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Vinyl cyanide (CH_2CHCN) in interstellar space: potential spectral lines for its detection

Mohit K. Sharma *

Amity Centre for Astronomy & Astrophysics, Amity Institute of Applied Sciences, Amity University, Sector 125, Noida 201313, U.P., India

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ABSTRACT

Vinyl cyanide is a molecule having planar geometry with electric dipole moment components, $\mu_a = 3.821$ D and $\mu_b = 0.687$ D. Thus, a-type transitions are very strong as compared to b-type transitions, and are considered in this investigation. The rotational levels for a-type transitions, may be divided into two distinct groups: one group having odd values of k_a and the other having even values of k_a. Using the known values of rotational and centrifugal distortion constant along with the electric dipole moment μ_a, we have calculated energies of lower 120 rotational levels, having energy up to 92 cm^{-1}, for each group, and the probabilities for radiative transitions between the levels. These radiative transition probabilities in conjunction with the scaled values of collisional rate coefficients are used in the Sobolev Large Velocity Gradient analysis. Out of a large number of lines, we have selected the strongest ones. In the low lying levels, besides the 4 observed lines of CH_2CHCN, we have discussed about 8 additional transitions, of which 2 showing the phenomenon of anomalous absorption and 6 showing emission feature are found. These lines may play important role for the search of vinyl cyanide in a cosmic object.

1. Introduction

Vinyl cyanide (CH_2CHCN), also known as the acrylonitrile or propenenitrile, may be the best candidate for the formation of cell-like membranes in Titan's hydrocarbon-rich lakes and seas [1]. Lai et al. [2] have performed the first spatial distribution mapping of CH_2CHCN in the atmosphere of Titan with the help of ALMA. Along with C_2H_5CN, HC_3N and CH_3CN, the new maps of CH_2CHCN has been spatially resolved on Titan and their abundances are derived using the radiative transfer modeling.

Outside the solar system, it is discovered towards the galactic center in Sgr B2 by Gardner & Winnewisser [3] through its transition 2_{11}–2_{12} at 1.372 GHz, in dense dark cloud TMC-1 by Matthews & Sears [4] and in carbon-rich star IRC +10216 by Agundez et al. [5]. Lopez et al. [8] detected vinyl cyanide in Orion-KL with IRAM-30 m in the frequency range between 80–280 GHz in its ground and vibrationally excited states. Because of its importance, laboratory spectrum of CH_2CHCN is studied from time to time [6, 7, 8]. The rotational and centrifugal distortional constants derived by Lopez et al. [8] in I^r representation, with Watson A-reduction Hamiltonian are given in Table 1, and are used in the present investigation. Vinyl cyanide is a planar molecule whose components of electric dipole moment, $\mu_a = 3.815$ D and $\mu_b = 0.894$ D were obtained by Stolze & Sutter [9] which are modified to be $\mu_a = 3.821$ D and $\mu_b = 0.687$ D by Krasnicki & Kisiel [10], showing that its a-type transitions are very strong as compared to the b-type transitions. Thus, in the present investigation, we have considered a-type transitions. The vinylcyanide may be produced by a reaction of propylene, ammonia and oxygen

$$CH_2 = CH\text{-}CH_3 + NH_3 + 1.5\ O_2 \longrightarrow CH_2 = CH - CN + 3H_2O \quad (1)$$

The rotational levels for a-type transitions, may be classified into two distinct groups: one group having odd values of k_a and the other having even values of k_a. There are no radiative as well as collisional transitions between the levels of these groups. Using the rotational and centrifugal distortion constants given in Table 1, and electric dipole moment μ_a, for each group, we have calculated energies of 120 lower rotational levels, having energy up to 92 cm^{-1}, and the Einstein coefficients for radiative transitions between the levels with the help of ASROT [11]. These radiative transition probabilities in conjunction with the scaled values of collisional rate coefficients are used for solving the statistical equilibrium equations coupled with the equations of radiative transfer.

* Corresponding author.
E-mail addresses: mohitkumarsharma32@yahoo.in, mksharma4@amity.edu.

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Table 1
Rotational and centrifugal distortion constants.

Constant	Value (MHz)	Constant	Value (MHz)
A	49850.69655	ϕ_K	3.7011×10^{-5}
B	4971.212565	L_J	-2.6315×10^{-14}
C	4513.828526	L_{JJK}	-1.077×10^{-12}
Δ_J	2.244058×10^{-3}	L_{JK}	4.279×10^{-10}
Δ_{JK}	-8.56209×10^{-2}	L_{KKJ}	1.2×10^{-11}
Δ_K	2.7154213	L_K	-6.141×10^{-8}
δ_J	4.566499×10^{-4}	l_J	-1.1602×10^{-14}
δ_K	2.44935×10^{-4}	l_{JK}	-9.56×10^{-13}
Φ_J	6.4338×10^{-6}	l_{KJ}	-1.436×10^{-10}
Φ_{JK}	-4.25×10^{-9}	l_K	8.91×10^{-9}
Φ_{KJ}	-7.7804×10^{-6}	P_{KJ}	-1.56×10^{-14}
Φ_K	3.84762×10^{-4}	P_{KKJ}	-1.977×10^{-13}
ϕ_J	2.36953×10^{-9}	P_K	8.67×10^{-12}
ϕ_{JK}	1.4283×10^{-7}		

In the low lying levels, besides the 4 observed lines of CH_2CHCN, we have discussed about 8 additional transitions, of which 2 are found to show anomalous absorption and 6 are found to show emission feature. These lines may play important role in the search of vinyl cyanide in a cosmic object. The transitions observed by Agundez et al. [5] are between higher levels, and 10 out of them are analyzed here.

2. Model

In the Sobolev Large Velocity Gradient (LVG) analysis, discussed in Sharma [16] and Sharma et al. [17], we have solved a set of statistical equilibrium equations coupled with the equations of radiative transfer. The required input data in the analysis are the radiative transition probability (Einstein A and B coefficients) discussed in section 2.2 and the collisional rate coefficients, discussed in section 2.3. The set of equations is solved through iterative method where initial population densities are taken as thermal ones.

2.1. Rotational levels

In a cosmic object where vinyl cyanide may be found, the kinetic temperature may be few tens of Kelvin, and thus, we are concerned with the rotational levels in the ground vibrational state and ground electronic state. For an asymmetric top molecule, $J_{k_ak_c}$ is the rotational level where J is the rotational quantum number, and k_a and k_c denotes the projections of J on the axis of symmetry in case of the prolate and oblate symmetric tops, respectively. These levels are connected through radiative as well as collisional transitions.

2.2. Radiative transitions

The electric dipole moment of vinyl cyanide has the components $\mu_a = 3.821$ Debye and $\mu_b = 0.687$ Debye, showing that its a-type transitions are much intense as compared to the b-types. In our calculations, we have considered only a-type transitions, governed by the selection rules:

$$J:\quad \Delta J = 0, \pm 1$$

$$k_a, k_c:\quad \text{odd, even} \longleftrightarrow \text{odd, odd} \qquad \text{(group I)}$$

$$\text{even, even} \longleftrightarrow \text{even, odd} \qquad \text{(group II)}$$

The levels in group I have odd value of k_a whereas in group II have even value of k_a. Between 120 levels, there are 393 and 405 radiative transitions, for the groups I and II, respectively. We have calculated radiative transition probabilities between the levels, using the rotational and centrifugal distortion constants given in Table 1, with the help of the software ASROT [11].

2.3. Collisional transitions

Besides the radiative transitions, the levels are connected through the collisional transitions due to collisions with the molecular hydrogen H_2, which is the most abundant in a molecular region. In the study of interstellar molecules, the calculation of collisional rate coefficients is the most difficult part [12, 13, 14] as collisional transitions do not follow any selection rules. The collisional rate coefficients for one direction (excitation or deexcitation) of the transitions has to be calculated, as the collisional rate coefficients for the reverse direction can be calculated with the help of the detailed equilibrium [15]. Collisional rate coefficients are not available for the vinyl cyanide. In absence of the collisional rate coefficients, the deexcitation rate coefficients for a kinetic temperature T are calculated following the procedure discussed by Sharma [16] and Sharma et al. [17].

2.4. Anomalous absorption

Anomalous absorption is an unusual phenomenon developed under some specific condition. The required condition for brightness temperature T_B of transition showing anomalous absorption is $0 < T_{ex} < T_B < T_{bg}$ (Sharma et al. [17]) where T_{ex} is the excitation temperature of transition and T_{bg} ($= 2.73$ K) is background temperature of Cosmic Microwave Background. The brightness temperature may be defined ass the temperature of a black body corresponding to the given intensity of radiation and is given by

$$T_B = \frac{h\nu}{k}\frac{1}{\ln[1 + 8\pi h\nu^3/Ic^3]} \tag{2}$$

where I is the intensity of radiation.

3. Results & discussion

For the kinetic temperature considered here, up to 50 K, 120 levels having energy up to 92 cm^{-1}, are sufficient for the LVG analysis. For each group of rotational levels, a set of 120 statistical equilibrium equations coupled with the respective equations of radiative transfer is solved with the help of iterative procedure, where the radiative transition probabilities and the collisional rate coefficients are used as input parameters. The iterative method is initiated with the thermal population densities of levels corresponding to the kinetic temperature in the region. In order to include a large number of cosmic objects, where the vinyl cyanide may be found, in the calculations, we have considered wide ranges of physical parameters. The molecular hydrogen density n_{H_2} is taken from 10^2 to 10^6 cm^{-3}; the kinetic temperatures T are 10, 20, 30, 40 and 50 K, values of $\gamma[= n_{mol}/(dv_r/dr)]$ are taken as 10^{-6} and 10^{-5} cm^{-3} $(km/s)^{-1}$ pc. Here n_{mol} denotes the density of vinyl cyanide, and dv_r/dr the velocity-gradient in the region. There are large number of emission and absorption lines, we have selected the strongest ones.

Fig. 1 shows the variation of brightness temperatures T_B (K) versus the molecular hydrogen density n_{H_2} for the kinetic temperatures of 10, 20, 30, 40 and 50 K for six transitions of group I. The vinyl cyanide was discovered by Gardner & Winnewisser [3] through its transition 2_{11}–2_{12} at 1.372 GHz in emission towards SgrB2. This transition, we have however found to show anomalous absorption. Two transitions 2_{12}–1_{11} at 18.513 GHz and 2_{11}–1_{10} at 19.427 GHz observed by Matthews & Sears [4] in the dense dark cloud TMC-1 are found to show emission feature. Other two lines 1_{10}–1_{11} at 0.457 GHz and 3_{12}–3_{13} at 2.744 GHz are found to shows anomalous absorption, one transition 3_{12}–2_{11} at 29.139 GHz is emission line.

In Fig. 2, we have given results for 6 lines of group II. All six transitions are found to show emission feature. The line 1_{01}–0_{00} at 9.485 GHz is found as intense as the line 2_{02}–1_{01} at 18.967 GHz observed by Matthews & Sears [4] in the dense dark cloud TMC-1. Other four lines, 3_{03}–2_{02} at 28.441 GHz, 3_{21}–2_{20} at 28.471 GHz, 3_{22}–2_{21} at 28.457 GHz, 4_{04}–3_{03} at 37.905 GHz are found with emission.

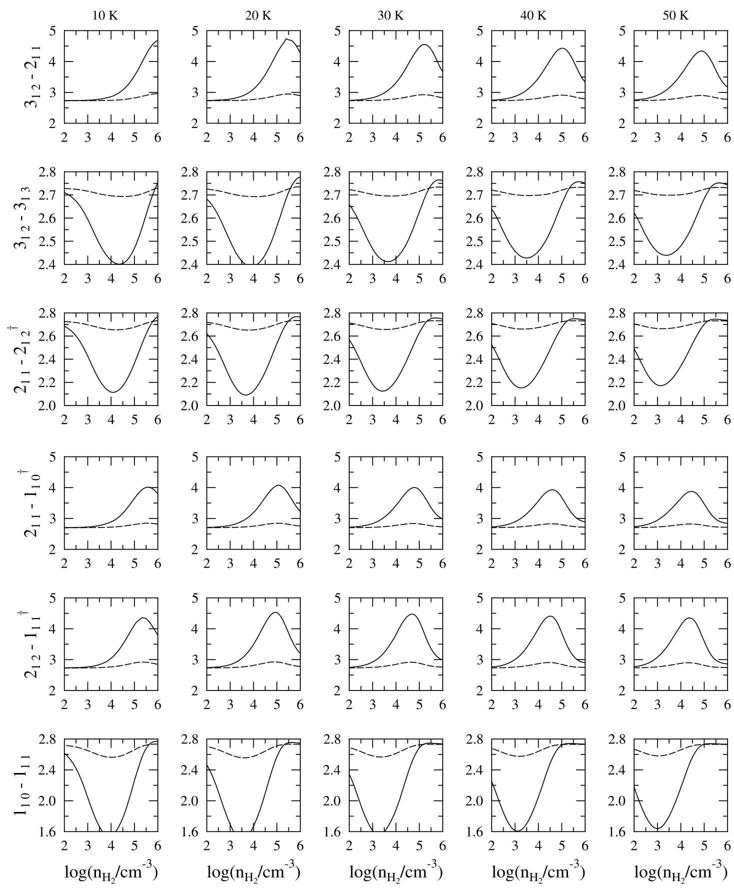

Fig. 1. Variation of brightness temperatures T_B (K) versus molecular hydrogen density n_{H_2} for kinetic temperatures of 10, 20, 30, 40 and 50 K, written at the top, for six transitions of group I, written on the left. Three transitions observed in a cosmic object are marked by the symbol †. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

Table 2
Frequency ν, A-coefficient A_{ul}, energy E_u of upper level, radiative life-time t_u of upper level and t_l of lower level for transitions.

Transitions	ν (GHz)	A_{ul} (s^{-1})	E_u (cm^{-1})	t_u (s)	t_l (s)
1_{10}–1_{11}	0.457	8.125E-12	1.827	1.23E+11	∞
2_{12}–$1^{\dagger}_{11}$	18.513	3.235E-07	2.429	3.09E+06	∞
2_{11}–$1^{\dagger}_{10}$	19.427	3.738E-07	2.475	2.67E+06	1.23E+11
2_{11}–$2^{\dagger}_{12}$	1.372	7.312E-11	2.475	2.67E+06	3.09E+06
3_{12}–3_{13}	2.744	2.925E-11	3.446	6.24E+05	7.22E+05
3_{12}–2_{11}	29.139	1.602E-06	3.446	6.24E+05	2.67E+06
1_{01}–0_{00}	9.485	4.834E-08	0.316	2.07D+07	∞
2_{02}–$1^{\dagger}_{01}$	18.967	4.638E-07	0.948	2.16D+06	2.07D+07
3_{03}–2_{02}	28.441	1.675E-06	1.896	5.97D+05	2.16D+06
3_{21}–2_{20}	28.471	9.338E-07	7.911	1.03D+06	7.35D+07
3_{22}–2_{21}	28.457	9.324E-07	7.910	1.04D+06	7.83D+07
4_{04}–3_{03}	37.905	4.113E-06	3.160	2.43D+05	5.97D+05

None of these lines is found to show any MASER action. With the increase of kinetic temperature, the strength of anomalous absorption is found to decrease and the position of trough is found to shift towards the low density. For the emission lines, the position of peak is found to shift towards the low density with the increase of kinetic temperature. Though the transitions 1_{10}–1_{11} and 1_{01}–0_{00} which are connecting the ground state in I and II groups are not detected in a cosmic object, but their probability for detection is quite good. These 8 transitions along with 4 observed, may play important role in the detection of vinyl cyanide in a cosmic object.

The frequency of transition, Einstein A-coefficient for the transition, energy of upper level, radiative life-times of upper and lower levels of the 12 transitions have been given in Table 2.

Out of the lines of CH_2CHCN detected by Agundez et al. [5] in the C-rich star IRC +10216, 5 lines group I are shown in Fig. 3 and lines group II are shown Fig. 4. All these lines are found to show emission feature. The intensities of lines are found to increase with the increase of kinetic temperature (Fig. 5).

Four lines $38_{1,38}$–$37_{1,37}$, $38_{0,38}$–$37_{0,37}$, $36_{2,34}$–$35_{2,33}$ and $37_{1,36}$–$36_{1,35}$ detected by Lai et al. [2] in the atmosphere of Titan lie at very high energy and are beyond the scope of our investigation.

4. Conclusions

We have solved a set of statistical equilibrium equations coupled with the equations of radiative transfer for two groups of rotational levels of CH_2CHCN. In the lower levels, besides the 4 observed lines, 8 lines are discussed. These lines may help in detection of vinyl cyanide in a cosmic object. In particular, the detection of lines connecting the ground state is highly probable.

Declarations

Author contribution statement

Mohit K. Sharma: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

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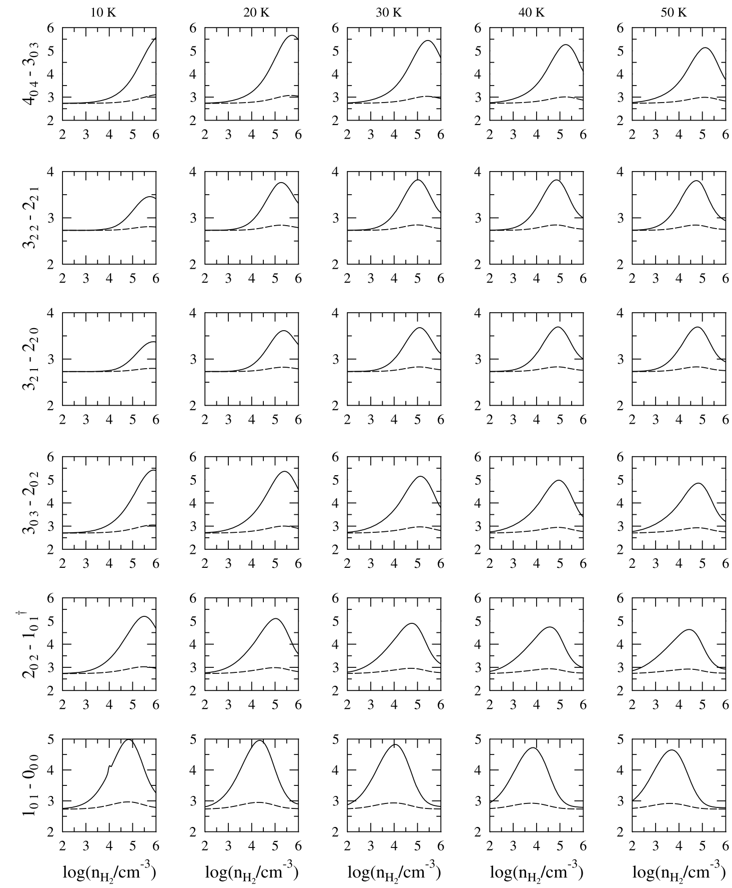

Fig. 2. Variation of brightness temperatures T_B (K) versus molecular hydrogen density n_{H_2} for kinetic temperatures of 10, 20, 30, 40 and 50 K, written at the top, for six transitions of group II, written on the left. One transitions observed in a cosmic object are marked by the symbol †. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

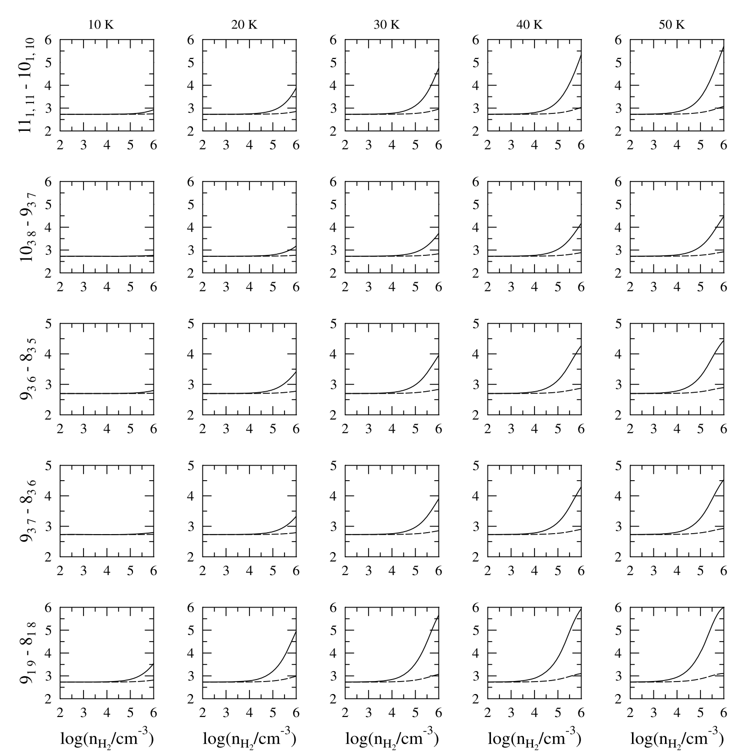

Fig. 3. Variation of brightness temperatures T_B (K) versus molecular hydrogen density n_{H_2} for kinetic temperatures of 10, 20, 30, 40 and 50 K, written at the top, for six transitions of group I, observed by Agundez et al. [5], written on the left. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

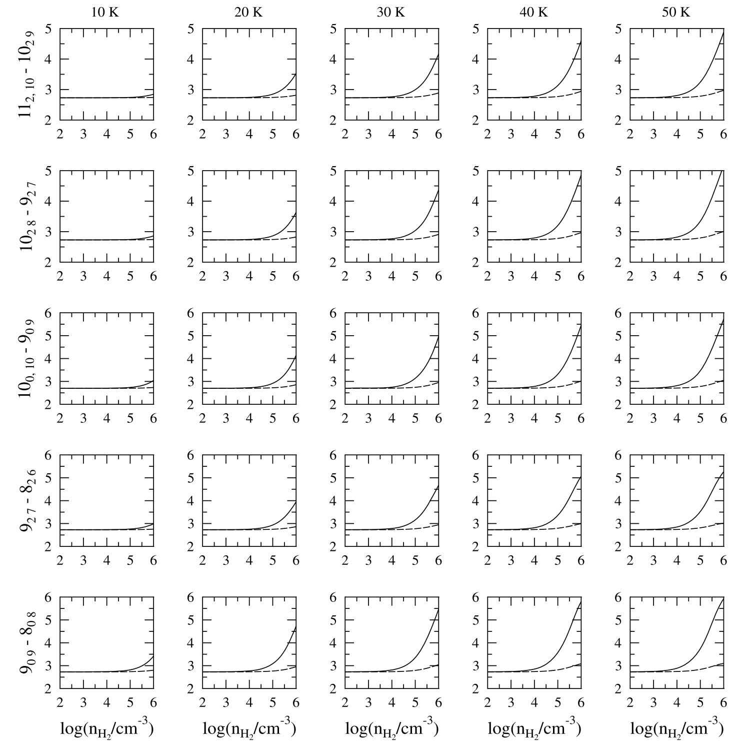

Fig. 4. Variation of brightness temperatures T_B (K) versus molecular hydrogen density n_{H_2} for kinetic temperatures of 10, 20, 30, 40 and 50 K, written at the top, for six transitions of group II, observed by Agundez et al. [5], written on the left. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

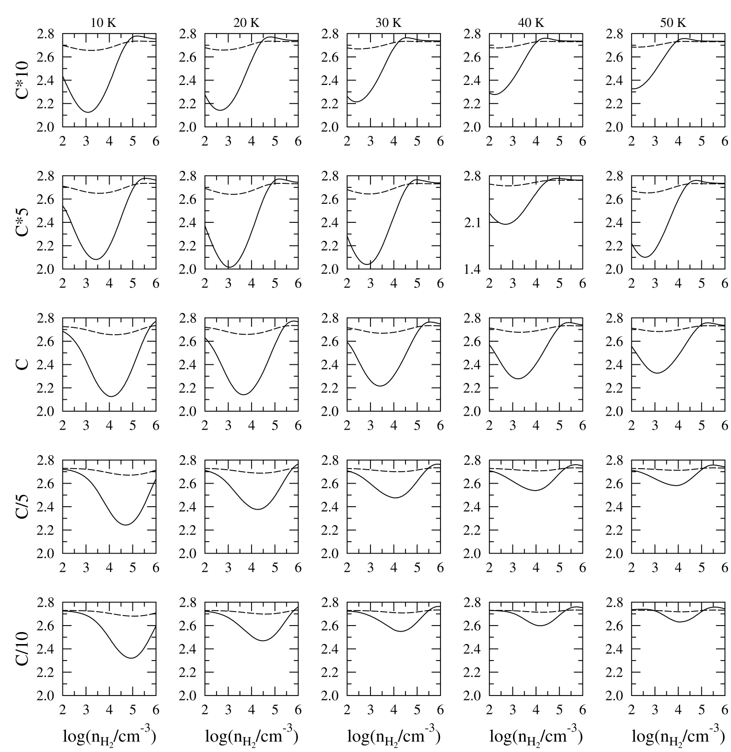

Fig. 5. Variation of brightness temperatures T_B (K) versus molecular hydrogen density n_{H_2} for kinetic temperatures of 10, 20, 30, 40 and 50 K, written at the top, for the transition $2_{11} - 2_{12}$ where collisional rate coefficients are multiplied and divided a factor 5 and 10 for the transitions with $\Delta k_a = 0$ besides the normal collisional rate coefficients. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-6}$ cm^{-3} (km/s)$^{-1}$ pc.

Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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