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Ammonia molecule and its applications in astrophysics

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Recently a new ammonia line list BYTe was reported comprising more than 1.1 billion transitions and designed for temperatures up to 1500 K. In this study we present an application of this line list for modelling spectra of cool star. We generated oscillator strengths of NH_3 using BYTe for a frequency range of 1–5 μm and applied it for computing synthetic spectra of cool carbon giants using the `WITA` program. A possibility of detection of ammonia in spectra of cool carbon giants is discussed.

Key words: molecular data; stars: atmospheres; stars: late-type

INTRODUCTION

A determination of chemical and physical properties of different astrophysical objects requires reliable molecular and atomic data for the important absorbers present in their environment. From an astrophysical perspective, satisfactory ammonia line lists are needed to accurately model the atmospheres of the Earth, late brown dwarfs, carbon stars, exoplanets, and other environments where ammonia can be thought as a significant source of opacity.

NH_3 is an important absorber present in the spectra of atmospheres of late T-type dwarfs, particularly in the 10.5 μm region [3, 13]. It has been found to exist in circumstellar envelopes of evolved stars [12], very young and low mass protostellar systems [15], in the atmospheres of solar system gas giant planets [4, 8], and also in comets. In cometary comae typical NH_3 number densities are $\sim$ 0.5% of that of gaseous H_2O [2, 7]. To-date, NH_3 has not been detected in atmospheres of extrasolar planets. However, theoretical investigations suggest the presence of ammonia in these objects [14].

There are a number of ammonia line lists available. One is the well-known HITRAN (high-resolution transmission molecular absorption database) [11]. It contains 27994 transitions covering the frequency range of 0–5295 cm^{-1}. Another experimental ammonia line list is of Irwin et al. [6] (1999) covering the 4000–11000 cm^{-1} spectral region but it is only suitable for use at temperatures below 300 K. Hargreaves et al. [5] recently reported a set of new experimental line lists for NH_3 obtained by recording Fourier transform infrared emission spectra for twelve temperatures between 300 and 1370 °C. They cover the frequency range from 740 to 2100 cm^{-1}.

The most complete theoretical NH_3 line list is BYTe (Barber-Yurchenko-Tennyson), which was created recently [16] at University College London (UCL). This 'hot' line list is able to be used for high resolution astronomical applications up to 1500 K. It comprises 1.1 billion transitions at wavelengths longer than 0.9 microns. The previous 'cool' NH_3 list reported by these authors [17] was accurate up to 300 K.

In this paper we apply BYTe in conjunction with the `WITA` program [9] for modelling synthetic spectra of cool astronomical objects.

THE OSCILLATOR STRENGTHS

The BYTe line list contains the transition probabilities of NH_3 in the form of Einstein coefficients A [1/s]. In order to make this line list compatible with the program `WITA` we generated corresponding oscillator strengths (gf) as follows [1]:

$$g_1 f_{12} = 1.499 \times 10^{-8}\, g_2\, A_{21}\, \lambda_{12}^2, \qquad (1)$$

where A_{21} is the Einstein coefficient of transition between states 1 and 2, λ_{12} is the wavelength of the transition ($1 \to 2$) in μm. The statistical weights of the state i is given by

$$g_i = g_{\rm ns}(2J+1), \qquad (2)$$

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where $g_{\rm ns}$ is the nuclear spin statistical weight factor and J is the total angular momentum quantum number. In case of $^{14}NH_3$ $g_{\rm ns}$ is defined as follows [16]: $g_{\rm ns} = 0$ for A_1' and A_1''; $g_{\rm ns} = 12$ for A_2' and A_2''; $g_{\rm ns} = 6$ for E' and E'', where A_1', A_1'', A_2', A_2'', E', and E'' are the irreducible representations of the molecular symmetry group $D_{3h}(M)$, which NH_3 belongs to (for more details see [16]).

The partition functions for NH_3, also required as an input for `WITA`, is computed by:

$$Q = \sum g_i \exp[-E_i/kT], \tag{3}$$

where g_i is the statistical weight defined in (2), E_i is the energy of the ro-vibrational state i, k is the Boltzmann's constant and T is the temperature. The Q values obtained using the BYTe energy values E_i are in perfect agreement with the HITRAN partition functions. The partition functions calculated using (3) is then approximated by the polynomial:

$$Q = (a + bT + cT^2), \tag{4}$$

where a, b and c are expansion constants.

TRANSMISSION SPECTRUM

Our calculations assumed a single layer, constant temperature, constant density NH_3 model approximation for the upper atmosphere of the cool carbon star.

The absorption coefficient in the centre of absorption line can be written as [1]:

$$\sigma_\nu = \int_0^\infty \alpha_\nu d\nu = \frac{\pi e^2}{mc} f_{nm} N_n, \tag{5}$$

where e is the electron charge, m is the electron mass, f_{nm} is the oscillator strength of the transition from the lower level n to the upper level m, and N_n is the population of the level n given by:

$$N_n = g_n N_{\rm tot} \exp(-E_n/kT)/Q. \tag{6}$$

Here g_n is the statistical weight of the level n, $N_{\rm tot}$ is the total number density of NH_3, E_n is the energy of the level n, Q is the partition function given by (4). In (5) α_ν is the line absorption coefficient, which outside the line core is given by:

$$\alpha_\nu = \sigma_\nu \phi_{mn}(\nu), \tag{7}$$

where $\phi_{mn}(\nu)$ is the line profile function. Assuming the Doppler line broadening $\phi_{mn}(\nu)$ is given by the Gaussian line profile:

$$\phi_{mn}(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} \exp\left[-\left(\frac{\nu - \nu_l}{\Delta\nu_D}\right)^2\right], \tag{8}$$

where $\Delta\nu_D = V_0\nu_0/c$ is the Doppler line width and ν_l is the frequency of the line centre. Taking into account the microturbulent gas motion and the Maxwell distribution, V_0 can be written as follows:

$$V_0^2 = \frac{2RT}{m} + V_{\rm turb}^2, \tag{9}$$

where R is the gas constant, m is the mass of the molecule, $V_{\rm turb}$ is the microturbulent gas motion velocity. In our model we assume $V_{\rm turb} = 2$ km/s. The transmission spectrum is then obtained as:

$$I_\nu = I_\nu^0 \exp(-\alpha L), \tag{10}$$

where I_ν^0 is the incoming light intensity (we adopt $I_\nu^=01$) and L is the light path (we adopt $L = 1$). The transition spectra of NH_3 were computed utilizing both the BYTe and HITRAN line lists for $T = 300$ K and $N_{tot} = 10^9$. The lines with $gf < 10^{-6}$ were rejected in both cases. The resulting synthetic spectra are shown on Fig. 1. It can be seen clearly that the BYTe list provides significantly more lines than HITRAN.

CARBON GIANT SYNTHETIC SPECTRA

To calculate the synthetic spectra of the carbon giant we used the procedure described in [10]. Apart from the NH_3 molecule our computational list of species includes C_2, CN, CS, HCN. We calculated two synthetic spectra of the cool carbon giant with $T_{eff} = 2000$ K, (i) with ammonia, utilizing the NH_3 equilibrium constants generated from the BYTe line list, and (ii) without it. The ratio of the corresponding computed fluxes is shown on Fig. 2. This figure demonstrates that the spectra of cool carbon giants will exhibit significant NH_3 absorption bands near 1.5 μm, 2 μm, 2.3 μm and 2.8–3.0 μm regions.

CONCLUSIONS

In this work we have applied the recently generated ammonia line list BYTe [16] for modelling spectra of cool astrophysical objects. We demonstrate that the NH_3 absorption bands will occur in the spectra of cool carbon giants near the 1.5 μm, 2 μm, 2.3 μm and 2.8–3.0 μm regions. The results of this work can also find application in studies of the atmosphere of the Earth, cool dwarfs, carbon stars, exoplanets, and other astrophysical objects.

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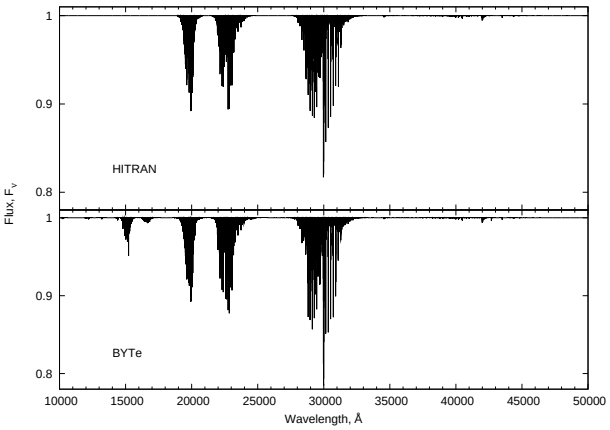

Fig. 1: Transmission spectra computed using BYTe line list and the line list from HITRAN for $T = 300$ K, $N_{tot} = 10^9$

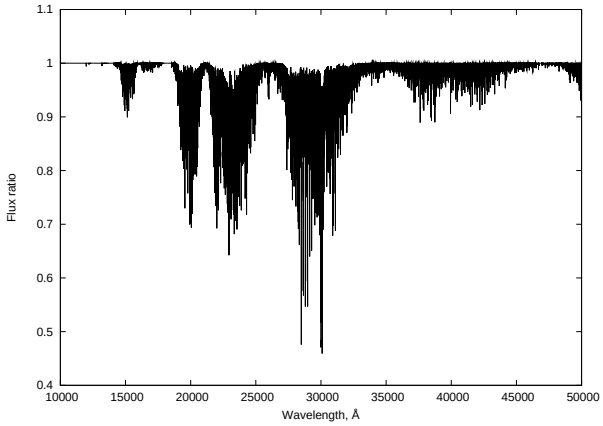

Fig. 2: The flux ratio of the carbon star spectrum with and without the NH_3 absorption considered.

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