Suggestions for an interstellar C₅H₂ search*

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Abstract. Laboratory detection of four isomers of C₅H₂ molecule have been reported by Travers et al. (1997), McCarthy et al. (1997), and Gottlieb et al. (1998). They suggested for detection of the ring-chain isomer of C₅H₂ (c-C₅H₂) in cosmic objects, as it is the most stable one in comparison to the others. Two transitions 3₁₃−₂₁₂ and 3₃₁₂−₂₀₂ at 19.147 GHz and 19.606 GHz, respectively, of c-C₅H₂ have been detected in TMC-1. We suggest that the c-C₅H₂ may be identified in cool cosmic objects through its transition 3₁₁₃−₄₀₄ at 4.3 GHz in absorption against the cosmic microwave background. Since in absence of availability of the collisional rates, we have used scaled values for them, we have checked the sensitivity of the lines on the rates by enhancing the rate for the transitions with Δκ_a = 0 by a factor of 10. Though the transitions are not found sensitive, our results may be treated as qualitative in nature. This absorption line may play an important role for identification of c-C₅H₂ in cosmic objects.

Key words. ISM: molecules

1. Introduction

After detection of C₄H₂ and C₆H₂ molecules in the expanding shell of the evolved carbon star IRC +10216 and in the rich-molecular-source TMC-1, search for C₅H₂ molecule in cosmic objects is being carried out. Out of the four isomers of C₅H₂ molecule, detected in laboratory by Travers et al. (1997), McCarthy et al. (1997), and Gottlieb et al. (1998), the ring-chain isomer (c-C₅H₂) is the most probable candidate for its detection in cosmic objects, as it is the most stable one as compared to the others. This isomer is an asymmetric top, planar molecule having, a large electric dipole moment μ = 3.5 Debye inclined with the axes of inertia so that its components along the a and b axes of inertia are μ_a = 2.04 Debye and μ_b = 2.89 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 in case of an a-type or b-type molecule. Hence, the investigation of this molecule is quite complicated. The molecular data derived by Travers et al. (1997) for c-C₅H₂ 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. We propose to identify C₅H₂ in cosmic objects through its transition 3₁₁₃−₄₀₄ in absorption against the cosmic 2.73 K background (also called the cosmic microwave background, denoted as CMB).

\[ \Psi_{JM}(\alpha, \beta, \gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{k=-J}^{J} g_{MK}^J D_{MK}^J(\alpha, \beta, \gamma) \]

where \( \alpha, \beta, \gamma \) are Euler angles specifying the orientation of the molecule, \( J \) the rotational quantum number, \( g_{MK}^J \) the expansion coefficients, \( D_{MK}^J \) the Wigner D-function and the pseudo quantum number \( \tau \) is defined by

\[ \tau = k_a - k_c \]

Table 1. Molecular data.

| A (MHz) | 34 638.7013 |
| B (MHz) | 3424.87684 |
| C (MHz) | 3113.63865 |
| \( \Delta J \) (MHz) | 2.888 \times 10^{-4} |
| \( \Delta_{JK} \) (MHz) | 2.952 \times 10^{-2} |
| \( \mu_a \) (Debye) | 2.04 |
| \( \mu_b \) (Debye) | 2.89 |

\* Tables 3 is only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/423/235

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Table 2. Energy levels of ring-chain isomer of C₅H₂.

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where \( k_a \) and \( k_- \) 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 \( J_{k_a,k_-} \) or \( J_{r} \). The rotational energy levels accounted in the present investigation are given in Table 2.

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

\[
J: \Delta J = 0, \pm 1
\]

\( k_a, k_- \): even, odd \( \leftrightarrow \) even, even

\( \text{odd, even} \leftrightarrow \text{odd, odd} \).

In the representation where the axis of quantization is along the \( a \)-axis of inertia, Einstein \( A \)-coefficient for the transition \( J'_r \to J_r \) is (Chandra & Sahu 1993; Chandra & Rashmi 1998)

\[
A(J'_r \to J_r) = \frac{64\pi^4 \mu_a^2 (J + 1)}{3 \hbar c^3 (2J + 1)} \left[ \sum_{k_- = -J}^{J} g_{r,K} g_{r,K+1} C_{J,K11}^J \right]^2
\]

where \( \mu_a \) is the electric dipole moment along the \( a \)-axis of inertia, and \( C \) is the Clebsch-Gordon coefficient. The \( b \)-type rotational transitions are governed by the selection rules

\[
J: \Delta J = 0, \pm 1
\]

\( k_a, k_- \): even, odd \( \leftrightarrow \) even, even

\( \text{odd, even} \leftrightarrow \text{odd, odd} \).

In the representation where the axis of quantization is along the \( a \)-axis of inertia, Einstein \( A \)-coefficient for the transition \( J'_r \to J_r \) is (Chandra & Sahu 1993; Chandra & Rashmi 1998)

\[
A(J'_r \to J_r) = \frac{32\pi^4 \mu_a^2 (2J + 1 + 1)}{3 \hbar c^3 (2J + 1)} \left[ \sum_{k_- = -J}^{J} g_{r,K} g_{r,K+1} C_{J,K11}^J \right]^2
\]

where \( \mu_a \) 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 18 cm⁻¹ are available in the electronic form in Table 3.

### 3. Collisional rate coefficients

Besides the radiative transition probabilities for optically allowed transitions between the rotational energy levels, data required as input for the present investigation are the rate coefficients for collisional transitions between the levels due to collisions with H₂ molecules. Though the collisional transitions are not restricted through any selection rules, computation of them 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 for the rate coefficients which do not favour 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 \( J'k'_a k'_- \to J_k k_- \) at a kinetic temperature \( T \) are taken as (Sharma & Chandra 2001)

\[
C(J'k'_a k'_- \to J_k k_-) = 1 \times 10^{-11} \sqrt{T/30}/(2J + 1)
\]

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 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 this paper. Moreover, in absence of accurate collisional rates, our results can be treated as qualitative in nature.

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

In our investigation, NLTE occupation numbers of the energy levels of the molecule under investigation are calculated in an on-the-spot approximation by using the escape probability method (see, e.g., Rausch et al. 1996), where the external radiation field, impinging on a volume element generating the lines, is the CMB only. Besides the normal features, some lines of a molecule may show anomalous features: (i) absorption against the CMB (called, anomalous absorption) and (ii) maser action.

4.1. Anomalous absorption

Observation of a spectral line in absorption against the CMB is an unusual phenomenon. The transition 10 → 11 of H₂CO and 20 → 21 of C₅H₂ are good examples of anomalous absorption. The intensity, I, of a line generated in an interstellar cloud, with homogeneous excitation conditions, is given by

\[ I(T) = I_{\text{bg}} - I_{\text{ex}}(1 - e^{-\tau_{\nu}}) \]

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

\[ B_{\nu}(T_{B}) - B_{\nu}(T_{\text{bg}}) = B_{\nu}(T_{\text{ex}}) - B_{\nu}(T_{\text{bg}})(1 - e^{-\tau_{\nu}}) \]

where \( B_{\nu} \) 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 \( T_{B} < T_{\text{bg}} \).) This obviously shows that for optically thin case, \( \tau_{\nu} \approx 0 \) and we have \( T_{\text{ex}} = T_{\text{bg}} \approx 2.7 \text{ K} \). Further, in the Rayleigh-Jeans limit \( \nu \text{GHz} < 21 \ T(K) \), Eq. (2) can be written as

\[ T_{B} = T_{\text{ex}} + (T_{\text{bg}} - T_{\text{ex}})e^{-\tau_{\nu}}. \]

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

4.2. Maser action

Maser action is another anomalous phenomenon shown by some molecules in the cosmic objects. The molecules OH, H₂O and SiO are good examples of masing molecules. We can rearrange the Eq. (3) as

\[ T_{B} = T_{\text{bg}}e^{-\tau_{\nu}} - T_{\text{ex}}e^{-\tau_{\nu}} - 1. \]

For maser action, we have population inversion and thus \( T_{\text{ex}} < 0 \) and \( \tau_{\nu} < 0 \), showing that \( T_{B} > T_{\text{bg}} \). When \( |\tau_{\nu}| \) is large (such that \( e^{-\tau_{\nu}} \approx 1 \)), then for the maser action, we have

\[ T_{B} = (T_{\text{bg}} - T_{\text{ex}})e^{-\tau_{\nu}}. \]

5. Numerical results and discussion

In our model, the free parameters are the hydrogen density \( n_{\text{H}} \), and \( \gamma \equiv n_{\text{mol}}/\langle d\nu_{l}/dr \rangle \), where \( n_{\text{mol}} \) is density of the molecule, and \( d\nu_{l}/dr \) the velocity gradient in the object. In order to include a large number of cosmic objects where \( c_{-}\text{C5H}_2 \) may be found, numerical calculations are carried out for wide ranges of physical parameters. We have taken two values \( 10^{-2} \) and \( 10^{-4} \text{ cm}^{-3} \text{ (km s}^{-1})^{-1} \text{ pc} \) for \( \gamma \). For each value of \( \gamma \), the molecular hydrogen density \( n_{\text{H}} \) is varied over the range from \( 10^{3} \) to \( 10^{6} \text{ cm}^{-3} \), and calculations are performed for two kinetic temperatures 10 and 20 K, as the temperature in the clouds cannot be larger than this. In the present investigation, a set of 64 linear equations coupled with 274 equations of radiative transfer is solved through the iterative procedure for given values of \( n_{\text{H}} \) and \( \gamma \).

5.1. Observations

For the observed two transitions \( 3_{12} \rightarrow 2_{11} \) and \( 3_{03} \rightarrow 2_{02} \) at 19.147 GHz and 19.606 GHz, respectively of \( c_{-}\text{C5H}_2 \) detected in TMC-1, Dickens et al. (2001) obtained \( \Delta \nu = 0.15 \text{ km s}^{-1} \), and the upper limits for the relative column density of \( c_{-}\text{C5H}_2 \) was obtained as \( 2 \times 10^{15} \text{ cm}^{-2} \) and \( 4 \times 10^{14} \text{ cm}^{-2} \), respectively. (Frequencies of these transitions given in Table 1 of Dickens et al. (2001) suffer from misprint as we discussed with them.) For these values of Dickens et al. (2001), the corresponding values of the free parameter \( \gamma \) are 4.5 \times 10^{-6} and \( 9 \times 10^{-6} \text{ cm}^{-3} (\text{km s}^{-1})^{-1} \text{ pc} \). This higher value \( 9 \times 10^{-6} \text{ cm}^{-3} \) is closed to our value \( 10^{-5} \text{ cm}^{-3} \), and our second value is larger by one order of magnitude.

For the observed lines \( 3_{13} \rightarrow 2_{12} \) and \( 3_{05} \rightarrow 2_{02} \), variation of brightness temperature \( T_{B} \) versus the hydrogen density \( n_{\text{H}} \), for \( T = 10 \text{ K} \) (row 1) and 20 K (row 2) is shown in Fig. 1. We found \( T_{B} > n_{\text{H}} \), although not very large for \( \gamma = 10^{-5} \), but showing emission feature for both the lines. Since both the lines are detected in emission, the reason for low value of \( T_{B} \) is that in our calculations can be assigned to the qualitative nature of our investigations. When \( \gamma \) (i.e., \( N(\text{C-C5H}_2)/\Delta \nu \)) is increased by one order of magnitude, \( T_{B} \) shows a remarkable increase where optical depth \( \tau_{\nu} \) goes up to 0.4 and 0.5 at \( T = 10 \text{ K} \), and 0.06 and 0.1 at \( T = 20 \text{ K} \) for \( 3_{13} \rightarrow 2_{12} \) and \( 3_{03} \rightarrow 2_{02} \) transitions, respectively. The results with the enhanced collisional rates for the lines are shown in rows 3 and 4 of Fig. 1. With the enhanced rates, a little increase in \( T_{B} \) is found; which is more remarkable on the two sides of the peak. The peak in \( T_{B} \) is found to shift towards the low density region, and at the peak, the optical depth is found to decrease.

5.2. The \( 7_{07} \rightarrow 6_{16} \) and \( 6_{06} \rightarrow 5_{15} \) transitions

A number of lines of \( c_{-}\text{C5H}_2 \) were found showing negative value for the excitation temperature (maser action). Though it was not large in magnitude, we have however investigated two transitions \( 7_{07} \rightarrow 6_{16} \) and \( 6_{06} \rightarrow 5_{15} \) at 17.4 GHz and 10.1 GHz, respectively. Other lines showing negative value for \( T_{\text{ex}} \) were insignificant. Variation of \( T_{B} \) versus \( n_{\text{H}} \) for these two lines is also shown in Fig. 1. The optical depth, at the peak, goes up
Fig. 1. Variation of brightness temperature $T_B$ (K) versus hydrogen density $n_{H_2}$ of the lines written at the top of each column for kinetic temperatures 10 K (rows 1 and 3) and 20 K (rows 2 and 4). Solid line is for $\gamma = 10^{-5}$ cm$^{-1}$ (km s$^{-1}$)$^{-1}$ pc, and the dotted line for $\gamma = 10^{-5}$ cm$^{-1}$ (km s$^{-1}$)$^{-1}$ pc. Lower rows (3 and 4) are for the case where collisional rates of the transitions with $\Delta
u_a = 0$ are increased by a factor of 10.

5.3. The $3_{13} - 4_{04}$ transition

A number of lines of $c$-C$_5$H$_2$ are found in absorption against the cosmic 2.7 K background. However, the transition $3_{13} - 4_{04}$ at 4.3 GHz has shown reasonably good absorption phenomenon. Einstein $A$-coefficient for this transition is $1.74 \times 10^{-9}$ s$^{-1}$. For this transition, we have plotted brightness temperature $T_B$ (Col. 1), excitation temperature $T_{ex}$ (Col. 2), optical depth $\tau_\nu$ (Col. 3) and again $T_B$ where the enhanced collisional rates are used (Col. 4). Anomalous absorption is found to increase with $\gamma$. A moderate increase is found with the increase of kinetic temperature $T$, where the position of the minimum value of $T_B$ is found to shift towards the low density region.

It is interesting to have a note that the observed transition $3_{13} - 2_{12}$ ($A = 1.30 \times 10^{-7}$ s$^{-1}$) is detected in emission whereas the transition $3_{13} - 4_{04}$, having the common upper level $3_{13}$ shows absorption against the CMB. The process of absorption can be understood in the following manner. The level $3_{13}$, besides to $4_{04}$, decays radiatively to the levels $2_{12}$ and $2_{02}$ ($A = 3.49 \times 10^{-6}$ s$^{-1}$). The lower level $4_{04}$ has only one radiative decay to $3_{03}$ ($A = 3.84 \times 10^{-7}$ s$^{-1}$). The radiative life time of the level $3_{13}$ ($2.8 \times 10^3$ s) of the transition is one order of magnitude smaller than that of the level $4_{04}$ ($2.6 \times 10^6$ s). Thus, the molecule in the lower level exists longer and can absorb the
radiations corresponding to the transition 3\textsubscript{13}−4\textsubscript{404} coming from the background.

6. Conclusion

Here, we have used scaled values of collisional rates, and therefore, our results are qualitative in nature. We have obtained emission feature of the observed lines qualitatively. We found that detection of c-C\textsubscript{5}H\textsubscript{2} is likely in cool cosmic objects through anomalous absorption of the transition 3\textsubscript{13}−4\textsubscript{404}. In absence of accurate collisional rates, our investigation provides information that this transition may play important role for identification of c-C\textsubscript{5}H\textsubscript{2} in cool cosmic objects.

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