), HCN molecules should be much more abundant than HCO\(^+\) molecules \(y_{\text{HCN}} \gg y_{\text{HCO}^+}\). For example, if we take \(y_{\text{HCO}^+} = 2 \times 10^{-8}\), Figure 2 means that \(y_{\text{HCN}}\) should be as large as \(\gtrsim 10^{-7}\) (or \(y_{\text{HCN}} \gtrsim 10y_{\text{HCO}^+}\)) for a high ratio \(R_{\text{HCN/HCO}^+} \approx 2\).

### 3.2. The Line Ratio \(R_{\text{HCN/HCO}^+}\) in the Bright Regions

Figure 1 (left) shows that the torus has many bright spots of several parsecs in size in the integrated intensity distribution. The line-ratio distribution has a smoother structure with \(R_{\text{HCN/HCO}^+} \approx 1\) (Fig. 1, right). Unfortunately, the observational beam size of present instruments is too large to resolve such small structures inside a compact torus (for instance, \(\Delta \theta_{\text{HPBW}} = 2'' - 6''\) for the Nobeyama Millimeter Array and Rainbow interferometers typically corresponds to several hundred parsecs except for Local Group members). Observational estimations of the line ratio would be practically governed by the ratio of the bright regions within the unresolved torus. In the following paragraph we examine the line ratio \(R_{\text{HCN/HCO}^+}\) in the bright region, which is expected to be close to the observational estimation in the unresolved molecular gas.

We show the two-dimensional probability distribution function of the integrated intensity \(I(x, y)\) and the ratio \(R_{\text{HCN/HCO}^+}(x, y) = I_{\text{HCN}(x, y)} / I_{\text{HCO}^+(x, y)}\) in Figure 3 [where \(I(x, y)\) is the integrated intensity at position \((x, y)\) in the field of view]. The three panels in Figure 3 are for different molecular abundances, \(y = 2 \times 10^{-10}\), \(2 \times 10^{-9}\), and \(2 \times 10^{-8}\), respectively. Figure 3 shows the line ratio \(R_{\text{HCN/HCO}^+} \leq 1\) for almost all pixels irrespective of the integrated intensity \(I(x, y)\). When \(y\) is very small \((2 \times 10^{-10})\), pixels of high ratio up to \(R_{\text{HCN/HCO}^+} \leq 1.4\) remain at the bright end. As \(y\) approaches the realistic abundance value \(y = 2 \times 10^{-8}\) inferred

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**TABLE 1**

| Molecule | \(2B\) (GHz) | \(\mu_\nu\) | \(A_{10}\) (Hz) | \(B_{10}\) |
|----------|--------------|------------|----------------|----------|
| HCN      | 88.63        | 2.99 \times 10^{-18} | 2.40 \times 10^{-5} | 2.35 \times 10^{4} |
| HCO\(^+\) | 89.19        | 3.93 \times 10^{-18} | 4.25 \times 10^{-5} | 4.25 \times 10^{4} |

**NOTES.** — The value \(2B\) is twice the rotation constant and is identical to \(v_{10}\). The electric dipole moment \(\mu_\nu\) is measured in cgs units, \(A_{10}\) measures the number of spontaneous transitions per unit time, and \(B_{10}\) is the stimulated radiative transition coefficient per unit time and per unit intensity.

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**FIG. 2** — Spatially averaged integrated intensity \(\langle I \rangle\) over the entire field of view as a function of molecular abundance \(y\). The line with squares displays the \(\langle I \rangle\) of HCO\(^+\)(1–0) emission, and that with crosses presents the \(\langle I \rangle\) of HCN(1–0) emission.
by observational results (e.g., NGC 1068; Usero et al. 2004), however, the line ratio at the bright end falls below $R_{\text{HCN}/\text{HCO}^+} \leq 0.8$. The lower $R_{\text{HCN}/\text{HCO}^+}$ toward the brighter points in the case of $y = 2 \times 10^{-8}$ may indicate a possible underestimation of the line ratio $R_{\text{HCN}/\text{HCO}^+}$ in the current observations of spatially unresolved tori. This trend in Figure 3 might even strengthen the necessity for abundant HCN over HCO$^+$ to obtain a high ratio ($R_{\text{HCN}/\text{HCO}^+} \sim 2$). On the other hand, it might be possible that different spatial distributions of HCN and HCO$^+$ molecules will loosen this requirement, but this topic is not in the scope of this paper and will be discussed in a subsequent paper.

3.3. The Population Distribution in the Radiative Transfer Calculations

In this subsection we demonstrate the population distribution of our non-LTE calculation results (the basic characteristics of the multilevel population distribution in statistical equilibrium in the optically thin limit are summarized in the Appendix). In Figure 4 we plot the ratio $n_1/n_0$ against the density $n_{\text{H}_2}$ for three models with $y = 2 \times 10^{-10}$, $2 \times 10^{-9}$, and $2 \times 10^{-8}$. The level population in the optically thin limit is also shown with lines. Figure 4 exhibits two distinct features of the ratio $n_1/n_0$ from radiative transfer calculations compared with optically thin cases: (1) larger values of $(n_1/n_0)_{\text{peak}} < (n_1/n_0)_{\text{peak, thin}}$ at $n_{\text{H}_2} \sim n_{\text{crit}}$. The departure from the optically thin distribution escalates with the molecular abundance $y$. These features on the diagram can be elucidated by an increase in the radiation-induced transition rate ($\sigma \bar{J}$) by the propagation of line emission in the torus.

The effect of frequent radiation-induced transitions appears on the diagrams as (1) the broad dispersion in the $n_1/n_0$ distribution on the low-density side ($n_{\text{H}_2} \lesssim 10^4$ cm$^{-3}$) and (2) the decrease in the local peak value of $n_1/n_0$ at $n_{\text{H}_2} \sim n_{\text{crit}}$. In the low-density regime ($n \ll n_{\text{crit}}$), collisional transitions are negligible, and the rate equation becomes

$$n_0B_{01}\bar{J} = n_1A_{10} + n_1B_{10}\bar{J}, \quad (11)$$
and the ratio $n_1/n_0$ is written as

$$\frac{n_1}{n_0} = \frac{g_1/g_0 B_{10} \bar{J}}{A_{10} + B_{10} \bar{J}}. \quad (12)$$

Equation (12) means that $n_1/n_0$ increases with the average intensity $\bar{J}$, and can become as large as $n_1/n_0 \leq g_1/g_0 = 3$. Therefore, $n_1/n_0$ can take a value ranging from 0.67 (when $\bar{J}$ is equal to the background radiation, $J_{\text{MKB}}$, see eq. [A1]) to 3 according to $\bar{J}$. In the denser regime, the decrement of the local peak value of $n_1/n_0$ at $n_{H_2} \sim \rho_{\text{crit}}$ is explained by an argument similar to that in § A.1: A large radiative excitation rate $\left[ \bar{J}_{10} = 1/(4\pi) \int I_0 \phi \left( \nu_{10} \right) d\nu d\Omega \right]$ increases the ratio $n_1/n_0$, and then the excitation rate from the level $J = 1$ (not from the ground level $J = 0$) increases as well. The increase in the excitation rate from level $J = 1$ obstructs the downward cascade $J = 2 \rightarrow 1$, and thus leads to the reduction of particle accumulation at $J = 1$ (see § A.1 for details).

An increase in molecular abundance $y$ raises the local emission rate $\left( J_y = \alpha_y g_y I_{10} \right)$ in eq. [5] as $n_{\text{mol}} H_2 \propto y n_{\text{mol}} H_2$, and then the average $\bar{J}$ increases with $y$ as well (eqs. [3] and [5]). Hence, the radiation-induced transition rate due to $J$ increases with $y$. The increase in $J_{10}$ reduces the peak value of $n_1/n_0$ at $n_{H_2} \sim \rho_{\text{crit}}$. The dispersion of $n_1/n_0$ at the low-density regime and the degree of reduction in the peak value of $n_1/n_0$ at $n_{H_2} \sim \rho_{\text{crit}}$ become larger for a larger $y$ in Figure 4. This behavior also supports the importance of radiation-induced transitions $\left( \propto \bar{J} \right)$ in determining the excitation conditions in the inhomogeneous torus.

In addition to the increased radiation-induced transitions, local photon trapping can also affect the distribution of $n_1/n_0$ for a large-$y$ case. The effect of local photon trapping can be described in terms of the escape probability $\beta$ (Goldreich & Kwan 1974; Periai 2002). Local photon trapping reduces the effective critical density as $\rho_{\text{crit}}(\text{eff}) \approx \beta A_{10}/\gamma_{10}$.

The escape probability $\beta$ is described as $\beta = (1 - e^{-\Delta n})/\beta_{\gamma_0}$ for a gas slab and $\beta = (1 - e^{-\Delta n})/\gamma_{10}$ for a spherical volume of gas (e.g., Periai 2002). Although our model torus is neither a slab nor a sphere, both formulae provide limiting values of $\beta \approx 1$ for small $\gamma_{10}$ ($\gamma_{10} \lesssim 1$) and $\beta \approx \gamma_{10}^{-1}$ for large $\gamma_{10}$ ($\gamma_{10} \gg 1$). The average optical thickness in the field of view is estimated to be $\langle \gamma_{10} \rangle = 2.00$ for the face-on data at the line center of HCN in our simulations for a large $y = 2 \times 10^{-4}$ result. An average optical thickness of order unity in our calculations results in a similar value of $\beta$, so that only a negligible effect due to $\beta$ is expected in the diagrams of Figure 4.

3.4. The Effects of Inhomogeneous Structure on Optical Thickness and Intensity Distributions

In the previous subsections we have examined the statistical characteristics of excitation conditions in the torus. In order to examine the connection between the resulting emission and the input torus properties, in Figure 5 we present the integrated intensity as a function of column density $N_{H_2}$. Figure 5 shows that while the integrated intensity $I$ is tightly correlated with $N_{H_2}$ in the low-$N_{H_2}$ regime ($N_{H_2} \lesssim 10^{23}$ cm$^{-2}$), a dispersion of $I$ appears in the larger $N_{H_2}$ regime ($N_{H_2} \gtrsim 10^{23}$ cm$^{-2}$). The origin of this dispersion is further investigated in the relations of integrated intensity, optical thickness, and column density (Fig. 6). Figure 6a shows a dispersion in the optical thickness $\tau_0 = \int \alpha_0 dS$ at large column density ($N_{H_2} \gtrsim 10^{23}$ cm$^{-2}$). This dispersion is obviously produced by the diversity of the absorption coefficients $\alpha_0(n_{H_2}, T)$ due to the non-LTE level population in the inhomogeneous torus.

The drastic increase in integrated intensity appearing at $\tau_0 \lesssim 0$ (Fig. 6b) is owed to the stimulated emission from population inversion (§ A.2). In the two panels of Figure 6, the crosses indicate the values of the average integrated intensity $\langle I \rangle = 42.0$ K km s$^{-1}$, the average optical thickness $\langle \tau_0 \rangle = 0.37$, and the average column density $\langle N_{H_2} \rangle = 9.27 \times 10^{22}$ cm$^{-2}$ in the face-on field of view. Our three-dimensional non-LTE radiative transfer calculations reveal large dispersions around the average values of $I$, $\tau_0$, and $N_{H_2}$. These results imply that high angular resolution observations of ALMA are of crucial importance to studying the structure of the torus.

The spatial correlations of the optical thickness and integrated intensity also show a wide variety in our results. In Figure 7 we plot the spatial distributions of the integrated intensity of HCN(1–0) and the optical thickness $\tau_0$. The disagreement of the integrated intensity distribution (color scale) and the optically thick region ([$\tau_0 \gtrsim 1$]) is obvious in this panel. This disagreement is reasonably well explained by the different dependence of $\tau_0$ and $I$ on density and the line-of-sight structure of the molecular torus as follows.

In the three panels of Figure 8 the distributions of $\Delta \tau_0$ (the optical thickness per single grid) and the density along three lines of sight are displayed. The locations of the three lines of sight are indicated in Figure 7. The three lines of sight represent different circumstances in the inhomogeneous torus. In Figure 8a emission from a clump of $n_{H_2} \lesssim 10^3$ cm$^{-3}$ is visible through a tenuous and optically thin ambient medium, in Figure 8b a tenuous atmosphere encompasses a large scale height in the outer torus, and in Figure 8c the stimulated emission due to population inversion inside a high-density region around the $z = 0$ plane dominates the intensity. Since the local emission rate $J_y = \alpha_y g_y I_{10}$ ($\propto n_{\text{mol}} H_2 \times n_{H_2}^3$) and the optical thickness $\tau_0$ ($\propto n_{H_2} \times n_{H_2}^3$),

2 In our simulation the gain factor $e^{-\Delta n}$ due to population inversion is at most several factors of 10 (see Fig. 6b). This gain factor might be underestimated because of the adopted microturbulence, $\sigma_{\text{turb}} = 20$ km s$^{-1}$, when calculating $\tau_0$ in a grid (eq. [6]). Higher resolution simulations might find even stronger maser spots amplified by population inversion and velocity coherence, although this kind of calculation is computationally too difficult a task at present.
depend differently on density, the integrated intensity can be strong even if \( \tau_0 \) is not large in the inhomogeneous torus (Figs. 8a and 8c). When population inversion \( (\alpha_y < 0) \) occurs (in Fig. 8c), the integrated intensity can be much larger than that simply estimated from the column density (Fig. 5). This is because while the intensity rises rapidly in proportion to \( e^{\Delta \tau_0} \), the optical thickness \( \tau_0 = \int \alpha_0 ds \) only weakly increases due to the negative \( \alpha_0 \) in the integrand.

Our results show that even if the chemical abundance distribution is uniform, the distribution of the intensity and the optical thickness can significantly differ. Hence, it would be possible for the line ratio to reflect neither the ratio of the corresponding amount of gas of density higher than the critical density, nor the ratio of the area of the \( \tau_0 = 1 \) surface. Conventional arguments about the amount of dense gas or the \( \tau_0 = 1 \) surface area are applicable only if the optical thickness is assured to be quite small \( (\tau_0 \ll 1) \) or large \( (\tau_0 \gg 1) \). However, if the ISM is thermally populated and/or has \( \tau_0 \sim 1 \) (which would be the case in the molecular torus), one should take account of the large dispersion of \( \alpha_y \), and especially of population inversion.

4. DISCUSSION

We performed three-dimensional radiative transfer calculations with the assumption of a spatially uniform chemical abundance and closely examined how an inhomogeneous torus structure affects the excitation conditions and the line ratio \( R_{\text{HCN}/\text{HCO}^+} \). Our results in § 3 are briefly summarized as follows: (1) the expected line ratio for the same molecular abundance \( y \) is \( R_{\text{HCN}/\text{HCO}^+} \leq 1 \) over a wide range of \( y \); and (2) the intensity can be strongly affected by the stimulated emission from population inversion. The arguments in § 3.2 and Figure 3 indicate a smaller line ratio \( R_{\text{HCN}/\text{HCO}^+} \leq 1 \) in bright regions, and thus, the observational estimation of the line ratio of the unresolved torus cannot be the “true” average ratio \( R_{\text{HCN}/\text{HCO}^+} \) including the faint regions. Even if we consider the inhomogeneous thermal structure in the torus, a ratio of \( R_{\text{HCN}/\text{HCO}^+} > 1 \) is quite difficult to achieve with the assumption of a spatially uniform chemical abundance (§ 3.2).

4.1. The HCN and HCO\(^+\) Line Ratio as a Probe of the Chemistry of Molecular Gas

Molecular line intensities could reflect the chemical evolution of molecular gas under the irradiation of X-ray and UV emission from the galactic center. This kind of study began with the pioneering work of Kohno (2005) on the “HCN diagram” of nearby Seyfert and starburst galaxies. His “HCN diagram” shows a trend of stronger HCN line emission in nearby galaxies with little signature of starbursts \( (R_{\text{HCN}/\text{CO}} \gtrsim 2.0 \) and \( R_{\text{HCN}/\text{CO}} \gtrsim 0.4 \)), compared with those with starburst regions (see also Imanishi et al. 2006; Imanishi & Nakanishi 2006; Graciá-Carpio et al. 2006). In addition to local Seyfert galaxies, a number of other types of galaxies show high ratios \( R_{\text{HCN}/\text{HCO}^+} > 1 \) (for example, NGC 4418 [Imanishi et al. 2004], UGC 5101 and Mrk 273 [Imanishi & Nakanishi 2006], IC 342, Maffei 2, and NGC 2903 [Nguyen-Q-Rieu et al. 1992], and NGC 1097, NGC 1068, and NGC 5194
around the large scale height, and in (c) the intensity is strong because of the stimulated emission from population inversion within a dense region \( (n_h \leq n_{cr}) \) around \( z = 0 \).

Our results show the ratio \( R_{\text{HCN}}/\text{HCO}^{+} \leq 1 \) for the same molecular abundance \( \gamma \) over 2 orders of magnitude (the right panels of Figs. 1 and 3). The arguments in § A.1 derive the reason for the convergence of the ratio \( n_1/n_0 \) of HCN and HCO\(^{+}\) in the extremes of both low and high densities in the optically thin limit (Fig. 11). Since the intensity \( I_{10} \) increases as \( n_1 \), the intensity ratio \( R_{\text{HCN}}/\text{HCO}^{+} \) roughly agrees with the fractional level population ratio \( n_1/n_0 \) of HCN and HCO\(^{+}\). Hence, for the same value of \( \gamma \), the line ratio \( R_{\text{HCN}}/\text{HCO}^{+} \) becomes of order unity (Fig. 3).\(^3\) This result means that in order to obtain a high ratio \( R_{\text{HCN}}/\text{HCO}^{+} > 1 \), HCN should be much more abundant than HCO\(^{+}\) (\( \gamma_{\text{HCN}} \gg \gamma_{\text{HCO}^{+}} \)). Recently, Graciá-Carpio et al. (2007) found that a high line ratio requires an HCN fractional abundance about 10 times larger than that for HCO\(^{+}\) from their large velocity gradient analysis of \( J = 3 \to 2 \) and \( J = 1 \to 0 \) transitions of LIRGs and ULIRGs. Our results are approximately consistent with theirs.

Several groups discussed the chemical evolution scenario for a high ratio \( R_{\text{HCN}}/\text{HCO}^{+} \). Meijerink et al. (2007) recently examined the chemical evolution of X-ray- and UV-irradiated molecular gas with a wide variety of input parameters. They calculated the thermal and chemical evolutions of plane-parallel gas slabs. Their results show that in a photodissociation region (PDR) the ratio tends to be high \( (R_{\text{HCN}}/\text{HCO}^{+} > 1) \), but in an X-ray-dominated region (XDR) the tendency is the reverse \( (R_{\text{HCN}}/\text{HCO}^{+} < 1) \), except for a small number of models of high density and strong X-ray emission. Although the majority of these kinds of calculations assume a simple geometry for the molecular gas (e.g., Maloney et al. 1996; Meijerink & Spaans 2005; Meijerink et al. 2007), PDR and XDR chemistry currently do not seem to explain the “HCN diagram” classification (Kohno 2005) of AGNs and starburst galaxies. As for alternative scenarios, intense ionization flux from nearby supernova remnant shock waves (and the accordingly high ionization degree; Lepp & Dalgarno 1996) and shock chemistry have been proposed (e.g., Nguyen-Q-Rieu et al. 1992), but it is still uncertain whether these ISM chemistry models can find the evolutionary path for yielding \( \gamma_{\text{HCN}}/\gamma_{\text{HCO}^{+}} > 1 \). Besides chemical abundance models, Aalto et al. (2007) discussed the possible role of mid-IR photons from the dusty torus in determining the excitation conditions of the emitting molecules for LIRGs/ULIRGs.

We expect the molecular torus to have an inhomogeneous structure, and then the shielding of high-energy (UV and X-ray) photons that affects the chemical and thermal structures would be significantly different from that predicted by one-zone or one-dimensional cloud models. Three-dimensional chemical abundance effects, such as simple models of PDRs and XDRs, will be investigated with a three-dimensional scheme in a subsequent paper.

### 4.2. Implications for Future Observations

We mainly examine molecular-line emission in the millimeter band on the basis of the non-LTE radiation transfer simulation so far. If we consider a nearby galaxy at the distance \( D = 20 \) Mpc,

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig8d.png}
\caption{Distributions of \( \Delta \gamma \) (lines with crosses) and the density (lines with diamonds) along the three lines of sight indicated in Fig. 7. The lowest density \( (n_h = 10^{18} \text{ cm}^{-3}) \) seen in these panels is the cutoff density adopted in the hydrodynamic simulation. These three panels represent different circumstances: in (a) emission from a dense clump at \( z \approx 3 \) is seen through a tenuous ambient medium, in (b) the optical thickness is large due to an accumulation low-density atmosphere encompassing the large scale height, and in (c) the intensity is strong because of the stimulated emission from population inversion within a dense region \( (n_h \leq n_{cr}) \) around \( z = 0 \).}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig9a.png}
\caption{Distribution of line profiles at grid points with 10 pc spacing. The abscissa denotes the velocity component along the line of sight measured from the position of the torus. The binning size of \( F_r \) is taken to be 16 km s\(^{-1}\). In each panel black lines show HCO\(^{+}\) \( (1 \to 0) \) and red lines show HCN \( (1 \to 0) \). The multi-peak profiles at the points labeled “A” and “B” reflect the inhomogeneous structure of the torus.}
\end{figure}

\(^3\) The brightness temperature \( T_b \) is proportional to \( v^2 \), and therefore, \( R_{\text{HCN}}/\text{HCO}^{+} \) is accordingly reduced for the same value of \( n_1/n_0 \).
the sizes of the bright spots in our results (Fig. 1), of radius \( \approx 1 \text{ pc} \), correspond to angular sizes \( \Delta \theta \approx 0.03'' \). Therefore, the internal structures of a torus will be resolvable with ALMA in line-intensity distributions. The dispersions of \( N_{\text{H}_2} \) and \( \alpha_v \) and the intensities presented in Figures 7 and 8 will be revealed in detail by ALMA’s high angular resolution observation as well. We briefly discuss the properties relevant to future observations.

Equation (6) means that our radiative transfer calculations take into account the turbulent velocity field inside the molecular torus. Figure 9 demonstrates the line profiles with 10 pc spacing. We assume a nearby galaxy at the distance \( D \approx 20 \text{ Mpc} \) and take the binning size of the velocity component along the line of sight to be \( 16 \text{ km s}^{-1} \). The line profiles in Figure 9 show an extremely complicated structure, reflecting the inhomogeneous structure and turbulent velocity field in the torus. Since a line of sight can pass through more than one dense clump, multiple peaks appear in the line profile, even if the molecular abundance is uniform. Figure 10 presents the average profile over the entire field of view. The compiled profile in Figure 10 shows a Gaussian-like structure of single components: this means that even if current observational results present Gaussian-like profiles, future high-resolution observations will be able to reveal the internal substructures of the compact molecular torus (\( R \leq 100 \text{ pc} \)).

5. SUMMARY AND CONCLUSION

We performed three-dimensional non-LTE radiative transfer calculations for HCN and HCO\(^+\) rotational lines based on a high-resolution hydrodynamic simulation of an AGN molecular torus. An AGN molecular torus is expected to have exceedingly inhomogeneous density and temperature structures, and accordingly complicated energy-level populations. In this article we examined the non-LTE level population distribution in an inhomogeneous molecular torus and its effects on the line ratio \( R_{\text{HCN}/\text{HCO}^+} \), with the assumption of a spatially uniform chemical abundance distribution. The results are summarized as follows: (1) The ratio of the HCN and HCO\(^+\) rotational lines becomes \( R_{\text{HCN}/\text{HCO}^+} \approx 1 \) for a wide range of molecular abundance \( y(10^{-11} \leq \gamma_{\text{HCN}} = \gamma_{\text{HCO}^+} \leq 10^{-7}) \); thus, obtaining the high ratio \( R_{\text{HCN}/\text{HCO}^+} \approx 2 \) observed in some galaxies (such as NGC 5194 and NGC 1068; Kohno 2005) requires more abundant HCN than HCO\(^+\) \( (\gamma_{\text{HCN}} \approx 10 \gamma_{\text{HCO}^+}) \).

(2) The spatial distribution of the line ratio \( R_{\text{HCN}/\text{HCO}^+} \) is inhomogeneous, reflecting the spatially inhomogeneous structure of the molecular torus. (3) Inhomogeneity in the structure of the molecular torus generates a dispersion around the linear relations between intensity and column density. The stimulated emission from population inversion can dominate the integrated intensity where \( n_{\text{H}_2} \sim n_{\text{crit}} \) (Fig. 8c). When the gas is subthermally populated and marginally thick \( (\gamma_i - 1) \), the line ratio may indicate neither the fraction of high-density molecular gas nor the ratio of the surface area of \( \gamma_i - 1 \) regions. Furthermore, our three-dimensional non-LTE calculations demonstrate the complex line profile distribution in the synthetic image of the torus (Fig. 9), even with the uniform abundance assumption. The forthcoming ALMA’s high-resolution observations will reveal such complex structures. The compilation of high-resolution hydrodynamic simulations and three-dimensional radiative transfer calculations will open a powerful way to study the compact molecular gas in the central regions of external galaxies.

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APPENDIX

EXCITATION TEMPERATURE DISTRIBUTION

In this Appendix we describe the fundamental mechanisms that determine non-LTE level population or excitation temperature distribution in the optically thin limit. We especially investigate the superthermal level population appearing at \( n \sim n_{\text{crit}} \) because the stimulated emission due to the superthermal population plays an important role in the line intensities of high-density tracers. In order to provide a simple description of the populating processes, we focus here on low energy level excitation in terms of the ratio \( n_1/n_0 \), compared with the two-level system.

A1. POPULATION DISTRIBUTION IN THE OPTICALLY THIN LIMIT

We first study how the ratio \( n_1/n_0 \) behaves according to the increase in number density of collisional excitation partners \( n_{\text{H}_2} \) in the optically thin limit. In Figure 11 the fractional population \( n_1/n_0 \) is plotted as a function of density for various temperatures. We solve equations (1) and (2) ignoring the average line intensity \( J \) except for the cosmic microwave background radiation \( J = B_s(T_{\text{CMB}}) \equiv J_{\text{CMB}} \). In Figure 11 the HCO\(^+\) and HCN populations are shown with black and blue lines, respectively. It is obvious in Figure 11 that the
fractional population \( n_1/n_0 \) of HCN coincides with that of HCO\(^+\) at the extremes of low \((n_{\text{H}_2} \leq 10^2 \text{ cm}^{-3})\) and high \((n_{\text{H}_2} \geq 10^7 \text{ cm}^{-3})\) densities for the same temperature. This fact can be easily understood in terms of the multilevel population of pure rotational transitions as follows:

In the low-density limit, collisional excitation by molecular hydrogen is negligible, and the level population distribution can be calculated by the balance of radiative excitation by CMB photons and spontaneous emission decay (eq. [11]). Inserting \( J = J_{\text{CMB}} \) into equation (11), the ratio \( n_1/n_0 \) becomes constant for both HCN and HCO\(^+\):

\[
\frac{n_1}{n_0} = \frac{g_1/g_0 B_{10} J_{\text{CMB}}}{A_{10} + B_{10} J_{\text{CMB}}} = 0.67. \tag{A1}
\]

In the second equality in equation (A1) we use the fact that the Einstein \( A\)- and \( B\)-coefficients for the HCN and HCO\(^+\) rotational transitions are almost the same (Table 1).

On the other hand, in the high-density limit the level population converges to the Boltzmann distribution:

\[
\frac{n_J}{n_{J'}} = \frac{g_J}{g_{J'}} \exp\left(-\frac{E_J - E_{J'}}{k_B T}\right) = \frac{2J + 1}{2J' + 1} \exp\left(-\frac{Bh(J(J + 1) - J'(J' + 1))}{k_B T}\right).
\]

From Table 1, rotational constant \( B(\text{HCN}) \simeq B(\text{HCO}^+) \), and then the Boltzmann distributions of the two lines are in perfect agreement:

\[
\frac{\langle n_1 \rangle_{\text{LTE}}}{n_0} = 3 \exp\left(-\frac{2Bh}{k_B T}\right). \tag{A2}
\]

Equations (A1) and (A2) explain the natural concordance of \( n_1/n_0 \) of HCN(1\( \rightarrow \)0) and HCO\(^+\)(1\( \rightarrow \)0) in both low- and high-density extremes.

Figure 11 exhibits a peak of \( n_1/n_0 \) higher than expected for \( n_1/n_0 \) in LTE, at the intermediate density \((10^2 \text{ cm}^{-3} \leq n_{\text{H}_2} \leq 10^7 \text{ cm}^{-3})\) for each temperature. This peak is a result of a combination of two effects, namely, the energy level cascade in a multilevel system and the strong \( J\)-dependence of critical densities for pure rotational transitions.

The energy level cascade originates in the selection rule of radiative transitions. Pure rotational transitions have a selection rule of \( J = \pm 1 \). The selection rule significantly simplifies the rate equation in the low-density and optically thin limit (Yamada et al. 2007):

\[
n_J A_{J,J-1} = \sum_{J' > J} C_{0,J'J} n_0. \tag{A3}
\]

Equation (A3) means that a collisionally excited particle from the ground state should cascade down all the steps of the energy level ladder with \( \Delta J = -1 \) accompanied by spontaneous emission photons.
As density increases, collisional de-excitation begins to modify the simple form of rate equation (A3). As shown in equations (9) and (10), the Einstein $A$-coefficient for pure rotational transition is strongly dependent on $J$. $A_{J,J-1} \propto J^3$. On the other hand, the collisional transition constant only weakly depends on $J$ (Goldreich & Kwan 1974; McKee et al. 1982). Thus, the critical density for LTE, $n_{\text{crit}}(J,J-1) = A_{J,J-1}/g_{J,J-1}$, sharply increases with $J$ ($\propto J^3$). Figure 12 displays the fractional level population distribution $f_J$ as a function of $J$ for various densities ($n_{\text{H}_2} = 10^5, 10^7, 10^9 \text{ cm}^{-3}$). The overall distribution of $f_J$ approaches the Boltzmann distribution (Fig. 12, solid line) as the density increases. In Figure 12 it is also shown that while $f_J$ is close to the Boltzmann distribution for low $J$, $f_J$ deviates from the Boltzmann distribution for high $J$. This is another expression for the reason the peak of $n_1/n_0$ appears (Fig. 11): for a fixed density $n$, the low-$J$ levels that satisfy $n > n_{\text{crit}}(J,J-1)$ approach the Boltzmann distribution (Fig. 12, solid line), and further downward level cascades from the corresponding level come to a halt. However, at higher $J$ levels where the LTE condition is not satisfied, the downward cascades by spontaneous emission accumulate cascading particles at the density $n_c/n_{\text{mol}}$. Accumulation of the extra cascaded particles in addition to the Boltzmann distribution generates the peak of $n_1/n_0$ shown in Figure 11.

A2. POPULATION INVERSION

The source function $S_v$ and the absorption coefficient $\alpha_v$ from the level $J$ to $J-1$ are denoted by

$$S_v = \frac{2\hbar \nu^3}{c^2} \left( \frac{g_J}{g_{J-1}} \frac{n_{J-1}}{n_J} - 1 \right)^{-1},$$

$$\alpha_v = \frac{\hbar \nu}{4\pi} n_{J-1} B_{J-1,J}(\nu) \left( 1 - \frac{g_{J-1}}{g_J} \frac{n_J}{n_{J-1}} \right).$$

(A4)

(A5)

These equations imply negative $S_v$ and $\alpha_v$, if $\delta_{\text{pop}} = n_J g_{J-1}/n_{J-1} g_J$ exceeds unity (population inversion; Rybicki & Lightman 1979). In Figure 13 we plot $\delta_{\text{pop}}$ for HCN(1–0) and HCO$^+$(1–0) in the optically thin limit as a function of density and temperature. In our torus...
model, the density and temperature are \( n_{\text{H}} \leq 2 \times 10^{6} \text{ cm}^{-3} \) and \( 20 \text{ K} \leq T_{\text{kin}} \leq 1000 \text{ K} \), respectively. Figure 13 suggests \( \delta_{\text{pop}} \) is likely to become larger than unity in this density and temperature regime.

When population inversion occurs at the \( i \)th grid cell \( (\delta_{\text{pop}} > 1) \), the optical thickness at the grid cell \( \Delta \tau_{\nu} = \alpha_{\nu}' \Delta s \) becomes negative due to a negative absorption coefficient \( \alpha_{\nu}' \). It is apparent in terms of the formal solution of radiative transfer \( I_{\nu}(\tau_{\nu}) = I_{\nu}(0) e^{-\tau_{\nu}} + S_{\nu}(1 - e^{-\tau_{\nu}}) \) that a negative optical thickness \( \tau_{\nu} < 0 \) strongly enhances the specific intensity \( I_{\nu} \). Since population inversion can significantly affect the intensity, it should be treated correctly in the line transfer calculations. As described in § A.1, one of the origins of population inversion between \( J \) and \( J - 1 \) (or the peak of \( n_{1}/n_{0} \) in Fig. 11) is a downward energy level cascade from higher levels \( J \rightarrow J \). Therefore, the maximum energy level \( J_{\text{max}} \) in the radiative transfer calculation has to be as large as possible to obtain a precise level population, especially when population inversion is expected. Preliminary radiative transfer calculations reveal that the lower limit of the maximum energy level should be \( J_{\text{max}} \geq 8 \) in our model torus. In this paper we take the upper limit of \( J_{\text{max}} = 10 \).

Intense population inversion \( (\delta_{\text{pop}} \geq 1) \) occasionally takes place during the iterative calculations before the solution of the level population meets the final convergence. This sort of temporal population inversion sometimes induces numerical divergence of the intensity due to a factor \( e^{-\tau_{\nu}} \). We avoid the temporal numerical divergence using a way similar to that of Hogerheijde & van der Tak (2000): we set numerical upper bounds on \( \tau_{\nu} \) to \( J_{\text{max}} \). Numerical experiments with several sets of upper bounds present an excellent convergence, thus confirming the stability of the obtained solutions against the variation of the numerical limiters.

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