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Suggestions for an interstellar C_7H_2 search

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Abstract

Laboratory detection of the ring-chain molecule c-C_7H_2 has been reported by McCarthy et al. [McCarthy, M.C., Travers, M.J., Gottlieb, C.A., Thaddeus, P., 1997. A&A 483, L139]. Two ring-chain molecules c-C_3H_2 and c-C_5H_2 of this series have already been detected in the cosmic objects. We suggest that the c-C_7H_2 may be identified in cool cosmic objects through its transitions 4_{14}–5_{05}, 5_{15}–6_{06}, 6_{16}–7_{07} and 7_{17}–8_{08} at 23.241, 21.105, 18.953 and 16.787 GHz, respectively, in absorption against the CMB. Since, in absence of the availability of collisional rates, we have used scaled values for them, we have checked the sensitivity of the results on the collisional rates, by enhancing the rates for the transitions with $\Delta k_a = 0$ by a factor of 10. Though the transitions are not found sensitive to the collisional rates, our results still may be treated as qualitative in nature. These absorption lines may play an important role for identification of c-C_7H_2 in cool cosmic objects.

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Keywords: ISM; Molecules

1. Introduction

The 2_{20}–2_{11} transition of c-C_3H_2 at 21.587 GHz has been found in absorption against the CMB by Matthews et al. (1986) and Madden et al. (1989) in all the objects investigated, except the Planetary Nebula NGC 7027 where Cox et al. (1987) found this transition in emission. Two transitions 3_{13}–2_{12} and 3_{03}–2_{02} at 19.147 and 19.606 GHz, respectively, of c-C_5H_2 have been detected in TMC-1 by Dickens et al. (2001). Chandra and Shinde (2004) have proposed detection of 3_{13}–4_{04} transition at 4.314 GHz of c-C_5H_2 in absorption against the

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cosmic microwave background (CMB). After detection of c-C_3H_2 and c-C_5H_2 in the cosmic objects, scientists are now interested in the identification of c-C_7H_2 in cosmic objects (Fig. 1). This ring-chain molecule c-C_7H_2 is an asymmetric top, planar molecule having a large electric dipole moment $\mu = 3.8$ Debye equally inclined with the axes of inertia so that its components along the a and b axes of inertia are $\mu_a = 2.69$ and $\mu_b = 2.69$ Debye. Thus, this isomer has both a-type and b-type radiative transitions, and therefore, the rotational energy levels cannot be separated into two different groups, as was the case for c-C_3H_2. Hence, the investigation of this molecule, likewise c-C_5H_2, is quite complicated. The molecular and distortional constants derived by McCarthy et al. (1997) for c-C_7H_2 are given in Table 1. Since the kinetic temperature in dark molecular clouds is rather low, only rotational transitions in the ground electronic and ground vibrational states take place.

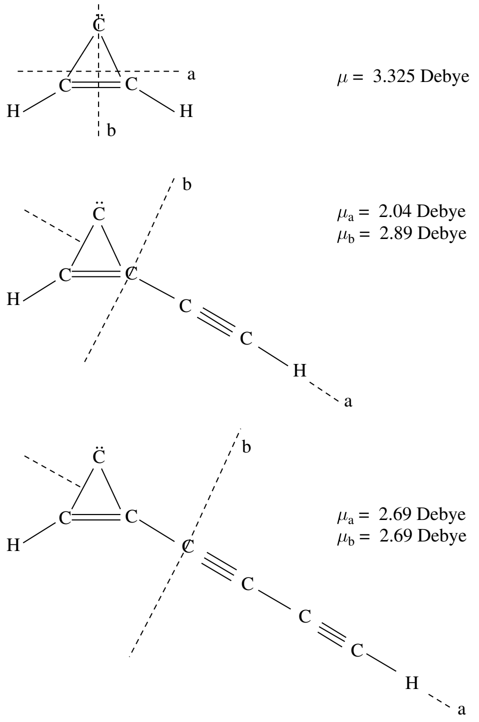

Fig. 1. The ring-chain molecules c-C_3H_2, c-C_5H_2 and c-C_7H_2 along with their inertial axes dipole moments (not to the scale). The c-C_3H_2 is a b-type asymmetric top molecule whereas c-C_5H_2 and c-C_7H_2 have both a- and b-type radiative transitions.

Table 1
Molecular data

A (MHz)	34722.136
B (MHz)	1045.20523
C (MHz)	1014.25700
Δ_J (MHz)	17.2×10^{-6}
Δ_{JK} (MHz)	7.06×10^{-3}
μ_a (Debye)	2.69
μ_b (Debye)	2.69

We propose that c-C_7H_2 may be identified in the cool cosmic objects through its transitions 4_{14}–5_{05}, 5_{15}–6_{06}, 6_{16}–7_{07} and 7_{17}–8_{08} at 23.241, 21.105, 18.953 and 16.787 GHz, respectively, in absorption against the CMB.

2. Basic formulation

The rotational energy levels of c-C_7H_2 accounted in the present investigation are given in Table 2. In our investigation, NLTE occupation numbers of the levels are calculated in an on-the-spot approximation by using the escape probability method (see, e.g., Rausch et al., 1996; Chandra and Shinde, 2004), where the external radiation field, impinging on a volume element generating the lines, is the CMB only. In the present investigation, a set of 53 linear equations coupled with 308 equations of radiative transfer is solved through the iterative procedure for given values of n_{H_2} and $\gamma \equiv n_{mol}/(dv_r/dr)$, where n_{mol} is density of the molecule and dv_r/dr the velocity gradient in the object. The input data required in the present investigation are the radiative transitions probabilities (Einstein A-coefficients) and the collisional rate coefficients.

2.1. Einstein A-coefficients

Rotational wave functions for an asymmetric top molecule can be described by linear combinations of symmetric top wave functions (Chandra et al., 1984a,b)

Table 2
Energy levels of ring-chain molecule c-C_7H_2

J	k_a	k_c	E (cm^{-1})	J	k_a	k_c	E (cm^{-1})
0	0	0	0.00000	1	0	1	0.06870
2	0	2	0.20609	3	0	3	0.41217
4	0	4	0.68695	5	0	5	1.03042
1	1	1	1.19204	1	1	0	1.19307
2	1	2	1.32840	2	1	1	1.33149
6	0	6	1.44257	3	1	3	1.53293
3	1	2	1.53913	4	1	4	1.80565
4	1	3	1.81598	7	0	7	1.92340
5	1	5	2.14655	5	1	4	2.16203
8	0	8	2.47291	6	1	6	2.55562
6	1	5	2.57730	7	1	7	3.03287
7	1	6	3.06177	9	0	9	3.09109
8	1	8	3.57829	8	1	7	3.61545
10	0	10	3.77535	9	1	9	4.19188
9	1	8	4.23833	11	0	11	4.53033
2	2	1	4.70151	2	2	0	4.70151
10	1	10	4.87364	3	2	2	4.90760
3	2	1	4.90760	10	1	9	4.93042
4	2	3	5.18238	4	2	2	5.18238
5	2	4	5.52584	5	2	3	5.52584
11	1	11	5.61985	11	1	10	5.68799
6	2	5	5.93801	6	2	4	5.93801
7	2	6	6.41886	7	2	5	6.41886
8	2	7	6.96841	8	2	6	6.96841
9	2	8	7.58664	9	2	7	7.58664
10	2	9	8.27288	10	2	8	8.27288
11	2	10	9.02866	11	2	9	9.02866
3	3	1	10.52687	3	3	0	10.52687
4	3	2	10.80164	4	3	1	10.80164
5	3	3	11.14510	5	3	2	11.14510
6	3	4	11.55726	6	3	3	11.55726
7	3	5	12.03811	7	3	4	12.03811
8	3	6	12.58765	8	3	5	12.58765
9	3	7	13.20589	9	3	6	13.20589
10	3	8	13.89282	10	3	7	13.89282
11	3	9	14.64757	11	3	8	14.64757

$$\Psi_{J\tau M}(\alpha,\beta,\gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^{J} g^J_{\tau K} D^J_{MK}(\alpha,\beta,\gamma),$$

where α, β, γ are Euler angles specifying the orientation of the molecule, J the rotational quantum number, $g^J_{\tau K}$ the expansion coefficients, D^J_{MK} the Wigner D-functions and the pseudo quantum number τ is defined by

$$\tau = k_a - k_c,$$

where k_a and k_c are projections of J on the axis of symmetry in case of prolate and oblate symmetric tops, respectively. Rotational levels in an asymmetric top molecule are specified as J_{k_a,k_c} or J_τ.

Since the electric dipole moment of the molecule is inclined with its axes of inertia, it has both a-type as well as b-type rotational transitions. The a-type rotational transitions are governed by the selection rules

$$\begin{array}{ll} J: & \Delta J = 0, \pm 1 \\ k_a, k_c: & \text{even, odd} \leftrightarrow \text{even, even} \\ & \text{odd, even} \leftrightarrow \text{odd, odd.} \end{array}$$

In the representation where the axis of quantization is along the *a*-axis of inertia, Einstein *A*-coefficient for the transition $J'_{\tau'} \to J_\tau$ is (Chandra and Sahu, 1993; Chandra and Rashmi, 1998)

$$A(J'_{\tau'} \to J_\tau) = \frac{64\pi^4 \nu^3 \mu_a^2 (2J+1)}{3hc^3(2J'+1)} \left[\sum_{K=-J}^{J} g^{J}_{\tau K} g^{J'}_{\tau' K} C^{J'K}_{JK10} \right]^2,$$

where μ_a is the electric dipole moment along the *a*-axis of inertia, and $C^{\cdot\cdot}_{\cdots}$ the Clebsch Gordon coefficient. The *b*-type rotational transitions are governed by the selection rules

$$\begin{array}{ll} J: & \Delta J = 0, \pm 1 \\ k_a, k_c: & \text{even, odd} \leftrightarrow \text{odd, even} \\ & \text{even, even} \leftrightarrow \text{odd, odd.} \end{array}$$

In the representation where the axis of quantization is along the *a*-axis of inertia, Einstein *A*-coefficient for the transition $J'_{\tau'} \to J_\tau$ is (Chandra et al., 1984b; Chandra, 2002)

$$A(J'_{\tau'} \to J_\tau) = \frac{32\pi^4 \nu^3 \mu_b^2 (2J+1)}{3hc^3(2J'+1)} \times \left[\sum_{K=-J}^{J} g^{J}_{\tau K} \left(g^{J'}_{\tau' K+1} C^{J'K+1}_{JK11} + g^{J'}_{\tau' K-1} C^{J'K-1}_{JK1,-1} \right) \right]^2,$$

where μ_b is the electric dipole moment along the *b*-axis of inertia. Calculated values of Einstein *A*-coefficients for *a*-type as well as *b*-type rotational transitions between the levels up to 15 cm^{-1} are available in the electronic form[2] in Table 3.

2.2. Collisional rate coefficients

Though the collisional transitions are not restricted through any selection rules, computation of the coefficients for collisional transitions between the levels due to collisions with H_2 molecules is quite cumbersome task. The required collisional rate coefficients are not available in the literature. In absence of them, qualitative investigations can however be carried out by choosing some scaling laws for the rate coefficients which do not create any anomalous behaviour from their own. As and when the collisional rate coefficients would be available, the investigation can be repeated for quantitative results. In the present investigation, the rate coefficients for downward transitions $J'k'_a k'_c \to J k_a k_c$ at a kinetic temperature *T* are taken as (Sharma and Chandra, 2001)

$$C(J'k'_a k'_c \to J k_a k_c) = \frac{1 \times 10^{-11}}{2J'+1} \sqrt{\frac{T}{30}}.$$

These rate coefficients can be interpreted as the cross section times a thermal velocity. The factor $(2J' + 1)$ is the degeneracy of the upper level of the transition. These rates have no selectivity and do not create any anomalous behaviour from their own.

For collisional rate coefficients in the upward direction, we accounted for the fact that downward and upward collisional rate coefficients are related through the detailed equilibrium (Chandra and Kegel, 2000).

3. Anomalous absorption

Observation of a spectral line in absorption against the CMB is an unusual phenomenon. The transition $1_{10} \to 1_{11}$ of H_2CO and $2_{20} \to 2_{11}$ of *c*-C_3H_2 are good examples of anomalous absorption. The intensity, I_ν, of a line generated in an interstellar cloud, with homogeneous excitation conditions, is given by

$$I_\nu - I_{\nu,\mathrm{bg}} = (S_\nu - I_{\nu,\mathrm{bg}})(1 - \mathrm{e}^{-\tau_\nu}), \tag{1}$$

where $I_{\nu,\mathrm{bg}}$ is the intensity of the continuum against which the line is observed, τ_ν the optical depth of the line, and S_ν the source function. For positive optical depth, observation of an interstellar line in absorption against the CMB (i.e., $I_\nu < I_{\nu,\mathrm{bg}}$), obviously, implies the excitation temperature T_{ex} of the line to be less than the CMB-temperature T_{bg}, but positive ($0 < T_{\mathrm{ex}} < T_{\mathrm{bg}}$). It requires rather peculiar conditions in the molecule generating the line. Eq. (1) may also be expressed as

$$B_\nu(T_\mathrm{B}) - B_\nu(T_{\mathrm{bg}}) = \left[B_\nu(T_{\mathrm{ex}}) - B_\nu(T_{\mathrm{bg}})\right](1 - \mathrm{e}^{-\tau_\nu}), \tag{2}$$

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[2] Table 3 can be found at doi:10.1016/j.newast.2004.12.005.

where B_ν represents a Planck's function corresponding to various temperatures and T_B is the brightness temperature of the line. (For absorption against the CMB, we have $T_B < T_{bg}$.) This obviously shows that for optically thin case, $\tau_\nu \approx 0$ and we have $T_B = T_{bg} \equiv 2.7$ K. Further, in the Rayleigh–Jeans limit [$\nu\,(\text{GHz}) \ll 21T\,(\text{K})$], Eq. (2) can be written as

$$T_B = T_{ex} + (T_{bg} - T_{ex})\, e^{-\tau_\nu}. \tag{3}$$

For anomalous absorption, we have $T_{ex} < T_{bg}$ and $\tau_\nu > 0$, and therefore, $T_B > T_{ex}$. When τ_ν is very large, then for the anomalous absorption, we have $T_B = T_{ex}$. It shows that for anomalous absorption, the brightness temperature of the line lies between T_{ex} of the line and $T_{bg}(T_{ex} \leqslant T_B \leqslant T_{bg})$.

4. Numerical results and discussion

In our model, the free parameters are the hydrogen density n_{H_2} and γ. In order to include a large number of cosmic objects where c-C_7H_2 may be found, numerical calculations are carried out for wide ranges of physical parameters. In our earlier work (Chandra and Shinde, 2004) for c-C_5H_2, we had taken $\gamma = 10^{-5}$ and 10^{-4} cm^{-3} (km/s)$^{-1}$ pc. These values are taken

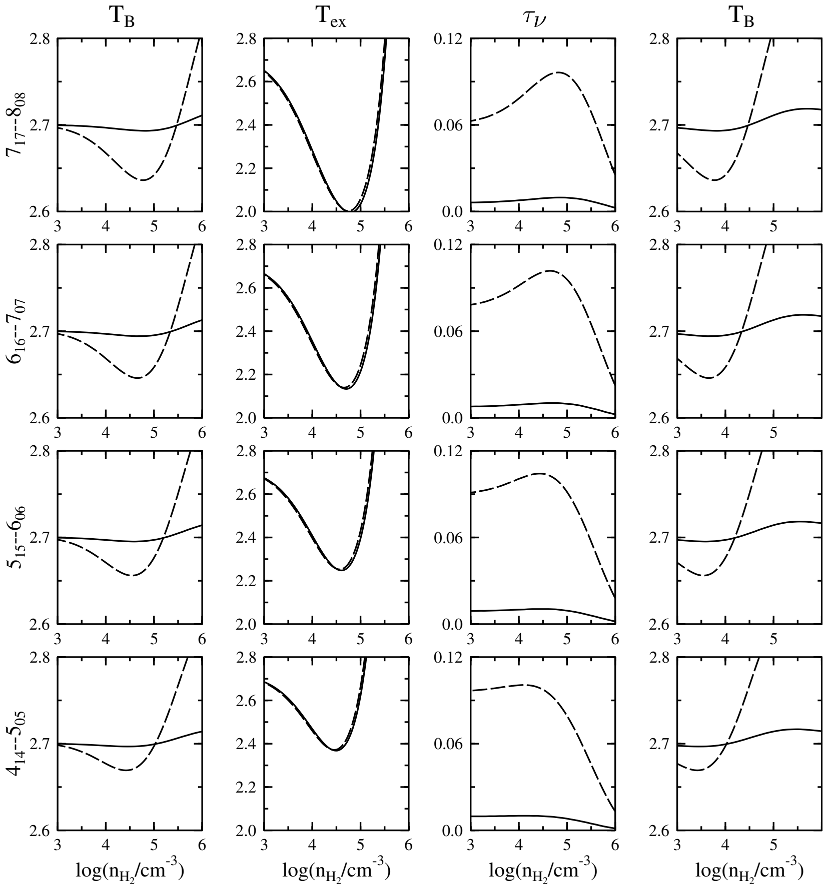

Fig. 2. Variation of brightness temperature T_B (K) (column 1), excitation temperature T_{ex} (K) (column 2), optical depth τ_ν (column 3) versus hydrogen density n_{H_2} for kinetic temperature of 10 K for the transitions written on the left. Solid line is for $\gamma = 10^{-5}$ cm^{-3} (km/s)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-4}$ cm^{-3} (km/s)$^{-1}$ pc. For the brightness temperature T_B in column 4, the collisional rates for the transitions with $\Delta k_a = 0$ are increased by a factor of 10.

here for c-C_7H_2 also. The later one corresponds to a little higher column density of the molecule. For lower value of the column density, the intensity of the line may not be observable. The molecular hydrogen density n_{H_2} is varied over the range from 10^3 to $10^6\,cm^{-3}$, and calculations are performed for the kinetic temperature 10 K, as the temperature in a cool cosmic object would be around that.

4.1. Anomalous absorption in c-C_7H_2 molecule

A number of lines of c-C_7H_2 are found in absorption against the CMB. However, the transitions 4_{14}–5_{05}, 5_{15}–6_{06}, 6_{16}–7_{07} and 7_{17}–8_{08} have shown good absorption phenomenon. For these transitions, we have plotted T_B (Fig. 2, column 1), T_{ex} (column 2) and τ_v (column 3). For the lines, the largest value of the optical depth τ_v is found ≈0.1 around $n_{H_2} = 10^{4.5}\,cm^{-3}$. Hence, the lines are optically thin. Thus, the collisional excitations take the molecules to the upper levels and the process of radiative cascading takes place. For these transitions, the radiative cascading is as shown in Fig. 3, where A and C correspond to the upper and lower levels, respectively, of the transition. The upper level A goes radiatively to the levels B and E whereas the lower level C goes radiatively to the level D only. The ratios of the radiative life times of the upper level A to the lower level C for 4_{14}–5_{05}, 5_{15}–6_{06}, 6_{16}–7_{07} and 7_{17}–8_{08} transitions are 47.61, 29.41, 20.40 and 22.72, respectively. Hence, the system remains in the lower level for a longer time and waits for absorption of the corresponding radiation coming from the CMB.

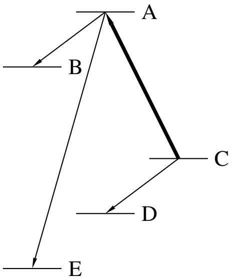

Fig. 3. Radiative cascading of the levels of the transition between A and C, which shows anomalous absorption.

4.2. Sensitivity to the collisional rates

Though the collisional rates have no selectivity and do not support any anomalous behaviour from their own. However, some transitions between the low lying levels may be sensitive to the collisional rates.

In order to investigate sensitivity of our results to the collisional rates, we enhanced the collisional rates for the transitions with $\Delta k_a = 0$ by a factor of 10 (i.e., by one order of magnitude), which may be taken as an extreme case. The results with these enhanced rates are also given in Fig. 2 (column 4). The absorption feature of the lines remains unaffected. However, the position of the minimum value of T_B is found to shift towards the low density region. Moreover, in absence of accurate collisional rates, our results can be treated as qualitative in nature.

5. Conclusions

Here, we have used scaled values of collisional rates, and therefore, our results are qualitative in nature. We found that detection of c-C_7H_2 is likely in cool cosmic objects through anomalous absorption of the transitions 4_{14}–5_{05}, 5_{15}–6_{06}, 6_{16}–7_{07} and 7_{17}–8_{08} in cool cosmic objects where density is around $10^{4.5}\,cm^{-3}$. In absence of accurate collisional rates, our investigation provides information that these transitions may play important role for identification of c-C_7H_2 in cool cosmic objects.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version at doi:10.1016/j.newast.2004.12.005.

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