

Anomalous absorption in rhomboidal SiC₃ molecules

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Received 5 November 2007; accepted 16 January 2008

Abstract. Laboratory detection of two isomers of cyclic SiC₃ molecule have been reported by McCarthy et al. (1999a, 1999b) and Apponi et al. (1999b). Seven transitions of the isomer-I have been detected in IRC+10216 by Apponi et al. (1999a). However, to date, the second isomer is not detected in the interstellar space. Here, we propose identification of isomer-I through the transition $4_{22} - 4_{23}$ at 0.2 GHz and of isomer-II through the transitions $2_{20} - 2_{21}$ at 4.44 GHz and $4_{40} - 4_{41}$ at 2.16 GHz, in absorption against the cosmic microwave background (CMB). In absence of the availability of the collisional rates, we have used scaled values for them. However, we have checked the sensitivity of the lines on the rates by enhancing the rates for transitions with $\Delta k_a = 0$ by a factor of 10 and the results are not found sensitive.

Keywords : interstellar molecules - SiC₃

1. Introduction

The isomer-I of cyclic SiC₃ is the fifth and the most stable ring molecule so far identified in the interstellar space. The structure of isomer-I is planar, rhomboidal with a transannular bond and C_{2v} symmetry (Fig. 1). This is an a -type asymmetric top molecule (nearly symmetric prolate top, $\kappa = -0.945$) with electric dipole moment $\mu = 4.2$ Debye (Alberts et al. 1990). In a search with the NRAO 12 m telescope at Kitt Peak, seven transitions of this unusual molecular ring in the rich molecular envelope of the evolved carbon star IRC+10216 have already been detected (Apponi et al. 1999a).

The isomer-II of cyclic SiC₃ is also a planar rhomboid with a transannular bond and C_{2v} symmetry (Fig. 1). The transannular bond is between the Si and the opposite C. This is also an a -type asymmetric top molecule ($\kappa = 0.654$) with electric dipole moment of $\mu = 2.2$ Debye (Alberts et al. 1990).

Here, we propose identification of isomer-I through the transition $4_{22} - 4_{23}$ at 0.2 GHz and of isomer-II through the transitions $2_{20} - 2_{21}$ at 4.44 GHz and $4_{40} - 4_{41}$ at 2.16 GHz, in absorption against the CMB.

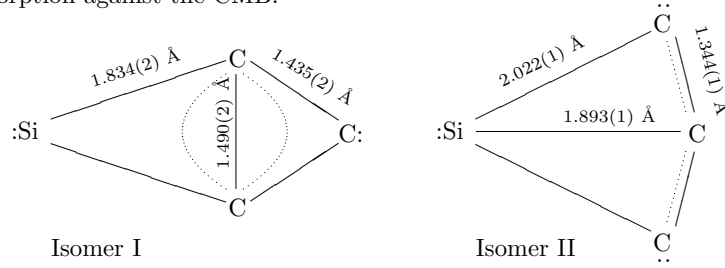


Figure 1. Structure of isomers I and II of SiC_3 , adapted from Fig. 1 of McCarthy et al. (1999b).

2. Basic formulation

We have calculated rotational energy levels for isomer-I using the molecular and distortion constants given by Apponi et al. (1999b). For calculations of rotational energy levels for isomer-II, we have used the molecular and distortion constants given by McCarthy et al. (1999b). The energy levels accounted for are given in Tables 1 and 2.

In the present investigation, for isomer-I, a set of 39 linear equations coupled with 105 equations of radiative transfer is solved through iterative procedure (Chandra et al. 2006). For the isomer-II, a set of 48 linear equations coupled with 186 equations of radiative transfer is solved through iterative procedure. The statistical equilibrium equations coupled with equations of radiative transfer can be expressed as the following.

$$n_i \sum_{\substack{j=1 \\ j \neq i}}^z P_{ij} = \sum_{\substack{j=1 \\ j \neq i}}^z n_j P_{ji} \quad i = 1, 2, \dots, z$$

where $z = 39$ for isomer-I and $z = 48$ for isomer-II. Here, n 's are the population densities of the rotational levels and the parameter P is:

(i) For optically allowed transitions

$$P_{ij} = \begin{cases} (A_{ij} + B_{ij} I_{\nu, bg}) \beta_{ij} + n_{H_2} C_{ij} & i > j \\ B_{ij} I_{\nu, bg} \beta_{ij} + n_{H_2} C_{ij} & i < j \end{cases}$$

(ii) For optically forbidden transitions

$$P_{ij} = n_{H_2} C_{ij}$$

where A 's and B 's are Einstein coefficients,

$$A_{ul} = \frac{2h\nu^3}{c^2} B_{ul} \qquad B_{ul} = \frac{g_l}{g_u} B_{lu}$$

C 's the collisional rate coefficients, n_{H_2} the density of hydrogen molecules, and the escape probability β for the transition is

$$\beta_{lu} = \beta_{ul} = \frac{1 - \exp(-\tau_\nu)}{\tau_\nu}$$

where optical thickness τ_ν is

$$\tau_\nu = \frac{hc}{4\pi(dv_r/dr)} [B_{lu}n_l - B_{ul}n_u].$$

Here, (dv_r/dr) is the velocity gradient in the region. By solving these coupled equations, population densities of the levels are calculated. This set of equations is solved through iterative procedure for the given values of n_{H_2} and $\gamma \equiv n_{\text{mol}}/(dv_r/dr)$, where n_{mol} is density of the molecule. In our investigation, NLTE occupation numbers of energy levels for each molecule are calculated in an on-the-spot approximation by using the escape probability method (Rauch et al. 1996) where the external radiation field, impinging on a volume element generating lines, is the CMB only.

The input data required are the radiative transitions probabilities (Einstein A-coefficients) and the collisional rate coefficients.

3. Einstein A-coefficients

Both the isomers of SiC₃ are a -type asymmetric top molecules and the rotational radiative transitions are governed by the selection rules:

$$\begin{aligned} J : & \quad \Delta J = 0, \pm 1 \\ k_a, k_c : & \quad \text{even, odd} \longleftrightarrow \text{even, even} \\ & \quad \text{odd, even} \longleftrightarrow \text{odd, odd.} \end{aligned}$$

In the representation, where the axis of quantization is along the a -axis of inertia, Einstein A-coefficient for the transition $J'_{\tau'} \rightarrow J_\tau$ is given by (Chandra et al. 1993, 1998)

$$A(J'_{\tau'} \rightarrow J_\tau) = \frac{64\pi^4\nu^3\mu^2(2J+1)}{3hc^3(2J'+1)} \left[\sum_{K=-J}^J g_{\tau K}^J g_{\tau' K}^{J'} C_{JK10}^{J'K} \right]^2 \quad (1)$$

where μ is the electric dipole moment of the molecule, $C_{JK10}^{J'K}$ the Clebsch Gordon coefficient and $\tau = k_a - k_c$ is a pseudo quantum number.

Table 1. Rotational energy levels of isomer-I of Sic₃.

| $J_{k_a k_c}$ | Energy in cm^{-1} | $J_{k_a k_c}$ | Energy in cm^{-1} | $J_{k_a k_c}$ | Energy in cm^{-1} |
|-----------------|-------------------------------|--------------------|-------------------------------|--------------------|-------------------------------|
| 0 ₀₀ | 0.000 | 1 ₀₁ | 0.389 | 2 ₀₂ | 1.167 |
| 3 ₀₃ | 2.332 | 4 ₀₄ | 3.883 | 2 ₂₁ | 5.452 |
| 2 ₂₀ | 5.453 | 5 ₀₅ | 5.817 | 3 ₂₂ | 6.620 |
| 3 ₂₁ | 6.623 | 6 ₀₆ | 8.131 | 4 ₂₃ | 8.176 |
| 4 ₂₂ | 8.186 | 5 ₂₄ | 10.121 | 5 ₂₃ | 10.143 |
| 7 ₀₇ | 10.822 | 6 ₂₅ | 12.454 | 6 ₂₄ | 12.497 |
| 8 ₀₈ | 13.885 | 7 ₂₆ | 15.174 | 7 ₂₅ | 15.251 |
| 9 ₀₉ | 17.318 | 8 ₂₇ | 18.280 | 8 ₂₆ | 18.408 |
| 4 ₄₁ | 21.030 | 4 ₄₀ | 21.030 | 10 _{0,10} | 21.117 |
| 9 ₂₈ | 21.772 | 9 ₂₇ | 21.970 | 5 ₄₂ | 22.977 |
| 5 ₄₁ | 22.977 | 11 _{0,11} | 25.278 | 6 ₄₃ | 25.315 |
| 6 ₄₂ | 25.315 | 10 ₂₉ | 25.649 | 10 ₂₈ | 25.940 |
| 7 ₄₄ | 28.043 | 7 ₄₃ | 28.043 | 11 _{2,10} | 29.909 |

Einstein A -coefficients for 104 radiative transitions between 39 energy levels of the isomer-I are calculated. Einstein A -coefficients for 186 radiative transitions between 48 energy levels of isomer-II are calculated.

4. Collisional rate coefficients

In the present investigation, besides the radiative transition probabilities, the collisional rate coefficients are required as input. Though the collisional transitions are not restricted through any selection rules, computation of them is a quite cumbersome task. These required collisional rate coefficients are not available in the literature. In absence of collisional rate coefficients, qualitative investigations can be carried out by choosing some scaling laws, which do not favour any anomalous behaviour from their own. In the present investigation, the rate coefficients for downward transitions $J'_{k'_a k'_c} \rightarrow J_{k_a k_c}$ at a kinetic temperature T_k are taken as (Chandra et al. 2007)

$$C(J'_{k'_a k'_c} \rightarrow J_{k_a k_c}) = 1 \times 10^{-11} (2J + 1) \sqrt{\frac{T_k}{30}}. \quad (2)$$

These rates have no selectivity and do not support any anomalous behaviour from their own. In order to check the 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, which may be taken as an extreme case. Moreover, in absence of the accurate collisional rates, our results can be treated as qualitative in nature. For the upward collisional rate coefficients, we

Table 2. Rotational energy levels of isomer-II of SiC₃ with k_a even.

| $J_{k_a k_c}$ | Energy in cm ⁻¹ | $J_{k_a k_c}$ | Energy in cm ⁻¹ | $J_{k_a k_c}$ | Energy in cm ⁻¹ |
|-----------------|-------------------------------|------------------|-------------------------------|--------------------|-------------------------------|
| 0 ₀₀ | 0.000 | 1 ₀₁ | 0.576 | 2 ₀₂ | 1.581 |
| 2 ₂₁ | 2.241 | 2 ₂₀ | 2.389 | 3 ₀₃ | 2.970 |
| 3 ₂₂ | 3.970 | 3 ₂₁ | 4.458 | 4 ₀₄ | 4.753 |
| 4 ₂₃ | 6.139 | 5 ₀₅ | 6.931 | 4 ₂₂ | 7.079 |
| 4 ₄₁ | 7.947 | 4 ₄₀ | 8.019 | 5 ₂₄ | 8.714 |
| 6 ₀₆ | 9.506 | 5 ₂₃ | 10.085 | 5 ₄₂ | 11.136 |
| 5 ₄₁ | 11.480 | 6 ₂₅ | 11.685 | 7 ₀₇ | 12.476 |
| 6 ₂₄ | 13.461 | 6 ₄₃ | 14.847 | 7 ₂₆ | 15.052 |
| 6 ₄₂ | 15.645 | 8 ₀₈ | 15.843 | 6 ₆₁ | 16.943 |
| 6 ₆₀ | 16.967 | 7 ₂₅ | 17.227 | 8 ₂₇ | 18.815 |
| 7 ₄₄ | 18.999 | 9 ₀₉ | 19.605 | 7 ₄₃ | 20.301 |
| 8 ₂₆ | 21.387 | 7 ₆₂ | 21.527 | 7 ₆₁ | 21.713 |
| 9 ₂₈ | 22.974 | 8 ₄₅ | 23.556 | 10 _{0,10} | 23.763 |
| 8 ₄₄ | 25.304 | 9 ₂₇ | 25.943 | 8 ₆₃ | 26.722 |
| 8 ₆₂ | 27.302 | 10 ₂₉ | 27.529 | 11 _{0,11} | 28.317 |
| 9 ₄₆ | 28.510 | 8 ₈₁ | 29.249 | 8 ₈₀ | 29.256 |

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

5. Anomalous absorption

Observation of a spectral line in absorption against the CMB is an unusual phenomenon. The intensity, I_ν , of a line generated in an interstellar cloud, with homogeneous excitation conditions, is given by

$$I_\nu - I_{\nu,bg} = (S_\nu - I_{\nu,bg})(1 - e^{-\tau_\nu}) \quad (3)$$

where $I_{\nu,bg}$ 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.*, $I_\nu < I_{\nu,bg}$), obviously, implies the excitation temperature T_{ex} of the line to be less than the CMB-temperature T_{bg} , but positive ($0 < T_{ex} < T_{bg}$). It requires rather peculiar conditions in the molecule generating the line. In the Rayleigh-Jeans limit ($h\nu \ll kT$), we have

$$T_B = T_{ex} + (T_{bg} - T_{ex})e^{-\tau_\nu}. \quad (4)$$

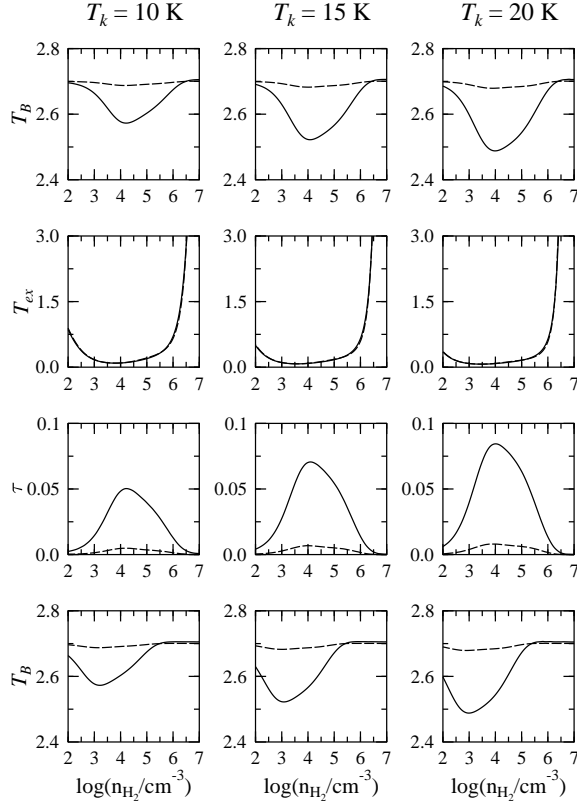


Figure 2. Variation of brightness temperature T_B (row 1), excitation temperature T_{ex} (row 2) and optical depth τ (row 3) versus hydrogen density n_{H_2} for the transition $4_{22} - 4_{23}$ of isomer-I of SiC_3 molecule for kinetic temperatures 10, 15, and 20 K. For the brightness temperature T_B (row 4), the collisional rates for the transitions with $\Delta k a = 0$ are increased by a factor of 10. Comparison of rows 1 and 4 shows that the results are not sensitive to the collisional rates. Solid line is for $\gamma = 10^{-5} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$ and the dotted line for $\gamma = 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$.

This obviously shows that for the optically thin case, $\tau_\nu \approx 0$ and we have $T_B = T_{bg}$. For anomalous absorption, the excitation temperature T_{ex} , brightness temperature T_B and the background temperature T_{bg} satisfy the condition $0 < T_{ex} < T_B < T_{bg}$.

6. Results and discussion

In our model, the free parameters are the molecular hydrogen density n_{H_2} and γ . We have taken $\gamma = 10^{-5}$ and $10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$. In order to include a large number

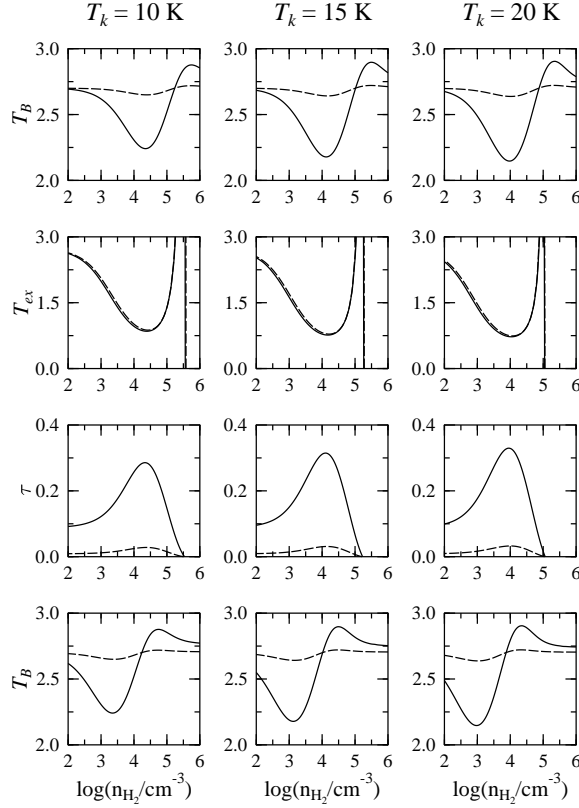


Figure 3. Same as Figure 2 but for the transition $2_{20} - 2_{21}$ of isomer-II of SiC_3 .

of molecular clouds where these molecules may be found, n_{H_2} is varied over a wide range from 10^2 to 10^6 cm^{-3} , and calculations are performed for different kinetic temperatures.

For both the isomers, we have plotted brightness temperature T_B , excitation temperature T_{ex} and optical depth τ versus the logarithm of molecular hydrogen density n_{H_2} for kinetic temperature 10, 15, and 20 K. To check the sensitivity of the collisional rate coefficients, we have plotted the brightness temperature T_B for enhanced collisional rates ($\Delta k_a = 0$ are increased by a factor of 10) in the fourth row. The transition $4_{22} - 4_{23}$ of isomer-I shows anomalous absorption, *i.e.*, the brightness temperature goes below 2.73 K, which is shown in Fig. 2. For the second isomer, anomalous absorption shown by the transitions $2_{20} - 2_{21}$ and $4_{40} - 4_{41}$, is plotted in Figs 3 and 4, respectively. In all the cases, when the kinetic temperature increases, anomalous absorption also found to increase. Comparison of first and fourth row shows that the collisional rate coefficients do not affect the anomalous absorption.

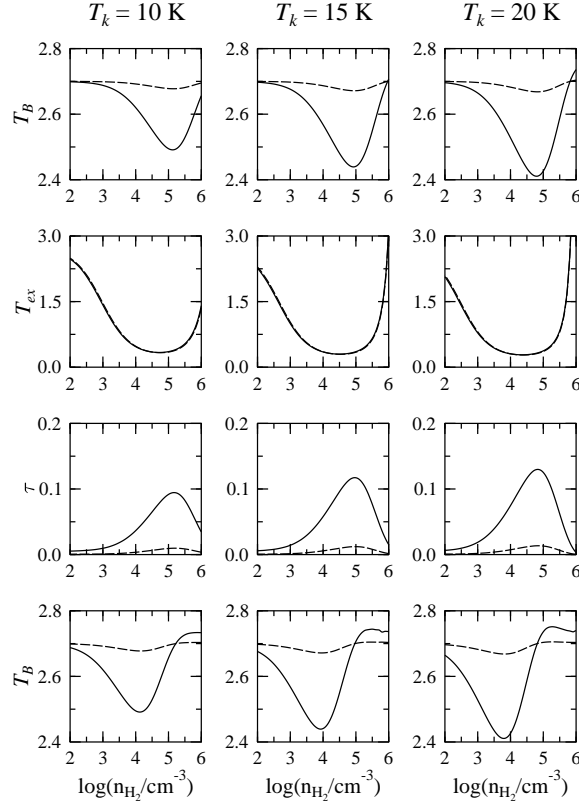


Figure 4. Same as Figure 2 but for the transition $4_{40} - 4_{41}$ of isomer-II of SiC_3 .

Acknowledgments

We are grateful to Prof. Jayant Narlikar and Prof. W.H. Kegel for their encouragement. Thanks are due to the Indian Space Research Organization, Bangalore and Department of Science and Technology, New Delhi for financial assistance in the form of research projects.

References

- Alberts, I. L., Grev, R. S., & Schaefer, H. F., 1990, JChPh, 93, 5046
- Apponi, A. J., McCarthy, M. C., Gottlieb, C. A., & Thaddeus, P. 1999a, ApJ, 516, L103
- Apponi, A. J., McCarthy, M. C., Gottlieb, C. A., & Thaddeus, P. 1999b, JChPh, 111, 3911
- Chandra, S., & Sahu, A., 1993, A&A, 272, 700
- Chandra, S., & Rashmi, 1998, A&AS, 131, 137

- Chandra, S., & Kegel, W.H., 2000, A&AS, 142, 113
Chandra, S., Musrif, P. G., & Shinde, S. V., 2006, BASI, 34, 11
Chandra, S., Shinde, S.V., Kegel, W.H., & Sedlmayr, E., 2007, A&A, 467, 371
McCarthy, M. C., Apponi, A. J., & Thaddeus, P., 1999a, JChPh, 110, 10645
McCarthy, M. C., Apponi, A. J., & Thaddeus, P., 1999b, JChPh, 111, 7175
Rausch, E., Kegel, W.H., Tsuji, T., & Piehler, G., 1996, A&A, 315, 533