Hyperfine Group Ratio (HFGR): A Recipe for Deriving Kinetic Temperature from Ammonia Inversion Lines

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ABSTRACT

Ammonia is a classic interstellar thermometer. The estimation of the rotational and kinetic temperatures can be affected by the blended Hyperfine Components (HFCs). We developed a new recipe, referred to as the Hyperfine Group Ratio (HFGR), which utilizes only direct observables, namely the intensity ratios between the grouped HFCs. As tested on the model spectra, the empirical formulae in HFGR can derive the rotational temperature ($T_{\text{rot}}$) from the HFC group ratios in an unambiguous manner. We compared HFGR to the two conventional methods, hyperfine fitting and line intensity ratio, based on both real data and simulated spectra. The HFGR has three major improvements. First, HFGR does not require modeling the HFC or fitting the line profiles, thus is more robust against the effect of HFC blending. Second, the simulation-enabled empirical formulae are much faster than fitting the spectra over the parameter space, so the computer time and human time can be both largely saved. Third, the statistical uncertainty of the temperature $\Delta T_{\text{rot}}$ as a function of the signal-to-noise ratio (SNR) are also provided. HFGR can keep an internal error of $\Delta T_{\text{rot}} \lesssim 0.5$ K over a broad parameter space of temperature (10 to 70 K), line width (0.3 to 4 km s$^{-1}$), and optical depth (0 to 5). When applied to the noisy spectra, HFGR can keep an uncertainty of $\Delta T_{\text{rot}} \lesssim 1.0$ K (1 $\sigma$) when SNR > 4.

Key words: ISM: molecules (Ammonia) – ISM: individual objects (Orion) – ISM: evolution

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1 INTRODUCTION

Gas temperature is a fundamental parameter of molecular clouds. An accurate temperature measurement is indispensable for studying all the physical and chemical aspects of a cloud. As the first polyatomic molecule discovered in interstellar medium (Cheung et al. 1968), Ammonia (NH$_3$) is considered to be an ideal temperature tracer for the dense molecular gas (Ho & Townes 1983a; Li et al. 2003; Mangum & Shirley 2015). NH$_3$ has several inversion transitions, which have largely different excitation energies, but are concentrated in a relatively small frequency range of 23-25 GHz. In the meantime, the NH$_3$ inversion lines are split into hyperfine components (HFCs) due to the varied alignment between the nitrogen and hydrogen nuclei (Ho & Townes 1983a; Li et al. 2003; Mangum & Shirley 2015, also see Figure 1). The HFCs can be used to estimate the optical depth so that the temperature measurement become more accurate (Ho & Townes 1983a). Due to these attributes, ammonia is an invaluable tool of probing the physical conditions in molecular clouds, especially the dense molecular gas.

In practical, there are currently two major options in calculating the temperature: (1) starting from the observed spectra, using the intensity ratios between high- and low-excitation lines to derive the temperature based on Boltzmann distribution (e.g. Ho & Townes 1983a; Busquet et al. 2009; Ragan et al. 2011); (2) starting from the radiative transfer function to generate the model spectra, and adjusting the temperature and other parameters to fit the observed spectra (e.g. Rosolowsky et al. 2008; Keown et al. 2017; Camacho et al. 2020). This method is now included in the Python Package Pyspeckit (Ginsburg & Mirocha 2011). The two methods are denoted as methods of Intensity ratio and HF fitting, respectively.

These two methods are widely applied in analyzing the observed NH$_3$ lines in a variety of molecular clouds (Ho & Townes 1983a; Rosolowsky et al. 2008; Busquet et al. 2009; Ragan et al. 2011; Keown et al. 2017; Camacho et al. 2020). But they still have some major aspects to be improved. The Intensity ratio method involves an approximation that the each HFCs group has one average intensity and optical depth. This assumption would cause potential uncertainty as described in Section 3.7. The hyperfine fitting requires to traverse over a broad parameter space to find the optimized values, which would be time-consuming, in particular when dealing with large spectral data cube.

To improve the accuracy and efficiency in calculation, we try to build a recipe which can more directly connect the physical parameters to the observed line intensities. One can see that the major connections between the spectral line profiles and the physical parameters lie in two aspects:

(i) the intensity ratios of NH$_3$ (2,2)/(1,1) lines increases with $T_{\text{rot}}$;

(ii) the intensity ratios between optically thin (satellites) and thick (main) hyperfine transitions increases with the optical depth.

In the current work, we try to more directly using these two relations instead of relying on additional assumptions about the optical depths.

In spectral modeling, it shows that $T_{\text{rot}}$ can sensitively determine the HFC intensities and its effect is not degenerated with the optical depth, so that the recipe can be expressed in a group of empirical formulae, which are comparatively simple as the Intensity ratio, but more stable over a broad parameter space. The recipe is named as the Hyperfine Group Ratio (HFGR). It is described in details in the following sections. The physical background of the ammonia inversion lines is described in Section 2. The spectra modeling is introduced in 3.1. The empirical formulae of deriving $T_{\text{rot}}$ from the spectra are derived in Section 3.2 to 3.4 and its intrinsic accuracy is inspected in Section 3.5 to 3.6. A comparison between HFGR and other two methods are presented in 3.7. And HFGR is applied to the observed data in Orion A in Section 3.8. A summary is given in Section 4.
2 BACKGROUND OF THE AMMONIA TEMPERATURE CALCULATION

2.1 Physical Basis of the NH$_3$ Inversion Transitions

Ammonia is a symmetric top molecule and has relatively simple rotational energy level structures. The energy levels are characterized by the total rotation momentum $J$ and the component along the molecular axis $K$. The two lowest metastable levels have quantum numbers of $(J, K) = (1, 1)$ and $(2, 2)$, and excitation energy of $E = 24.35$ K and 65.34 K above the ground state, respectively. In typical cold dense clouds with number density of $n$(H$_2$) $\sim 10^4$ cm$^{-3}$ and $T_{\text{gas}} < 20$ K, the NH$_3$ molecules are mainly populated on the $(1,1)$ and $(2,2)$ levels. NH$_3$ $(1,1)$ and $(2,2)$ are mainly excited by the collision, and these transitions have similar frequencies thus can be observed simultaneously with the same telescope.

The physical basis of the population and line transitions are specified in a series of papers (Kukolich 1967; Rydbeck et al. 1977; Ho & Townes 1983a; Stahler & Palla 2005; Mangum & Shirley 2015). The energy level distributions of the $(1,1)$ and $(2,2)$ are shown in Figure 1. For each level, the line emission is generated by the transition between different parities of the nitrogen wave function through the plane of three hydrogen atoms. As measured by Rydbeck et al. (1977), there are 18 HFCs in the $(1,1)$ transitions and 24 HFCs in the $(2,2)$. The right panels in Figure 1 show the synthetic spectra for the two transitions. For both $(1,1)$ and $(2,2)$ lines, the HFCs can be divided into the main group (mg), the inner satellite group (isg) and outer satellite group (osg) as labeled in Figure 1.

The intrinsic strengths of the hyperfine groups are measured from the laboratory spectra assuming all the transitions to have the same excitation temperature, total gas number density and NH$_3$ column density. We adopt the normalized line strengths listed in the review paper of Mangum & Shirley (2015, Table 19 and Table 20 therein). The information of 18 HFCs in $(1,1)$ and 24 HFCs in $(2,2)$ are presented in Table 2.1.
Table 1. Hyperfine intensities for NH$_3$ (1,1) and (2,2).

| Hyperfine Group | HFC number | $F' \rightarrow F$ | Frequency (kHz) | Relative Intensities$^a$ | Velocity km s$^{-1}$ | HFC number | $F' \rightarrow F$ | $F'_{1} \rightarrow F_{1}$ | Frequency (kHz) | Relative Intensities$^a$ | Velocity km s$^{-1}$ |
|-----------------|------------|---------------------|-----------------|--------------------------|---------------------|------------|---------------------|---------------------------|-----------------|--------------------------|---------------------|
| NH$_3$ (1, 1)   |            |                     |                 |                          |                     | NH$_3$ (2, 2) |                     |                           |                 |                          |                     |
| o5g.1           | 1          | 1/2, 1/2            | (0,1)           | -1568.49                 | 1/27                | -19.84     | 1                   | 3/2, 3/2                  | (1,2)           | -2099.03                 | 1/300               | -26.53                 |
|                 | 2          | 1/2, 3/2            | (0,1)           | -1526.96                 | 2/27                | -19.32     | 2                   | 3/2, 5/2                  | (1,2)           | -2058.26                 | 3/100               | -26.01                 |
|                 | 3          | 1/2, 3/2            | (1,2)           | -1523.46                 | 1/60                | -25.95     | 3                   | 1, 2, 3/2                 | (0,1)           | -2056.46                 | 1/300               | -25.95                 |
| isg.1           | 3          | 3/2, 1/2            | (2,1)           | -623.31                  | 5/108               | -7.89      | 4                   | 7/2, 5/2                  | (3,2)           | -1297.08                 | 4/135               | -16.39                 |
|                 | 4          | 5/2, 3/2            | (2,1)           | -590.34                  | 1/12                | -7.47      | 5                   | 5/2, 3/2                  | (3,2)           | -1296.10                 | 14/675              | -16.38                 |
|                 | 5          | 3/2, 3/2            | (2,1)           | -580.92                  | 1/108               | -7.35      | 6                   | 5/2, 5/2                  | (3,2)           | -1255.33                 | 1/675               | -15.86                 |
| mg              | 6          | 1/2, 1/2            | (1,1)           | -36.54                   | 1/54                | -0.46      | 7                   | 3/2, 1/2                  | (1,1)           | -44.51                   | 1/60                | -0.56                  |
|                 | 7          | 3/2, 1/2            | (1,1)           | -25.54                   | 1/108               | -0.32      | 8                   | 5/2, 3/2                  | (2,2)           | -41.81                   | 1/108               | -0.53                  |
|                 | 8          | 5/2, 3/2            | (2,2)           | -24.39                   | 1/60                | -0.31      | 9                   | 7/2, 5/2                  | (3,3)           | -41.44                   | 8/945               | -0.52                  |
|                 | 9          | 3/2, 3/2            | (2,2)           | -14.98                   | 3/20                | -0.19      | 10                  | 5/2, 5/2                  | (2,2)           | -1.05                    | 7/54                | 0.011                  |
|                 | 10         | 1/2, 3/2            | (1,1)           | 5.85                     | 1/108               | 0.07       | 11                  | 3/2, 3/2                  | (2,2)           | -1.05                    | 1/12                | -0.013                 |
|                 | 11         | 5/2, 5/2            | (2,2)           | 10.52                    | 7/30                | 0.13       | 12                  | 7/2, 7/2                  | (3,3)           | 0.31                     | 8/35                | 0.0039                 |
|                 | 12         | 3/2, 3/2            | (1,1)           | 16.85                    | 5/108               | 0.21       | 13                  | 5/2, 5/2                  | (3,3)           | 0.31                     | 32/189              | 0.0039                 |
|                 | 13         | 3/2, 5/2            | (2,2)           | 19.93                    | 1/60                | 0.25       | 14                  | 3/2, 3/2                  | (1,1)           | 1.05                     | 1/12                | 0.013                  |
|                 | 14         | 1/2, 3/2            | (1,2)           | 571.79                   | 5/108               | 7.23       | 19                  | 5/2, 5/2                  | (2,3)           | 1254.58                  | 1/675               | 15.85                  |
|                 | 15         | 3/2, 3/2            | (1,2)           | 582.79                   | 1/108               | 7.37       | 20                  | 3/2, 5/2                  | (2,3)           | 1295.34                  | 14/675              | 16.37                  |
|                 | 16         | 3/2, 5/2            | (1,2)           | 617.70                   | 1/12                | 7.81       | 21                  | 5/2, 7/2                  | (2,3)           | 1296.33                  | 4/135               | 16.38                  |
| isg.2           | 14         | 1/2, 3/2            | (1,2)           | 571.79                   | 5/108               | 7.23       | 19                  | 5/2, 5/2                  | (2,3)           | 1254.58                  | 1/675               | 15.85                  |
|                 | 15         | 3/2, 3/2            | (1,2)           | 582.79                   | 1/108               | 7.37       | 20                  | 3/2, 5/2                  | (2,3)           | 1295.34                  | 14/675              | 16.37                  |
|                 | 16         | 3/2, 5/2            | (1,2)           | 617.70                   | 1/12                | 7.81       | 21                  | 5/2, 7/2                  | (2,3)           | 1296.33                  | 4/135               | 16.38                  |
| os5g.2          | 17         | 1/2, 1/2            | (1,0)           | 1534.05                  | 1/27                | 19.41      | 22                  | 3/2, 1/2                  | (2,1)           | 2053.46                  | 3/100               | 25.75                  |
|                 | 18         | 3/2, 1/2            | (1,0)           | 1545.05                  | 2/27                | 19.55      | 23                  | 3/2, 3/2                  | (2,1)           | 2058.26                  | 3/100               | 26.01                  |
|                 | 19         | 3/2, 3/1            | (2,2)           | 1534.05                  | 1/27                | 19.41      | 22                  | 3/2, 3/2                  | (2,1)           | 2053.46                  | 3/100               | 25.75                  |

$^a$ The Hyperfine intensities are taken from Kukolich (1967); Poynter & Kakar (1975); Mangum & Shirley (2015). The sum of the relative intensities is 1.0.
2.2 The Previous Methods: Aspects to be Improved

The Intensity ratio method uses the intensities of the (1, 1) and (2, 2) HFCs to derive $T_{\text{rot}}$ assuming that the two levels obey the Maxwell-Boltzmann distribution (Ho & Townes 1983a; Mangum et al. 1992; Ragan et al. 2011), that is

$$T_{\text{rot}} = -\Delta E \pm \ln\left[\frac{0.282}{\tau(1, 1, \text{mg})} \ln[1 - \frac{T_B(2, 2, \text{mg})}{T_B(1, 1, \text{mg})}(1 - e^{-\tau(1, 1, \text{mg})})]\right].$$

(1)

The NH$_3$ (1,1) transition often has a high optical depth, which has to be estimated from the ratio between the main and satellite groups of HFCs in (Ho & Townes 1983a, also see Figure 2)

$$T_B(1, 1, \text{mg}) = 1 - e^{-\tau(1, 1, \text{mg})} = 1 - e^{-\tau(1, 1, \text{isg})},$$  

(2)

where $a = 0.278$ is the intensity ratio between NH$_3$ (1,1) main and inner satellite groups, $T_B(1, 1, \text{mg})$ and $T_B(1, 1, \text{isg})$ are the observed brightness temperatures of the two groups, respectively.

Equation (2) assumes that each HFC group has a unique optical depth $\tau_{\text{group}}$. This is an approximation since each group actually contains several internal HFCs with slightly different frequencies (Table 2.1 and Figure 1 right panels), corresponding to an average velocity difference of $\Delta V_{\text{HFC}} = 0.3$ km s$^{-1}$. If the line width is relatively large ($\Delta V > \Delta V_{\text{HFC}}$), the HFCs would be overlapped and the group could be regarded as an integrate spectral feature. In contrast, if $\Delta V < \Delta V_{\text{HFC}}$, the internal HFCs would be further separated and have individual $\tau$ values, which are not necessarily equal. In this case, it would be less accurate to assume the HFC group to have a unified $\tau_{\text{group}}$. The two cases, namely separated and overlapped HFCs are presented in Figure 3a.

For HF fitting, we estimated its $T_{\text{rot}}$ deviation due to $\Delta V$. The NH$_3$ (1, 1) and (2, 2) model spectra can be generated using the radiative transfer functions as described in Section 3.1. The output $T_{\text{rot}}$ is calculated from the model spectra using Equation (1) and (2). Figure 3b exhibits the variation of output $T_{\text{rot}}$ as a function of $\Delta V$. As expected, when $\Delta V$ is relatively small, the output $T_{\text{rot}}$ has a large deviation from the actual value with a scale of $\Delta T_{\text{rot}} = 8$ to 10 K. As shown in Figure 3b, $\Delta T_{\text{rot}}$ is also affected by $\tau$. When $\tau$ increases a factor of 10, the derived $T_{\text{rot}}$ varies for a scale of $\Delta T_{\text{rot}} = 2$ K. The variation of $\Delta T_{\text{rot}}$ suggests the requirement to improve Intensity ratio method, in particular in the case of low $\Delta V$.

The HF fitting method requires a traversal over the broad parameter space of ($\Delta V$, $T_{\text{rot}}$, $N$(NH$_3$)) to look for the best-fit spectra. The complexity of this algorithm should be proportional to the parameter space, which is estimated to be $O(n(\text{channels}) \times n(\Delta V) \times n(T_{\text{rot}}) \times n(N$(NH$_3$))), wherein $n(\text{channels})$ is the number of channels in the spectrum. For other parameters, i.e., $\Delta V$, $T_{\text{rot}}$, and $N$(NH$_3$), $n(X)$ represents the number of data points to be sampled over its suspected range. One can attempt to reduce the calculation by carefully selecting the initial values of the parameters and combining the channels to more quickly approach the optimized values, but the overall $O(n(X))$-complexity is unlikely to be largely reduced.

In this work, we try to combine the advantages of the two methods. Following the simplicity in the Intensity ratio method, we also adopt the strategy of using the HF groups to derive $T_{\text{rot}}$, but we do not assume an average optical depth for each HF group. Instead, we look for direct connection between $T_{\text{rot}}$ and the HFC intensities. This is based on the intuitive connections between the line intensities and the physical parameters, which include two main aspects:

(i) the intensity ratio of $T_{b}(2, 2)/T_{b}(1, 1)$ lines increases with $T_{\text{rot}}$;

(ii) the intensity ratio of $T_{mb}(1, 1, \text{isg})/T_{mb}(1, 1, \text{mg})$ increases with the optical depth or column density $N$(NH$_3$).

Like in HF fitting, one needs to adjust the physical parameters in the model spectra to fit these two relations. But once they can be described in empirical formulae with acceptable accuracy, the formulae would be adopted to
Figure 2. An example of (1,1) and (2,2) spectra, with HF groups are labeled on each HF group. The red solid line represent the best-fit spectra from the HF fitting method. The major equations in the two methods are also presented on the figure, including the equations used to calculate $T_{\text{rot}}$ from the HF groups in the Intensity ratio method and the equations to produce the model spectra in the HF fitting method.

Figure 3. The $T_{\text{rot}}$ deviation as a function of the line width $\Delta V$. (a) two model spectra to elucidate how $\Delta V$ can alter the line profile and HF-group intensities. (b) The $T_{\text{rot}}$ deviation as a function of $\Delta V$ in the intensity-ratio method. The real temperature is $T_{\text{rot}} = 20$ K. The deviation curve is calculated for two values of the optical depths.

be an independent method to derive $T_{\text{rot}}$, and the fitting over the parameter space is no longer needed.

3 RECIPE FOR AMMONIA ROTATIONAL TEMPERATURE

3.1 Modeling the NH$_3$ inversion spectra

There are three major steps to build the new recipe of estimating $T_{\text{rot}}$, including:
(i) generating the model spectra using radiation transfer functions based on the input parameters;
(ii) sampling the relation between $T_{\text{rot}}$ and the HFC intensities from the model spectra using the empirical formulae;
(iii) evaluating the $T_{\text{rot}}$ uncertainty in the empirical formulae and its variation in the parameter space.

The physical parameters to determine the line profiles include optical depth $\tau_0$, rotational temperature $T_{\text{rot}}$, and the intrinsic line width $\Delta V$. The optical depth as a function of the frequency is assumed to have a Gaussian profile for each HFC. The optical depth as a function of $\tau(v)$ over the spectral band is

$$\tau(v) = \tau_0 \sum_i s_i \exp \left[ -\frac{(v - \nu_i - \nu_0)^2}{2\sigma_v^2} \right],$$

wherein $\tau_0$ is the central optical depth of the (1,1) transition, $\nu_0$ is the observed central frequency of the mg component, $s_i$ is the relative intensity of each HFC, and $\nu_i$ is the frequency shift of each HFC relative to $\nu_0$. The values of $\nu_i$ and $s_i$ are adopted from Kukolich (1967) and are shown in Table 2.1. The spectral frequency is related to the radial velocity as $(\nu_0 - \nu)/\nu_0 = (V - V_0)/c$, and hence is the frequency dispersion $\sigma_v = (\nu_0/c)\sigma_V$. The velocity dispersion $\sigma_V$ is related to the full-width half-maximum (FWHM) line width $\Delta V$ as $\sigma_V = \Delta V/\sqrt{8\ln 2}$. Using the Planck-corrected brightness temperature

$$J(T) = \frac{h\nu_{\text{at}}/k}{\exp(h\nu_{\text{at}}/kT) - 1},$$

the (1,1) and (2,2) spectra can be modeled using the radiative transfer function as:

$$T_{\text{mb}}(v) = \eta_f [J(T_{\text{ex}}) - J(T_{\text{bg}})] [1 - e^{-\tau(v)}].$$

Wherein $\tau(v)$ is the optical depth as a function of frequency $v$, $T_{\text{ex}}$ is the excitation temperature, $T_{\text{bg}} = 2.73$ K is the cosmic background temperature, $\eta_f$ is the beam filling factor and is set to be $\eta_f = 1$ in modeling the line profile.

In the condition of Local Thermal Equilibrium (LTE), the (1,1) and (2,2) levels obey the Maxwell-Boltzmann distribution. Their column-density ratio is thus

$$\frac{N(2,2)}{N(1,1)} = \frac{g_{22}}{g_{11}} \exp \left[ \frac{\Delta E}{T_{\text{rot}}} \right],$$

wherein $\Delta E = (E_{22} - E_{11})/k = 40.99$ K is the energy difference; the statistic weight ratio is $g_{11}/g_{22} = 3/5$ (Pickett et al. 1998). On the other hand, for each energy level, the column density is related to the total optical depth as (Rosolowsky et al. 2008):

$$N(i, i) = \frac{8\pi\nu_0^2}{c^2} \frac{g_i}{g_u} \frac{A_i}{A_i} \left[ 1 - \exp \left( \frac{h\nu_i}{kT_{\text{ex}}} \right) \right]^{-1} \int_{v_{\text{min}}}^{v_{\text{max}}} \tau_v(i, i) \Delta \nu_{\text{FWHM}} dv$$

$$\times \left( \frac{8\pi\nu_0^2}{c^2} \frac{g_i}{g_u} \frac{A_i}{A_i} \right)$$

$$\times \left[ 1 - \exp \left( \frac{h\nu_i}{kT_{\text{ex}}} \right) \right]^{-1} \tau_0(i, i) \Delta \nu_{\text{FWHM}}.$$

The second term on the right side is obtained by using Equation (3) as the term of $\tau(v)$. From the NH$_3$ collisional coefficients $\gamma$ (Danby et al. 1988) and the Einstein coefficient $A_i$, the critical density is $n_{\text{crit}} = \gamma / \gamma$. The derived values are shown in Table 3.1. The value of $n_{\text{crit}}$ suggests that the level populations would be thermalized when $n($H$_2$) $\geq 7 \times 10^3$ cm$^{-3}$. This condition is supposed to be widely satisfied in cold dense molecular gas and young star-forming cores, which have $n($H$_2$) $> 10^4$ cm$^{-3}$ (e.g. Ragan et al. 2012).

An example of NH$_3$(1,1) and (2,2) model spectra is presented in Figure 2. The input parameters are $T_{\text{rot}} = T_{\text{ex}} = 28$ K, $\Delta V = 1.5$ km s$^{-1}$, $\tau_0(1,1) = 2.00$, and an rms noise of 0.1 K. Using Equation (6) and (7), one can derive $\tau_0(2,2) = 0.44$. For the (2,2) line, the satellite components appear to be much weaker compare to that in the (1,1) spectrum.

To make simulation more similar to observations, especially VLA observations, we set temperature as 20 K, $\Delta V$ as 1.0 km s$^{-1}$, channel width as 0.24 km s$^{-1}$ and rms as 0.2 K. We also set optical depth($\tau$) for NH$_3$(1,1) change from 0.2 to 4.0 as show in the Fig. 4 (An animation is shown in online version). It shows NH$_3$(2,2) satellite lines are not obvious like NH$_3$(1,1) satellite lines in most of time.
Table 2. The Physical Parameters of The NH$_3$ Transitions.

| Transition | Frequency$^a$ (×10$^6$ kHz) | $E_u$ (K) | $A_b^b$ (10$^{-7}$ s$^{-1}$) | $\gamma^c$ (10$^{-11}$ cm$^3$ s$^{-1}$) | $n_{cm}^d$ (10$^3$ cm$^{-3}$) |
|------------|-----------------------------|----------|-----------------------------|----------------------------------|-------------------------------|
| (1,1)      | 23.69449                    | 24.35    | 1.86,5.58                   | 8.3,9.5                          | 2.0,6.7                       |
| (2,2)      | 23.722633                   | 65.34    | 0.83,6.63                   | 11,13                            | 0.6,6.0                       |

$^a$. NH$_3$ (1,1) and (2,2) inversion transition frequencies given by (Kukolich 1967).

$^b$. Einstein $A$ coefficients were previously measured by Osorio et al. (2009); Poynter & Kakar (1975); Mangum & Shirley (2015). The current values are from Mangum & Shirley (2015). The two values correspond to the upper and lower limits for all the HFCs, respectively.

$^c$. Collisional coefficients $\gamma$ are taken from Danby et al. (1988). For each transition, the two values correspond to that at the temperature of $T_{kin} = 10$ to 100 K, respectively.

$^d$. Critical density of each transition, the two values correspond to the lower and upper limits among all the hyperfine groups.

Figure 4. The modeled spectra with a series of optical depths from 0.2 to 4.0. The spectra are generated using the radiative transfer modeling as shown in Equation (1) to (3). The physical parameters are $T_{rot} = 20$ K, $\Delta V = 1.0$ km s$^{-1}$. In each spectrum the rms noise is set to be 0.2 K. (This animation is available online.)
3.2 Relation between $T_{\text{rot}}$ and HFC intensities

Using Equation (5), the total optical depth can be manually connected to the observed line intensity as:

$$\int \tau_d d\nu \equiv \int \frac{\tau_d d\nu}{1 - e^{-\tau_d}} \frac{\int T_{\text{mb}}(\nu) d\nu}{J(T_{\text{ex}}) - J(T_{\text{bg}})}.$$

Using this form, the ratio between the (1,1) and (2,2) column densities can be written as

$$\frac{N(1,1)}{N(2,2)} = \left[ \frac{\nu_1^2 A_{22}}{\nu_2^2 A_{11}} \right] \frac{\int \tau_{\nu_1(1,1)} d\nu}{\int \tau_{\nu_2(2,2)} d\nu} \times \frac{\int T_{\text{mb}(1,1)} d\nu}{\int T_{\text{mb}(2,2)} d\nu}.$$

Combining Equation (9) and (6), we have

$$\exp \left[ \frac{\Delta E}{T_{\text{rot}}} \right] = \left[ \frac{g(2,2) \nu_1 A_{22}}{g(1,1) \nu_2 A_{11}} \right] \frac{\int \tau_{\nu_1(1,1)} d\nu}{\int \tau_{\nu_2(2,2)} d\nu} \times \frac{\int T_{\text{mb}(1,1)} d\nu}{\int T_{\text{mb}(2,2)} d\nu}.$$

In deriving Equation (10), we adopted an approximation that $1 - \exp(h\nu/kT_{\text{ex}}) = -h\nu/kT_{\text{ex}}$. This should be reasonable since the transition energy of $h\nu_{1,1}/k = h\nu_{2,2}/k = 1.1$ K should be usually much lower than $T_{\text{ex}}$.

To further reduce Equation (10), we define the correction factor $C_f$ as

$$C_f = \left[ \frac{g_{22}}{g_{11}} \frac{\nu_1 A_{22}}{\nu_2 A_{11}} \right] \frac{\int \tau_{\nu_1(1,1)} d\nu}{\int \tau_{\nu_2(2,2)} d\nu} \frac{1 - e^{-\tau_0(1,1)}}{1 - e^{-\tau_0(2,2)}}.$$

Using $C_f$, Equation (10) becomes

$$\exp \left[ \frac{\Delta E}{T_{\text{rot}}} \right] = C_f \times \frac{\int T_{\text{mb}(1,1)} d\nu}{\int T_{\text{mb}(2,2)} d\nu}.$$

Equation (12) is then transformed into an expression of $T_{\text{rot}}$.

$$T_{\text{rot}} = \frac{\Delta E}{\ln C_f \times \frac{\int T_{\text{mb}(1,1)} d\nu}{\int T_{\text{mb}(2,2)} d\nu}}.$$

Now the key step is to express $C_f$ using the observed quantities. Since a main purpose of this work is to circumvent the uncertainty due to the HFC-blending, we consider using the intensity ratios among the HFC groups (mg, isg, osg). Since $C_f$ is related to the optical depth, a natural option is to consider the intensity ratio between mg and sg which is also proportional to the optical depth, that is

$$R_{\text{sm}} = \left[ \frac{\int T_{\text{mb}}^{\text{isg+osg}} d\nu}{\int T_{\text{mb}}^{\text{mg}} d\nu} \right]_{(1,1)}.$$

Theoretically, the HFC groups of the (2,2) level can also trace $C_f$ as shown in Equation (11). They are not adopted mainly because the (2,2)-satellite groups are much weaker than in (1,1) (Figure 1 and 3).

The relation between $C_f$ and $R_{\text{sm}}$ can be numerically sampled from the model spectra over the $\tau_0$ range. In each sampling over the $\tau_0$ range, the other two parameters, $\Delta V$ and $T_{\text{rot}}$ are set to be constants. Then a number of samplings are carried out to obtain the $C_f(\tau_0)$ function at different $\Delta V$ and $T_{\text{rot}}$ values. Figure 5a shows the $C_f(R_{\text{sm}})$ relation sampled at temperatures from $T_{\text{rot}} = 10$ to 70 K. One can see that each $C_f(R_{\text{sm}})$ relation has a clear and smooth variation trend with $R_{\text{sm}}$. The slope of the $C_f(R_{\text{sm}})$ relation continuously varies with $T_{\text{rot}}$. When $T_{\text{rot}}$ is very high ($T_{\text{rot}} > 55$ K), the $C_f(R_{\text{sm}})$ relation turns to be slightly negative, which is mainly due to the increased (2,2) optical depth in the denominator of Equation (11). The average slope of the $C_f(R_{\text{sm}})$ relation declines from $C_f/R_{\text{sm}} = 0.7$ to $-0.1$ from $T_{\text{rot}} = 10$ to 70 K.

Figure 5b shows the $C_f(R_{\text{sm}})$ relations at line widths from $\Delta V = 0.5$ to 3.0 km s$^{-1}$. As shown in Figure 5b, the slope of the $C_f(R_{\text{sm}})$ relation increases from $C_f/R_{\text{sm}} = 0.45$ to 0.5 in the range of $\Delta V = 0.5$ to 3.0 km s$^{-1}$. The changing of $C_f(R_{\text{sm}})$ curves with $\Delta V$ should also reflect the changing of blending condition of the internal components in each HFC group as shown in Figure 3a. This effect is now included in $\Delta V$ in the expression of $C_f$.

Figure 5a and 5b also show that all the $C_f(R_{\text{sm}})$
curves are exactly converged at $(R_{\text{sm}}, C_f) = (1.0, 0.9524)$, which represents the line intensity ratio at extremely low optical depth. When $\tau_0$ is very small, the HFC group intensities would become independent of $\Delta V$ and $T_{\text{rot}}$.

Since $R_{\text{sm}}$ is a correction factor for optical depth $\tau_0$, we examined the relation between $R_{\text{sm}}$ and $\tau_0$. For each (1,1) model spectrum, $\tau_0$ can be estimated from Equation (7). As shown in Figure 5c, the two quantities are found to have a nearly linear relation of $\tau_0(1,1) = 3.52(R_{\text{sm}} - 1)$. Since $\tau_0$ can be uniquely determined by $R_{\text{sm}}$, it is not necessary to be independently considered in our calculation.

### 3.3 Coefficients in the Polynomial Expression of $T_{\text{rot}}$

At any $\Delta V$ and $T_{\text{rot}}$ values, the $C_f(R_{\text{sm}})$ relation exhibits a linear increasing or decreasing trend with a slight curvature. We thus tried to fit it using a two-order polynomial,

$$C_f = a_0 + a_1(R_{\text{sm}} - R_{\text{sm}0}) + a_2(R_{\text{sm}} - R_{\text{sm}0})^2,$$

wherein $R_{\text{sm}0} = 1.0$, $a_0 = 0.9524$ represent the values at the convergent point (Figure 5a). The coefficients $a_{1,2}$ are constants in an individual $C_f(R_{\text{sm}})$ relation, but would depend on $T_{\text{rot}}$ and $\Delta V$. In Figure 6, the solid dots represent $a_1$ and $a_2$ values sampled over the parameter space of $\Delta V$ and $T_{\text{rot}}$. The numerical functions of $a_{1,2}(T_{\text{rot}}, \Delta V)$ are also fitted by two-order polynomials,

$$a_i = h_0 + h_1\Delta V + h_2T_{\text{rot}} + h_3\Delta V^2 + h_4T_{\text{rot}}^2,$$

wherein coefficients $\{h_i\}$ are permanent constants that no longer depend on the parameters of $\tau_0$, $T_{\text{rot}}$, or $\Delta V$. Based on the numerically sampled $a_i$, we found that $T_{\text{rot}}$ and $\Delta V$ would have independent influence to $a_{1,2}$. Namely Equation (16) would not contain a crossing term of $T_{\text{rot}}\Delta V$.

The best-fit analytical functions of $a_i(\Delta V, T_{\text{rot}})$ are presented as false-color surfaces in each panel. The best-fit coefficients $\{h_i\}$ values are provided in Table 3. We see that the surface of $a_i(\Delta V, T_{\text{rot}})$ functions with the best-fit $\{h_i\}$ values are coincident with the sampled data points, suggesting that Equation (16) can closely describe the $a_i$ variation with $T_{\text{rot}}$ and $\Delta V$. Although $a_{1,2}$ can be estimated from $\{h_i\}$ using Equation (16), their numerical results are still presented in Table 3.3 and Table 3.3.

![Figure 5](image-url)

**Figure 5.** (a) The correction factor $C_f$ as a function of $R_{\text{sm}}$ at different $T_{\text{rot}}$ values, with the line width fixed to be $\Delta V = 1.0$ km s$^{-1}$ and $\tau = 2.0$. (b) The $C_f(R_{\text{sm}})$ function at $\Delta V = 0.5, 1.0, 1.5, 2.0, 2.5$, and $3.0$ km s$^{-1}$, with a fixed temperature of $T_{\text{rot}} = 20$ K. (c) The relation between the (1, 1) optical depth $\tau_0$ and $R_{\text{sm}}$ estimated at $T_{\text{rot}} = 20$ K and $\tau_{11} = 2.0$. The slope of $\tau_0$-$R_{\text{sm}}$ relation is almost not affected by $T_{\text{rot}}$.

### Table 3. $h_i$ values in Equation (16).

| $T_{\text{rot}}$ (K) | $h_0$ | $h_1$ | $h_2$ | $h_3$ | $h_4$ |
|----------------------|-------|-------|-------|-------|-------|
| in $a_1$             | 0.6857| -1.0001| 0.3413| 0.2797| -0.1051|
| in $a_2$             | -0.0836| -0.1592| -0.1387| -0.0429| 0.0804|
### 3.4 How to Perform the Recipe

The major steps of using the recipe are presented in a flow chart in Figure 7. In calculation, an initial value of $T_{\text{rot}}$ is provided. It can be calculated from Equation (11) assuming $C_f = 1.0$. And the line width $\Delta V$ can be measured from the (1,1) major group. As described above, compared to $T_{\text{rot}}, \Delta V$ has a minor influence to $C_f$. We only need to ensure that $\Delta V$ is not largely deviated from the actual value so that its influence to $C_f$ can be corrected. $a_{1,2}$ and $C_f$ are then derived using Equation (16) and (15), respectively. And $T_{\text{rot}}$ is recalculated using Equation (13). The calculation can be usually converged after several iteration. One can also estimate the kinetic temperature.
Table 5. Numerical $a_2$ values in Equation (15).

| $\Delta V$ (km s$^{-1}$) | 10 K | 20 K | 30 K | 40 K | 50 K | 60 K | 70 K |
|--------------------------|------|------|------|------|------|------|------|
| 0.2                      | 0.0101 | -0.1572 | -0.0756 | 0.1804 | 0.4946 | 0.8214 | 1.1428 |
| 0.4                      | -0.0836 | -0.1592 | -0.1387 | -0.0429 | 0.0804 | 0.2116 | 0.3426 |
| 0.6                      | -0.0792 | -0.1473 | -0.1557 | -0.1065 | -0.0350 | 0.0437 | 0.1236 |
| 0.8                      | -0.0722 | -0.1397 | -0.1581 | -0.1228 | -0.0665 | -0.0030 | 0.0621 |
| 1.0                      | -0.0671 | -0.1351 | -0.1578 | -0.1281 | -0.0778 | -0.0201 | 0.0393 |
| 1.2                      | -0.0650 | -0.1325 | -0.1572 | -0.1303 | -0.0828 | -0.0279 | 0.0289 |
| 1.4                      | -0.0727 | -0.1329 | -0.1584 | -0.1331 | -0.0876 | -0.0350 | 0.0196 |
| 1.6                      | -0.0923 | -0.1366 | -0.1617 | -0.1378 | -0.0945 | -0.0445 | 0.0069 |
| 1.8                      | -0.1170 | -0.1418 | -0.1655 | -0.1427 | -0.1016 | -0.0545 | -0.0066 |
| 2.0                      | -0.1388 | -0.1465 | -0.1681 | -0.1460 | -0.1066 | -0.0620 | -0.0170 |
| 2.2                      | -0.1533 | -0.1495 | -0.1688 | -0.1468 | -0.1087 | -0.0656 | -0.0224 |
| 2.4                      | -0.1599 | -0.1506 | -0.1677 | -0.1455 | -0.1078 | -0.0655 | -0.0231 |
| 2.6                      | -0.1602 | -0.1501 | -0.1652 | -0.1425 | -0.1050 | -0.0627 | -0.0202 |
| 2.8                      | -0.1560 | -0.1486 | -0.1619 | -0.1387 | -0.1099 | -0.0583 | -0.0151 |
| 3.0                      | -0.1488 | -0.1463 | -0.1583 | -0.1344 | -0.0962 | -0.0530 | -0.0087 |
| 3.2                      | -0.1393 | -0.1435 | -0.1544 | -0.1300 | -0.0912 | -0.0472 | -0.0017 |
| 3.4                      | -0.1269 | -0.1401 | -0.1502 | -0.1252 | -0.0858 | -0.0408 | 0.0062 |

Figure 7. The flow chart showing the calculation process of the recipe. $S_{mg}$, $S_{isg}$ and $S_{osg}$ are integrated intensities of main group (mg), inner satellite group (isg) and outer satellite group (osg). $C_f$ is a correction factor for optical depth. The coefficients $h_i$ are constants that no longer depend on physical parameters $\tau_0$, $T_{rot}$, or $\Delta V$. $\alpha_0 = 0.952406$ and $R_{sm0} = 1.000$. The output $T_{rot}$ and $T_{kin}$ are determined by whether $T_{rot}$ is convergent.
\( T_{\text{kin}} \). The recommended formula is from Tafalla et al. (2004),

\[
T_{\text{kin}} = \frac{T_{\text{rot}}}{1 - \frac{T_{\text{rot}}}{T_{\text{rot}} - 1} \ln[1 + 1.1 \exp(-16/T_{\text{rot}})]},
\]

which is obtained from a Monte Carlo sampling of the \((J,K)\)-level population as a function of \( T_{\text{kin}} \).

3.5 Accuracy of the recipe

In order to test the accuracy of HFGR, it is applied to a series of model spectra. The \((1,1)\) and \((2,2)\) model spectra are generated using Equation (3), (4), and (5). The input parameters include \( T_{\text{rot}}, \Delta V, \) and \( \tau_0 \). Figure 8a shows the output \( T_{\text{rot}} \) deviation as a function of \( N(\text{NH}_3) \) (or \( \tau_0 \)) at a number of \( T_{\text{rot}} \) values. The \( T_{\text{rot}} \) deviation turns out to increase moderately with \( N(\text{NH}_3) \) and remains at \( \Delta T_{\text{rot}} < 1.0 \) K throughout the temperature range. In the high-mass dense molecular cores, the column densities have an average level of \( N(\text{NH}_3) = 5 \times 10^{14} \text{ cm}^{-2} \) and only occasionally exceed \( 10^{15} \text{ cm}^{-2} \) (e.g. Lu et al. 2014, Table 6 therein). The \( N(\text{NH}_3) \) values in real cases are thus well covered in our calculation range, and the \( T_{\text{rot}} \) deviation due to the \( N(\text{NH}_3) \) would not be significant. Figure 8b shows the \( T_{\text{rot}} \) deviation over the \( (T_{\text{rot}}, \Delta V) \) parameter space at \( \tau_0 = 3.0 \). One can see that the \( T_{\text{rot}} \)-error is quite small in the major fraction of the parameter space, and the \( T_{\text{rot}} \)-error increases to a noticeable level only when \( \Delta V \) is very small and \( T_{\text{rot}} \) is very high. There is a physical constraint that \( \Delta V \) should be lower than the level of thermal motion, that is \( \Delta V > 8 \ln 2 kT_{\text{kin}} / (\mu m_{\text{NH}_3})^{1/2} \). The relation of \( \Delta V = 8 \ln 2 kT_{\text{kin}} / (\mu m_{\text{NH}_3})^{1/2} \), as plotted in Figure 8b, represent a lower limit for the available \( \Delta V \). The region bellow this curve would not exist in real conditions. Above this curve, the \( T_{\text{rot}} \) deviation is lower than 0.15 K and only slightly increases to \( \Delta T = 0.40 \) K at very high temperatures of \( T_{\text{rot}} \sim 90 \) K.

3.6 The Modification at Low Temperatures

At low temperatures, the \((2,2)\) line will become very weak so that the \( T_{\text{rot}} \) uncertainty would largely increase. This problem exists in all three methods. Figure 9 shows the output \( \Delta T_{\text{rot}} \) distribution as a function of the real \( T_{\text{rot}} \) in the low temperature range for the numerical recipe. One can see that \( \Delta T_{\text{rot}} \) dramatically increases when \( T_{\text{rot}} < 15 \) K. This is mainly due to the \((2,2)\) emission becoming very weak at low temperatures. To eliminate the uncertainty, one can use gaussian fitting to measure the HFC-group intensities. As a result, the \( \Delta T_{\text{rot}} \) distribution becomes more convergent towards the lower end of \( T_{\text{rot}} \) as shown in Figure 9b.

3.7 Comparison between the HFGR and other Methods

We compared HFGR with other two classical methods (Section 2) for the efficiency and accuracy. For Intensity ratio, most studies used the peak line intensity of each HFC group (e.g. Friesen et al. 2009; Ragan et al. 2011; Chira et al. 2013). Actually, as the second option, one can also use the integrated intensity of each HFC group instead of its peak value. This can increase the signal-to-noise ratio (SNR). For example, if the line emission in a group extends over \( N \) channels, the SNR of the integrated emission would be increased by a factor of \( \sqrt{N} \). It is worthwhile to have a comparison between the two options, namely using the peak value or integrated emission of each HFC group.

HFGR and other two methods are applied to the model spectra to make comparison of their accuracies. We first investigate the \( T_{\text{rot}} \) variation at constant SNR and \( \sigma_{\text{rms}} \) the three methods, wherein the input parameters are \( T_{\text{rot}} = 20 \) K, \( \Delta V = 1.0 \text{ km s}^{-1} \), \( \tau_0(1,1) = 1.5 \), and an rms noise of 0.2 K. The physical conditions are typical for dense molecular clouds. The rms level corresponds to SNR\(\approx\) 20 for the \((1,1)\)-isg group. In each of the 2000 samplings, the rms noise is independently generated and
added into the model spectra. In each sampling, $T\text{rot}$ is calculated from the noisy spectra using the three methods. Figure 10a shows the temperature variation $\Delta T\text{rot}$ relative to the actual value of $T\text{rot} = 20$ K in all the samplings. One can see that $HFGR$ and the $HF$ fitting turn out to have comparable variation of $\Delta T\text{rot} = \pm 0.5$ K at the half-maximum level. For the intensity-ratio method, the two options, (i) total emission, and (ii) the peak value for each $HF$ group are both investigated. As a result, option (i) exhibits a comparable $\Delta T\text{rot}$ variation, while option (ii) yields a much larger variation of $\Delta T\text{rot} = \pm 1$ K. The larger uncertainty is within our expectation since the peak $T\text{mb}$ of each hyperfine group is sensitive to the rms noise.

Figure 10b shows the $\Delta T\text{rot}$ distribution as a function of the rms noise. As expected, for each method, $\Delta T\text{rot}$ shows an increasing trend with the rms level. $HF$ fitting has the lowest $\Delta T\text{rot}$ over the rms range, while $HFGR$ and $Intensity$ ratio-option (i) have slightly higher $\Delta T\text{rot}$ than $HF$ fitting. For all three methods, the variation can maintain a reasonable level of $\Delta T\text{rot} \leq 2.0$ K if the SNR is not too low (SNR > 4). In comparison, $Intensity$ ratio-option (ii) has much larger $\Delta T\text{rot}$, and increases to $\pm 2.5$ K towards highest rms level (1.0 K). It indicates that the option (ii) would have large uncertainty if applied to very noisy spectra. Therefore, when using the $Intensity$ ratio method to derive $T\text{rot}$, one should first attempt to use option (i).

Figure 10c shows the average $\Delta T\text{rot}$ as a function of $\Delta V$. A notable feature is that $\Delta T\text{rot}$ becomes evidently deviated from the zero level over the $\Delta V$ range, in particular for $HF$ fitting and $Intensity$ ratio. And the three methods exhibit quite different variation trends. For $HF$ fitting, the value decreases to $\Delta T\text{rot} = -1.5$ K at $\Delta V = 2.9$ km s$^{-1}$. The $\Delta T\text{rot}$ deviation with $\Delta V$ should be mainly due to the change of HFC blending conditions. At small $\Delta V$, the internal HFCs within each group can be clearly resolved in the fitting. When $\Delta V$ becomes higher, the HFCs would gradually become blended. As a result, the line-profile fitting can only rely on overall morphology of each HFC group, the parameters would thus be less constrained.

The intensity ratio method, in contrast, exhibits a nearly opposite trend. It has relatively large deviation of $\Delta T\text{rot} = -1.7$ K at $\Delta V = 0.1$ to 0.5 km s$^{-1}$, and becomes converged within $\Delta T\text{rot} = \pm 0.5$ K at $\Delta V > 0.5$ km s$^{-1}$.
The $\Delta T_{\text{rot}}$ deviation at low $\Delta V$ is similar as that shown in Figure 3.

HFGR exhibits a smaller variation over the $\Delta V$ range. This is within our expectation since the effect of $\Delta V$ is already considered in its calculation (Fig. 3b). Its $\Delta T_{\text{rot}}$ slightly increases with a scale of 0.4 K only towards small $\Delta V$ ($\leq 0.2$ km s$^{-1}$). At larger values of $\Delta V > 0.5$ km s$^{-1}$, $\Delta T_{\text{rot}}$ stays in a narrow range of $-0.2$ to 0 K.

Figure 10d shows the calculation time $\Delta t_{\text{cal}}$ in the three methods. For each method, $\Delta t_{\text{cal}}$ is measured from an average of 100 times of calculations run in the same computer. The HFGR and Intensity ratio has comparable $\Delta t_{\text{cal}} = 1$ to $2 \times 10^{-4}$ seconds. HFGR has slightly higher $\Delta t_{\text{cal}}$ than the Intensity ratio because the HFGR contains several iterations to optimize $C_f$ (Figure 7). The HF fitting is much more time-consuming, with $\Delta t_{\text{cal}} = 3$–4 seconds, which is $10^4$ higher than the other two methods. This is because the HF fitting would traverse the large parameter space to look for the optimized parameters.

Figure 10d also shows a feature that for HF fitting, its $\Delta t_{\text{cal}}$ slightly increases towards the lowest SNR, while for Intensity ratio and HFGR, $\Delta t_{\text{cal}}$ appears to be constant throughout the SNR range. As an explanation, for Intensity ratio and HFGR, its $\Delta t_{\text{cal}}$ simply represents the time to run two or three analytical equations, thus would be clearly independent of the spectral noise. While HF fitting would be affected by spectral shape, thus would be slightly delayed if the spectral shape is largely disturbed by the rms noise.

As a short summary, in the comparison test, the HFGR shows a balanced advantage between efficiency and accuracy, and has a relatively stable performance over a broad range of $\delta V$ and SNR.

### 3.8 Comparison with the Dust Temperature and SED fitting

To further test the performance of HFGR, we applied it to the real observational data in OMC-2,3 region. This region contains compact and quiescent filament structures with moderate protostellar heating. The region is covered by both the NH$_3$ (1,1) (2,2) observations (Li et al. 2013) and the Herschel 70 to 500 $\mu$m continuum images (Arab et al. 2012; Lombardi et al. 2014). Sadavoy et al. (2016) measured the dust temperature ($T_{\text{dust}}$) distribution by fitting the Spectral Energy Distribution (SED) of the continuum emissions, allowing us to make a comparison between $T_{\text{dust}}$ and $T_{\text{rot(NH}_3)}$ estimated using HFGR.

Figure 11a show the NH$_3$ (1,1)-mg emission (contours) overlaid on the Herschel/SPIRE 250 $\mu$m image. We see that the dust and gas have similar spatial distributions. The NH$_3$ (1,1) and (2,2) spectra at FIR-6 are shown in Figure 12b. In this data set, the (1,1)-osg component is
not included in the observed frequency range. But one can still derive the total intensity of the satellites from the isg component as
\[
\int T_{mb}^{isg+osg} dv = \frac{9}{5} \int T_{mb}^{isg} dv, \tag{18}
\]
wherein the 9/5 is the intrinsic strength ratio of these HFC groups (see Table 2.1). Because the isg and osg have comparable intensities, their observed $T_{mb}$ ratios would not largely vary with the optical depth.

The $T_{dust}$ map in OMC-2 (Sadavoy et al. 2016) is shown in Figure 11d. The $T_{rot}(\text{NH}_3)$ maps derived from HFGR and HF fitting method are shown in Figure 11e and 11f, respectively. The three panels show comparable temperature distributions. They all exhibit an average level of 15 K over the entire region and increased value around 30 K at the dense core FIR-4.

For each method of $T_{rot}(\text{NH}_3)$, we examined its difference to the $T_{dust}$ distribution, as shown in Figure 12a and 12b. We see that HFGR and HF fitting both exhibit overall coherent distributions with $T_{dust}$, while the HF fitting tends to have systematically higher temperature values than $T_{dust}$. This difference is more clearly shown in Figure 12c. In this panel, the two methods exhibit sim-
Figure 11. (a) The NH$_3$ and dust continuum emissions of the Orion A OMC-2 region. The contours represent the integrated image of NH$_3$ (1, 1) mg components. The contour levels are 30, 50, 70, 90% of the peak value $0.45 \text{ Jy beam}^{-1} \text{ km s}^{-1}$. The color-scale image is the Herschel/SPIRE 250 μm continuum image in unit of Jy arcsec$^{-2}$. (b) The NH$_3$ and dust continuum emissions image of OMC-2 FIR-3,4,5 region. (c) The spectra of NH$_3$ (1,1),(2,2) lines at FIR-5. (d) The dust temperature of OMC-2 region. (e) The rotational temperature calculated by us using HFGR of OMC-2 region. (f) The rotational temperature calculated by Friesen et al. (2017) using HFC fitting of OMC-2 region.

Figure 12. $T_{\text{rot}}$ and $T_{\text{dust}}$ distribution for all the pixels with valid temperature estimate. The solid line is the linear fitting for the correlation that is $T_{\text{dust}} = 0.8 \times T_{\text{rot}}(\text{NH}_3) + 4.0$. The color scales of the data points represent their optical depth $\tau_0$. The temperature comparison of HFGR and HFC fitting with dust temperature of OMC-2 region pixel by pixel can prove that HFGR matches better than HF fitting in statistics.
ilar distributions, which are nearly symmetrical around $T_{\text{rot}} - T_{\text{dust}} = 0$ K, with a dispersion of $T_{\text{rot}} - T_{\text{dust}} = \pm 5$ K. This result suggests HFGR have a reliably derive $T_{\text{rot}}$ from the observed data. And the gas temperatures estimated from $T_{\text{rot}}$(NH$_3$) and $T_{\text{dust}}$ are reasonably consistent.

4 SUMMARY

In order to improve the accuracy and efficiency in calculating the gas temperature using NH$_3$, we build up a new recipe of using the hyperfine groups in NH$_3$ (1,1) and (2,2) inversion lines to derive $T_{\text{rot}}$. It is tested on the model spectra over a broad parameter space to guarantee the reliability. The python program for this calculation is provided freely$^1$. In building HFGR, we made three major efforts to improve the $T_{\text{rot}}$ calculation:

1. HFGR uses a group of empirical formulae (Equation 13 to 16) to derive $T_{\text{rot}}$. The equations only rely intensities of the HFC groups, thus the uncertainties related to the spectral profiles can be effectively prevented. HFGR can maintain an intrinsic uncertainty of $\Delta T_{\text{rot}} < 0.15$ K over a parameter space of $T_{\text{rot}} = 10$ to 70 K, $\Delta V = 0.5$ to 3.5 km s$^{-1}$, and $N$(NH$_3$) $< 2 \times 10^{15}$ cm$^{-2}$. In comparison, the two classic methods are both sensitive to the spectral shape, in particular the internal HFCs in each HFC group. The variation in $\Delta V$ would largely change the blending conditions of the HFCs and thereby affect the $T_{\text{rot}}$-accuracy in these methods.

2. As a comparison to HF fitting, the traversal over the parameters space is replaced by the empirical formulae in HFGR. A large amount of computational load is therefore reduced.

3. HFGR is further applied to the noisy spectra to estimate the relation between $T_{\text{rot}}$-uncertainty and the rms noise level. It shows that the uncertainty is maintained at the level of $\Delta T_{\text{rot}} \lesssim 1.0$ K (1 $\sigma$) when SNR $> 4$. The $T_{\text{rot}}$-rms relation is provided to directly estimate $\Delta T_{\text{rot}}$ when using HFGR, thereby to further reduce the human time.

HFGR is applied to the NH$_3$ lines observed in Orion A OMC-2,3 region. As a result, the derived $T_{\text{rot}}$ map exhibits a comparable result with the dust temperature, with a symmetrical distribution over the range of $T_{\text{dust}} - T_{\text{rot}} = \pm 5$ K. A comparable result is given by HF fitting. It suggests that HFGR can achieve an unbiased temperature measurement with the observed data.

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DATA AVAILABILITY

All the python codes are publicly available this web site: https://github.com/Workaholicws/AmmoniaProgram

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