Search for an interstellar Si₂C molecule: A theoretical prediction

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Abstract: We suggest that Si₂C molecule may be identified in astronomical objects through its transitions $4_{14} \rightarrow 5_{05}$, $5_{15} \rightarrow 6_{06}$, $2_{12} \rightarrow 3_{03}$, $3_{13} \rightarrow 4_{04}$, and $1_{11} \rightarrow 2_{02}$ at 15.9, 5.1, 33.6, 24.9, and 42.3 GHz in absorption even against the cosmic 2.7 K background, in a region having low temperature. The absorption phenomenon is found rather large in the first two transitions. Dependence of results on the set of molecular parameters is discussed.

Keywords. interstellar molecules - Si₂C

PACS No.: 32.30.Bv; 33.20.Bx; 33.20.Ea; 33.20.Sn

1. Introduction

Two molecules, SiC and SiC₂, comprising silicon and carbon atoms have been observed in astronomical objects [1-4]. SiC₂ is an *a*-type asymmetric top molecule. Einstein A-coefficients for rotational transitions in the ground vibrational state as well as in the vibrationally excited ν_3 state of SiC₂ are calculated by Chandra & Rashmi [5] and Chandra & Sahu [6], respectively. A number of lines in the observed spectra of astronomical sources are still unidentified. Some of these lines may come from Si₂C [7, 8]. Very little information about this molecule is known. Theoretical study for structure of Si₂C have been carried out by some scientists. In the event of observation of Si₂C in interstellar medium, information about spectra of the molecule is essentially needed.

Since temperature in interstellar molecular clouds is generally low, probability of observation of Si₂C through its rotational transitions is high. Hence, in the present investigation, we have investigated transfer of radiation through a medium containing the Si₂C molecule.

2. The Si₂C molecule

Geometry of Si₂C molecule is shown in Figure 1 where the angle α is obtuse. The axis of symmetry of the molecule lies in its plane and is denoted by 1. Another axis lying in the plane, perpendicular to the axis 1 and passing through the centre-of-mass, is denoted by 2. We have one more axis, denoted by 3, perpendicular to the plane of the molecule and passing through the centre-of-mass. The moments of inertia about these principal inertial axes are denoted by I_1 , I_2 , and I_3 , respectively. Since α is an obtuse angle, for Si₂C, we get $I_2 < I_1 < I_3$. Hence, Si₂C is a *b*-type asymmetric top molecule as its electric dipole

Figure 1: Geometry of Si_2C molecule

moment μ lies along the axis of intermediate moment of inertia. Because of differences between the molecular parameters of Si_2C reported by various scientists, we decided to look into the effect of the two sets of the parameters (Table 1) given by Spielfiedel [9] and Barone et al. [10].

Table 1. Molecular parameters

	S	B
	cm^{-1}	cm^{-1}
A	2.0390911	2.13131
B	0.1461906	0.14281
C	0.1364001	0.13384
Δ_J	0.273212×10^{-6}	0.2889×10^{-6}
Δ_{JK}	$-0.2072262 \times 10^{-4}$	-25.3641×10^{-6}
Δ_K	0.4909885×10^{-3}	675.1668×10^{-6}
δ_J	0.4275785×10^{-7}	-0.0446×10^{-6}
δ_K	0.1080399×10^{-5}	-0.0007×10^{-6}
μ	0.904 D	0.85 D

S - Spielfiedel [9]; B - Barone et al. [10]

In a b -type asymmetric top molecule, allowed radiative transitions are governed by the selection rules [11, 12]:

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

where J denotes the rotational quantum number, and k_a and k_c are sub-quantum numbers. Hence, rotational energy levels of the molecule are divided into two groups, called ortho and para, which behave like quite distinct from each other. Einstein A-coefficients for allowed transitions between the levels for both sets of molecular data are calculated and

are available with the author. In the present investigation, we accounted for 27 rotational energy levels connected by 49 radiative transitions for each of the ortho as well para species.

3. Basic formulation

NLTE occupation numbers of energy levels of the molecule under investigation are calculated in an on-the-spot approximation by using the escape probability method [13], where the external radiation field, impinging on a volume element emitting the lines, is the cosmic 2.7 K background only. Besides the radiative transition probabilities for optically allowed transitions between the rotational levels, data required as input for the present investigation are rate coefficients for collisional transitions between the energy levels due to collisions with H_2 molecules. Collisional rate coefficients are not available in literature. Therefore, the rate coefficients for downward transitions $J'k'_ak'_c \rightarrow Jk_ak_c$ at a kinetic temperature T are taken as [14]

$$C(J'k'_ak'_c \rightarrow Jk_ak_c) = 1 \times 10^{-11} \sqrt{T/30} / (2J' + 1)$$

For upward collisional rate coefficients, we accounted for the fact that downward and upward collisional rate coefficients are related through the detailed equilibrium.

4. Numerical results and discussion

In order to include a large number of cosmic objects where Si_2C may be found, numerical calculations are carried out for wide ranges for physical parameters. The molecular hydrogen density n_{H_2} has been varied over the range from 10^3 cm^{-3} to 10^6 cm^{-3} , and calculations are performed for three kinetic temperatures 10, 20, and 30 K. In the calculations, free parameters are the hydrogen density 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.

A number of lines of Si_2C are found in absorption against the cosmic 2.7 K background. However, the transitions $4_{14} \rightarrow 5_{05}$, $5_{15} \rightarrow 6_{06}$, $2_{12} \rightarrow 3_{03}$, $3_{13} \rightarrow 4_{04}$, and $1_{11} \rightarrow 2_{02}$ at 15.9, 5.1, 33.6, 24.9, and 42.3 GHz, respectively, have shown reasonably good absorption phenomenon. Variation of line-intensity against the cosmic 2.7 K background in the unit of Planck's function at the kinetic temperature of $T(K)$, i.e., $(I_\nu - I_{\nu,bg})/B_\nu(T)$, for three kinetic temperatures 10, 20, and 30 K is shown in Figure 2 for the lines of Si_2C , for $\gamma = 10^{-6}$, and $10^{-5} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$. There are two sets of curves, one for the data of Spielfiedel [9] and the other for the data of Barone et al. [10]. In each pair, the above curve for the data of Barone et al. [10]. Qualitative behaviour of the results in the two sets for the data of Spielfiedel [9] and of Barone et al. [10] is very similar.

Figure 2 shows that the transitions $4_{14} \rightarrow 5_{05}$, and $5_{15} \rightarrow 6_{06}$ have the strongest absorption phenomenon for the molecule. With the increase of kinetic temperature, position of minimum in the graph is found to shift toward the low density region, and the absolute value of absorption is found to decrease.

Thus, the lines $4_{14} \rightarrow 5_{05}$, $5_{15} \rightarrow 6_{06}$, $2_{12} \rightarrow 3_{03}$, $3_{13} \rightarrow 4_{04}$, and $1_{11} \rightarrow 2_{02}$ at 15.9, 5.1, 33.6, 24.9, and 42.3 GHz, respectively, may play important role for identification of Si_2C in astronomical objects in a region having low temperature.

Figure 2: Variation of line-intensity against the cosmic 2.7 K background in the unit of Planck's function at the kinetic temperature of $T(\text{K})$, i.e., $(I_\nu - I_{\nu,bg})/B_\nu(T)$, for the transition written at the top of the column for three kinetic temperatures 10, 20, and 30 K. Negative value of line-intensity shows absorption against the cosmic 2.7 K background. Solid line is for $\gamma = 10^{-6} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$, and dotted line for $\gamma = 10^{-5} \text{ cm}^{-3} (\text{km/s})^{-1} \text{ pc}$. There are two sets of curves, one for the data of Spielfiedel [9] and the other for the data of Barone et al. [10]. In each pair, the above curve for the data of Barone et al. [10].

Acknowledgments

I am grateful to Prof. J.V. Narlikar, Prof. S.A. Suryawanshi, and Prof. Dr. W.H. Kegel for encouragement. Thanks are due to Dr. H.O. Vats for his help.

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