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The excitation of NH₂ in the interstellar medium

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ABSTRACT

Accurate estimation of the abundance of the NH₂ radical in the interstellar medium requires accurate radiative and collisional rate coefficients. The calculation of hyperfine-resolved rate coefficients for the collisional (de-)excitation of NH₂ by both ortho- and para-H₂ are presented in this work. Hyperfine-resolved rate coefficients are calculated from pure rotational close-coupling rate coefficients using the M_j randomizing approximation. Rate coefficients for temperatures ranging from 5 to 150 K were computed for all hyperfine transitions among the first 15 rotational energy levels of both ortho- and para-NH₂ in collisions with ortho- and para- H₂. The new data were then employed in radiative transfer calculations to simulate the excitation of NH₂ in typical star-forming regions such as W31C. We compared the excitation and brightness temperatures for different NH₂ transitions obtained using the new and the previously available collisional data. It is found that the new rate coefficients increase the simulated line intensities. As a consequence, NH₂ abundance derived from the observations will be significantly reduced by the use of the present rate coefficients.

Key words: Molecular data - Molecular processes - radiative transfer - scattering.

1 INTRODUCTION

Observations of nitrogen hydrides are crucial to constrain the nitrogen chemistry in space since they are at the root of the nitrogen chemical network. Among nitrogen hydrides, NH₂ radical is one of the key molecules to understand such chemistry. Indeed, NH₂ is a light and floppy molecule thought to be an important reactant intermediate in the production/destruction of nitrogen-bearing molecules such as ammonia (NH₃).

Interstellar NH₂ was first detected by van Dishoeck et al. (1993) in absorption towards Sgr B2. Further, absorption lines of NH₂ were observed through the use of the long-wavelength spectrometer aboard ISO (Cernicharo et al. 2000; Goicoechea et al. 2004; Polehampton et al. 2007). More recently, the Herschel Space Observatory (Pilbratt et al. 2010) with the Heterodyne Instrument for the Far-Infrared (HIFI, De Graauw et al. 2010) offered the possibility to observe the ground-state rotational transitions with resolved hyperfine structure of NH₂. NH₂ is also well known in comets (Magee-Sauer et al. 1989; Swings et al. 1943), and have been observed in stellar photospheres via its electronic, vibration-rotation, and high rotational transitions.

Moreover, NH₂ exhibit spin symmetry states whose relative abundances are sensitive to the H₂ ortho-to-para ratio

(OPR) in the gas phase. NH₂ observations may then also be able to put constraints on the H₂ OPR in dense gas.

The absorption lines detected were employed to derive NH:NH₂:NH₃ abundance ratios of $\sim 2:1:1$ in lukewarm diffuse clouds (Persson et al. 2010) and $\sim 3:1:20$ in the cold envelope of low-mass protostars (Le Gal et al. 2014). Emission lines were also detected more recently in denser and hotter interstellar regions (Persson et al. 2016). Anomalous (i.e. non statistical) ortho-to-para ratios of NH₂ and NH₃ were derived in the diffuse gas (Persson et al. 2012; Persson et al. 2016). These ratios were however successfully reproduced by gas-phase models including a rigorous nuclear-spin chemistry (Faure et al. 2013; Le Gal et al. 2014), suggesting that NH₂, just like NH₃, is mainly formed in the gas-phase *via* a series of successive hydrogen abstraction $\text{NH}_n^+ + \text{H}_2$ ($n = 0 - 3$) reactions followed by electronic dissociation recombination. A recent work has also emphasized the importance of the H-exchange reaction $\text{NH}_2 + \text{H}$ in the ortho-para conversion of NH₂ (Le Gal et al. 2016).

Due to the low density of the interstellar medium (ISM) ($\simeq 10^2 - 10^6$ cm³), the energy levels of the NH₂ molecule are expected to be out local thermodynamical equilibrium (LTE). Hence, deriving NH₂ abundance from absorption and emission spectral lines requires excitation calculations that include collisional rate coefficients for transitions between the molecular energy levels induced by the most abundant ISM species, such H₂. As no collisional data were available

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for the NH₂ molecule and in order to perform non-LTE analysis of the NH₂ observations, [Persson et al. \(2016\)](#) crudely estimated rate coefficients assuming a quenching rate coefficient of $5 \times 10\text{--}11 \text{ cm}^3 \text{ s}^{-1}$ and state-specific downward rate coefficients for radiatively allowed transitions that scale in proportion to radiative line strengths.

However, it has been shown that the degree of excitation of molecules depends crucially on the set of collisional rate coefficients used ([Roueff & Lique 2013](#)). Consequently, inaccurate rates may induce important errors in the determination of the molecular abundance in molecular clouds. Hence, considering the sensitivity of the radiative transfer models to the collisional rate coefficients, it is very important to provide accurate values for the NH₂ collisional rate coefficients.

Recently, we presented quantum close-coupling calculations for the pure rotational excitation of NH₂ due to collisions with H₂ molecules ([Bouhafs et al. 2017](#), hereafter Paper I). The calculations were based on a recent, high-accuracy full-dimensional NH₄ potential energy surface (PES) adapted for rigid-rotor scattering calculations. Collisional cross sections were obtained for all transitions among the first 15 energy levels of both ortho- and para-NH₂ and for total energies up to 1500 cm^{-1} .

In this paper, we generate the first realistic set of rate coefficients of NH₂ in collisions with H₂ from the collisional cross sections of Paper I. Hyperfine-resolved rate coefficients are calculated from pure rotational close-coupling rate coefficients using the M_j randomizing approximation for temperatures ranging from 5 to 150 K.

The paper is organized as follows. In Section 2, we briefly present theoretical approach used to generate the collisional data. Section 3 presents rate coefficients for selected rotational and hyperfine-resolved transitions in NH₂ induced by collisions with ortho- and para-H₂. Finally, section 4 is devoted to an astrophysical applications and the conclusions of this work are drawn in Section 5.

2 METHODS

The scattering calculations are based on a five-dimensional (5D) PES determined from the nine-dimensional global PES of NH₄ ([Li & Guo 2014](#)). Ab initio calculations for the NH₂-H₂ complex in its ground electronic state were carried out at the explicitly correlated coupled cluster with single, double, and perturbative triple excitations [UCCSD(T)-F12a] ([Knizia et al. 2009](#)) level of theory with augmented correlation-consistent polarized valence- triple- ζ (aug-cc-pVTZ) basis set ([Dunning Jr 1989](#); [Kendall et al. 1992](#)). The collision partners were considered as rigid with geometries corresponding to the ground vibrational state. We refer the reader to [Li & Guo \(2014\)](#) and Paper I for more details about the PES.

In order to solve the close-coupling equations for scattering, the PES was expanded over angular functions using the expression ([Phillips et al. 1994](#)) :

$$V(R, \theta, \varphi, \theta', \varphi') = \sum v_{p_1 q_1 p_2 p} t_{p_1 q_1 p_2 p}(\theta, \varphi, \theta', \varphi') \quad (1)$$

where $t_{p_1 q_1 p_2 p}(\theta, \varphi, \theta', \varphi')$ is formed from coupled spherical functions $Y_{li, mi}(\alpha, \beta)$ which are associated with the rotational angular momenta of NH₂ and H₂.

The global minimum of the 5D PES corresponds to the most stable configuration of the NH₂-H₂ complex so that H₂ is approaching the N atom of the NH₂ molecule along the C_{2v} axis with a depth of 213 cm^{-1} .

The rotational energy levels of NH₂ are labelled by three numbers: the angular momentum N_1 and the pseudo-quantum numbers k_a and k_c which correspond to the projection of N_1 along the axis of the least and greatest moments of inertia, respectively. Two forms (ortho- and para-NH₂) caused by the different relative orientations of the hydrogen nuclear spins exist. The para states correspond to $k_a + k_c$ odd and the ortho states to $k_a + k_c$ even.

The calculations of pure rotational cross sections (i.e. neglecting the fine and hyperfine structure) that will be used in this paper to generate the rotational and hyperfine rate coefficients were performed with the MOLSCAT program ([Hutson & Green 1994](#)) using the close-coupling approach ([Green 1975](#)) (Paper I). Calculations were carried out for total energies ranging from 32 to 1500 cm^{-1} . Transitions among both the 15 lowest levels of ortho-NH₂ and para-NH₂ were considered. The convergence of the cross-sections with respect to the propagation parameters and with the NH₂ and H₂ rotational basis has been discussed in details in Paper I.

Here, from the calculated rotational cross-sections, one can obtain the corresponding thermal rate coefficients at temperature T by an average over the collision energy (E_c):

$$k_{\beta \rightarrow \beta'}(T) = \left(\frac{8}{\pi \mu k_B^3 T^3} \right)^{\frac{1}{2}} \times \int_0^\infty \sigma_{\beta \rightarrow \beta'} E_c e^{-\frac{E_c}{k_B T}} dE_c \quad (2)$$

where $\sigma_{\beta \rightarrow \beta'}$ is the collisional cross section. $\beta \equiv N_1 \alpha, j_2$ and $\beta' \equiv N_1' \alpha', j_2'$, unprimed and primed quantum numbers label initial and final states of the molecules, j_2 is the rotational angular momenta of H₂, and α specifies the NH₂ quantum numbers (e.g. k_a, k_c). μ is the reduced mass of the system and k_B is the Boltzmann's constant. Calculations up to 1500 cm^{-1} allow determining rotation rate coefficients from 5 to 150 K. The fine/hyperfine structure of the molecule was then considered using a statistical weight approximation that is presented below.

The electronic ground state of NH₂ is 2B_1 with a net unpaired electronic spin of 1/2, Hence, each rotational level is split by spin-rotation interaction in a fine structure of two sublevels identified by the the total angular momentum J_1 with $J_1 = N_1 \pm S$ (where N_1 is the rotational angular momentum, and $S = 1/2$ is the electronic spin). As the nitrogen atoms possess a non-zero nuclear spin ($I_N = 1$), the fine structure levels are further split into hyperfine levels, due to the coupling between the nitrogen nuclear spin and the total angular momentum J_1 characterized by the quantum number F_1 ($F_1 = J_1 \pm I_N$, I_N being the nuclear spin of the first nitrogen atom). The ortho-transitions also have additional splitting due to the the coupling with the net proton spin identified by the quantum number F ($F = F_1 \pm I_H$, $I_H = I_{H_1} + I_{H_2}$ being the nuclear spin of the hydrogen atom).

Since NH₂ hyperfine resolved rate coefficients can be crucial in detailed models of radiative transfer and in order to obtain a first overview of the impact of collisional rates on the astrophysical models, we have estimated from

the rotational collision rates the hyperfine collision rates using the so-called M_j randomizing limit. It is a statistical weight approximation which assumes that the hyperfine de-excitation rate coefficients are proportional to the degeneracy of the final hyperfine level (here, $2F' + 1$) and completely independent of the initial hyperfine level. Then, the de-excitation rate coefficients between hyperfine structure levels ($K_{N_{1ka}kcJ_1F_1F \rightarrow N'_{1ka'kc'}J'_1F'_1F'}^{RAN}$) are related to the close-coupling rate coefficients between rotational structure levels as follows (Faure & Lique 2012):

$$K_{N_{1ka}kcJ_1F_1F \rightarrow N'_{1ka'kc'}J'_1F'_1F'}^{RAN} = \frac{(2F' + 1)}{(2I_H + 1)(2I_N + 1)(2S + 1)(2N'_1 + 1)} K_{N_{1ka}kc \rightarrow N'_{1ka'kc'}}^{CC(3)}$$

Where, $K_{N_{1ka}kc \rightarrow N'_{1ka'kc'}}^{CC}$ are the rotational rate coefficients.

$I_H = H_1 + H_2$ and I_N is the nuclear spin of the hydrogen and nitrogen atom, respectively.

As the pure elastic rate coefficients $K_{N_{1ka}kc \rightarrow N_{1ka}kc}^{CC}$ are one to two orders of magnitude larger than inelastic rate coefficients, the quasi-elastic rate coefficients are set to zero, in order to avoid an overvalue for these transitions. We note also that Eq. (1) guarantees that the summed hyperfine rate coefficients are identical to the coupled-channel pure rotational rate coefficients.

3 RESULTS

We have obtained the rotational rate coefficients of NH₂ in collision with both para-H₂ and ortho-H₂ for the first 15 rotational levels and temperatures between 5 and 150 K.

The variation with temperature of typical NH₂-H₂ de-excitation rate coefficients is presented in fig.1 for both para-H₂ and ortho-H₂. We can notice that the rate coefficients vary smoothly with the temperature especially at temperature higher than 50 K. We also observe that the rate coefficients are generally two to three times smaller for collisions with para-H₂ ($j_2 = 0$) than for collisions with ortho-H₂ ($j_2 = 1$). This trend was already observed for several interstellar species like HCl (Lanza et al. 2014), SO₂ (Cernicharo et al. 2011) or H₂O (Dubernet et al. 2006). Even if ortho-H₂ is significantly less abundant than para-H₂ ($j_2=0$) in the cold ISM, the magnitude of the ortho-H₂ rate coefficients makes that this collisional partner has to be included as soon as the ortho-to-para ratio (OPR) of H₂ is larger than 0.1.

We can observe that the rate coefficients decrease while ΔN_1 increase for both para- and ortho-NH₂ in collision with both para- and ortho-H₂. Although we can retrieve the predominance of the $\Delta N_1=1$ transitions over the $\Delta N_1=2$ ones, no rigorous selection rules are defined although transitions with $\Delta k_c = 0$ seem to be slightly favored (already found in Paper I).

Using the approximate M_j randomizing method described above, we have obtained inelastic rates coefficients for transitions between the first 249 hyperfine levels of ortho

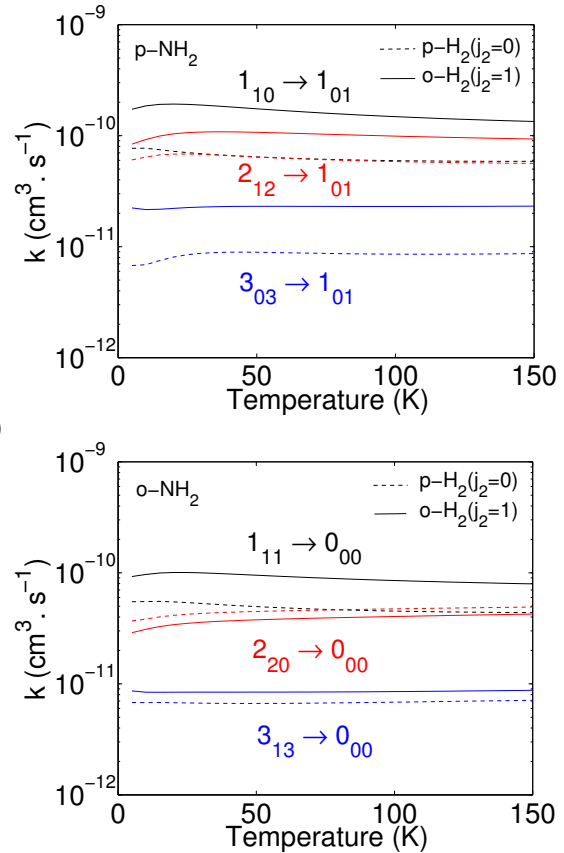


Figure 1. Typical rotational de-excitation rate coefficients of o- and p-NH₂ by H₂ ($j_2 = 0, 1$) as a function of temperature

and 88 first hyperfine levels for para-NH₂. The hyperfine-structure resolved rate coefficients display the same behavior than the rotationally inelastic rate coefficients. In particular, there is no temperature effect and the rate coefficients for collisions with para-H₂ and ortho-H₂ differ significantly, which was expected since the hyperfine de-excitation rate coefficients are proportional to the degeneracy of the final hyperfine state.

Therefore, the present results can be considered as a reasonable first estimate of collisional hyperfine rate coefficients, since the statistical method provide hyperfine resolved rate coefficients with an average accuracy, with respect to the memory and CPU cost of full recoupling calculations, and represents a suitable and low-cost alternative for this system. On the other hand, in terms of radiative transfer application, it should be noted that at moderate and high opacities, where the relative hyperfine populations can significantly depart from the statistical weights, the S-IOS method is notably better than the statistical approach (Faure & Lique 2012).

The complete set of (de-)excitation rate coefficients will be available online from the LAMDA (Schöier et al. 2005) and BASECOL (Dubernet et al. 2013) websites.

4 THE EXCITATION OF NH₂

As a first simple application, we have carried out radiative transfer calculations to simulate the excitation of NH₂ in interstellar molecular clouds. In particular, we focus on the physical conditions encountered in the massive star-forming region W31C that is a complex and extremely luminous sub-millimetre and infrared continuum source. The more highly excited ortho-lines are detected in emission from the hot cores, while the lowest ortho- and para-NH₂ lines at 953 and 1 444 GHz are in absorption and arise from the envelopes surrounding the hot cores.

Non-LTE calculations were performed with the RADEX code (Van der Tak et al. 2007) using the large velocity gradient (LVG) that simplifies the resolution of the statistical equilibrium equations by assuming that the velocity gradient is large enough to decouple the radiative transfer and the rotational level populations through the introduction of a photon escape probability.

Both collisional and radiative processes are taken into account. Einstein coefficients and frequencies were obtained from the Cologne Data base for Molecular Spectroscopy (Müller et al. 2005).

We include the cosmic microwave background radiation at 2.73 K and we assume a uniform spherical geometry of the cloud. A typical line width of 8.0 km s⁻¹ was considered.

We have chosen different kinetic temperatures (30 and 100 K) for the radiative transfer calculations. We varied the column density of ortho- and para-NH₂ from 10¹² to 10¹⁴ cm⁻² and we consider molecular hydrogen densities in a range from 10² to 10¹² cm⁻³.

In the radiative transfer calculations, we include all the energy levels for which both radiative and collisional data are available.

Figs. 2 displays the excitation temperatures (T_{ex}) and brightness temperatures (T_B) of the observed transition $N_{1ka kc J_1} = 1_{11}3/2$ as a function of molecular hydrogen density for temperatures of 30 and 100 K.

These hyperfine lines display classic behavior as a function of density. The excitation temperatures tend to be equal to the adopted value of background radiation field (2.73 K) at very low volume densities of molecular hydrogen. The excitation temperatures increase to higher values with increasing H₂ density, and hence the rate of collisional excitation. At densities greater than a critical value, where the rates of photon and collisional excitation become equal, the excitation temperatures approach the kinetic temperature, and then the LTE approximation becomes valid.

We have also found that the column density has almost no impact on the magnitude of the excitation temperature. In fact, the three curves cannot be distinguished in the plots. This can be explained by the fact that NH₂ lines are optically thin for the physical conditions considered in this work. At low temperatures (~ 30 K), the critical density lies at $\approx 10^8 - 10^9$ cm⁻³, while for higher temperatures, the critical density is slightly larger (up to a factor of 2).

Since the rate coefficients do not vary strongly with temperature, the critical densities are relatively independent of the temperature. These critical densities are considerably greater than typical densities in the interstellar medium. Hence, we expect that the NH₂ lines are not thermalized, and hence a non-LTE analysis is required even for analysis

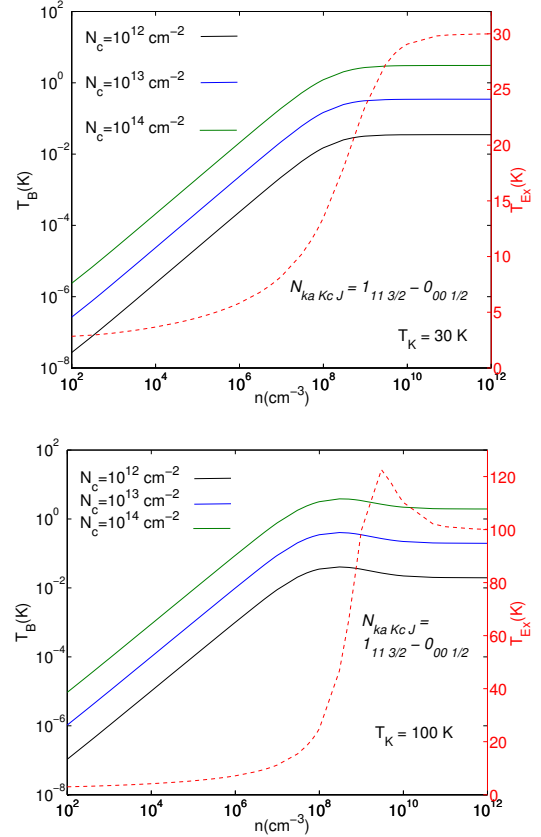


Figure 2. Excitation temperature (T_{ex} , dashed lines), brightness temperature (T_B , solid lines) for the lines of NH₂. The H₂ volume density varies between 10² and 10¹² cm⁻³ and the NH₂ column density from 10¹² to 10¹⁴ cm⁻² by a step factor of 10. The linewidth is 8 km s⁻¹.

of absorption spectra, as it was shown in the previous analysis of NH absorption lines in the pre-stellar core 16293N in L1689N (Bacmann et al. 2016). Figs 2 also show the brightness temperatures of the ortho-NH₂ lines as a function of molecular hydrogen density. T_B increases gradually with the density before being constant at around $n(\text{H}_2) = 10^7 - 10^8$ cm⁻³ when LTE conditions are reached. Effect of suprathermal excitation is also seen at $T_{kin} = 100$ K. This effect is due to the selection rules of the radiative and collisional transitions that will overpopulate one level with respect to another lower level and thus cause a sudden increase of the excitation temperature.

The two nuclear spin symmetries of NH₂ have been observed towards the high-mass star-forming regions W31C using the *Herschel*-HIFI instrument (Persson et al. 2016). They detected three transitions with fine and hyperfine structure resolved of ortho-NH₂ ($N_{1ka kc J_1} : 2_{11}3/2 \rightarrow 2_{02}3/2, 2_{02}5/2 \rightarrow 1_{11}3/2, 4_{22}9/2 \rightarrow 4_{13}9/2, 1_{11}3/2 \rightarrow 0_{00}1/2$) and one of para-NH₂ ($2_{12}5/2 \rightarrow 1_{01}3/2$).

Persson et al. (2016) modeled the emission line profiles using collision rates of NH₂-H₂ estimated from an assumed quenching rate coefficient of 5×10^{-11} cm³s⁻¹ and state-specific downward rates for radiatively allowed transitions that scale in proportion to radiative line strengths.

We were interested in the impact of the above approximate collisional rates on the excitation temperatures and

peak intensity of NH₂ hyperfine transitions, we have performed non-LTE radiative transfer calculations with the two sets of rate coefficients, namely the assumed data of Persson et al. (2016) and the present data.

From the observed spectra of W31C, we fix the basic parameters on which depend the LVG computation: the density of the collider H₂ = 10⁷ cm⁻³ (with an OPR = 1), the kinetic temperature is kept fixed at 80 K (typical of hot core molecular clouds) and the column density of o-NH₂ = 2 10¹⁴ cm⁻². The line width being set to 8 km s⁻¹.

Table 1 presents excitation temperatures (T_{ex}) of the hyperfine lines associated with different NH₂ rotational lines, computed with the present set of NH₂-H₂ and the earlier NH₂-H₂ rate coefficients of Persson et al. (2016).

In all cases, the excitation temperatures are greater than that of the CMB. Thus, these lines should be seen in emission, in agreement with the observations (Persson et al. 2016). All the lines are found to be optically thin.

It can be observed that the excitation temperatures and peak intensity based on the present rates are increased up to a factor of 30 with respect to those based on the assumed rates of Persson et al. (2016). These results clearly reflect the differences between the corresponding rates and highlight the importance of using computed NH₂-H₂ rate coefficients.

We conclude that the present rates will significantly improve the accuracy of the NH₂ abundances and H₂ densities derived from the observations and changes significantly the conclusions about the physical conditions in molecular clouds.

5 CONCLUSION

We have reported in this paper rate coefficients for the rotational excitation of ortho-, para-NH₂ by ortho- and para-H₂. The lowest 15 rotational levels of ortho-, para-NH₂ were included and kinetic temperatures up to 150 K were considered. Hyperfine resolved rate coefficients were also deduced using the M_j randomizing approximation. These calculations employed the PES for the interaction of NH₂ with H₂ computed by Li & Guo (2014) using the [UCCSD(T)-F12a] coupled-cluster method.

In order to evaluate the effect of these new data on the astrophysical modelling, we have performed radiative transfer calculations corresponding to typical physical conditions of the ISM where NH₂ emissions are detected. The simulated brightness temperatures obtained with our new rate coefficients are significantly larger than the ones obtained with previous rate coefficients assumed by Persson et al. (2016). The new rates lead to an increase by a factor of 1030 of the brightness temperatures, the NH₂ abundance derived from the observations will be substantially smaller than the current estimates.

It would be useful to re-analyze the astronomical observations of NH₂ rotational intensities to deduce the physical conditions in interstellar molecular clouds. A more complete treatment is now possible due to the availability of accurate NH₂-H₂ rate coefficients to model all detected lines, in absorption and emission, in order to improve the determination of the abundances and the physical conditions.

REFERENCES

- Bacmann A., et al., 2016, *Astronomy & Astrophysics*, 587, A26
 Bouhafs N., Lique F., Faure A., Bacmann A., Li J., Guo H., 2017, *The Journal of Chemical Physics*, 146, 064309
 Cernicharo J., Goicoechea J. R., Caux E., 2000, *The Astrophysical Journal Letters*, 534, L199
 Cernicharo J., et al., 2011, *Astronomy & Astrophysics*, 531, A103
 De Graauw T., et al., 2010, *Astronomy & Astrophysics*, 518, L6
 Dubernet M.-L., et al., 2006, *Astronomy & Astrophysics*, 460, 323
 Dubernet M.-L., et al., 2013, *Astronomy & Astrophysics*, 553, A50
 Dunning Jr T. H., 1989, *The Journal of chemical physics*, 90, 1007
 Faure A., Lique F., 2012, *Monthly Notices of the Royal Astronomical Society*, 425, 740
 Faure A., Hily-Blant P., Le Gal R., Rist C., Des Forêts G. P., 2013, *The Astrophysical Journal Letters*, 770, L2
 Goicoechea J. R., Rodríguez-Fernández N. J., Cernicharo J., 2004, *The Astrophysical Journal*, 600, 214
 Green S., 1975, *J. Chem. Phys.*, 62, 2271
 Hutson J. M., Green S., 1994
 Kendall R. A., Dunning Jr T. H., Harrison R. J., 1992, *The Journal of chemical physics*, 96, 6796
 Knizia G., Adler T. B., Werner H.-J., 2009, *The Journal of Chemical Physics*, 130, 054104
 Lanza M., Kalugina Y., Wiesenfeld L., Lique F., 2014, *The Journal of chemical physics*, 140, 064316
 Le Gal R., Hily-Blant P., Faure A., des Forêts G. P., Rist C., Maret S., 2014, *Astronomy & Astrophysics*, 562, A83
 Le Gal R., Herbst E., Xie C., Li A., Guo H., 2016, *Astronomy & Astrophysics*, 596, A35
 Li J., Guo H., 2014, *Physical Chemistry Chemical Physics*, 16, 6753
 Magee-Sauer K., Scherb F., Roesler F., Harlander J., Lutz B. L., 1989, *Icarus*, 82, 50
 Müller H. S., Schlöder F., Stutzki J., Winnewisser G., 2005, *Journal of Molecular Structure*, 742, 215
 Persson C. M., Black J. ., Cernicharo J., others. 2010, *Astronomy and Astrophysics*, 521, L45
 Persson C. M., et al., 2012, *Astronomy & Astrophysics*, 543, A145
 Persson C. M., et al., 2016, *A&A*, 586, A128
 Phillips T. R., Maluendes S., McLean A., Green S., 1994, *The Journal of chemical physics*, 101, 5824
 Pilbratt G., et al., 2010, *Astronomy & Astrophysics*, 518, L1
 Polehampton E. T., Baluteau J.-P., Swinyard B. M., Goicoechea J. R., Brown J. M., White G. J., Cernicharo J., Grundy T. W., 2007, *Monthly Notices of the Royal Astronomical Society*, 377, 1122
 Roueff E., Lique F., 2013, *Chemical reviews*, 113, 8906
 Schöier F. L., van der Tak F. F., van Dishoeck E. F., Black J. H., 2005, *Astronomy & Astrophysics*, 432, 369
 Swings P., McKellar A., Minkowski R., 1943, *Astrophysical Journal*, 98, 142
 Van der Tak F., Black J. H., Schöier F., Jansen D., van Dishoeck E. F., 2007, *Astronomy & Astrophysics*, 468, 627
 van Dishoeck E. F., Jansen D. J., Schilke P., Phillips T., et al., 1993

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W31C						
	present work		Persson et al.(2016)			
$N_{kakc}J_1F_1F \rightarrow N'_{ka'kc'}J'_1F'_1F'$	T_{ex} (K)	T_{b_1} (K)	T_{ex} (K)	T_{b_2} (K)	T_{b_1}/T_{b_2}	
$2_{11} 3/2 5/2 7/2 \rightarrow 2_{02} 3/2 5/2 7/2$	26.60	1.32E-01	13.13	3.99E-03	33.07	
$2_{11} 3/2 5/2 5/2 \rightarrow 2_{02} 3/2 5/2 5/2$	27.40	5.53E-02	12.94	1.83E-03	30.30	
$2_{11} 3/2 5/2 5/2 \rightarrow 2_{02} 3/2 5/2 5/2$	31.70	2.64E-02	12.80	8.73E-04	30.25	
$2_{11} 3/2 3/2 5/2 \rightarrow 2_{02} 3/2 3/2 5/2$	28.80	7.30E-02	13.35	2.43E-03	30.02	
$2_{11} 3/2 1/2 3/2 \rightarrow 2_{02} 3/2 1/2 3/2$	32.90	5.18E-02	13.15	2.09E-03	24.75	
$2_{02} 5/2 7/2 9/2 \rightarrow 1_{11} 3/2 5/2 7/2$	29.90	4.46E-01	15.40	4.19E-02	10.64	
$2_{02} 5/2 5/2 7/2 \rightarrow 1_{11} 5/2 3/2 5/2$	43.50	3.10E-01	15.30	3.40E-02	9.12	
$2_{02} 5/2 3/2 5/2 \rightarrow 1_{11} 3/2 1/2 3/2$	47.40	2.33E-01	14.97	3.53E-02	6.60	

Table 1. Comparison between excitation temperature and peak intensity for different ortho-NH₂ observed transitions obtained with the assumed collisional rates of [Persson et al. \(2016\)](#) and those computed in this work.