

## Search for an interstellar Si<sub>2</sub>C molecule: A theoretical prediction

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MS received 6 October 2003; revised 25 March 2004; accepted 8 April 2004

**Abstract.** We suggest that Si<sub>2</sub>C 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; Si<sub>2</sub>C.

**PACS Nos** 32.30.Bv; 33.20.Bx; 33.20.Ea; 33.20.Sn

### 1. Introduction

Two molecules, SiC and SiC<sub>2</sub>, comprising silicon and carbon atoms have been observed in astronomical objects [1–4]. SiC<sub>2</sub> 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  $\nu_3$  state of SiC<sub>2</sub> are calculated by Chandra and Rashmi [5] and Chandra and Sahu [6], respectively. A number of lines in the observed spectra of astronomical sources are still unidentified. Some of these lines may come from Si<sub>2</sub>C [7, 8]. Very little information about this molecule is known. Theoretical study of the structure of Si<sub>2</sub>C has been carried out by some scientists. In the event of observation of Si<sub>2</sub>C 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 Si<sub>2</sub>C through its rotational transitions is high. Hence, in the present investigation, we have investigated transfer of radiation through a medium containing the Si<sub>2</sub>C molecule.

## 2. The Si<sub>2</sub>C molecule

Geometry of Si<sub>2</sub>C molecule is shown in figure 1 where the angle  $\alpha$  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  $\alpha$  is an obtuse angle, for Si<sub>2</sub>C, we get  $I_2 < I_1 < I_3$ . Hence, Si<sub>2</sub>C is a *b*-type asymmetric top molecule as its electric dipole moment  $\mu$  lies along the axis of intermediate moment of inertia. Because of differences between the molecular parameters of Si<sub>2</sub>C 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].

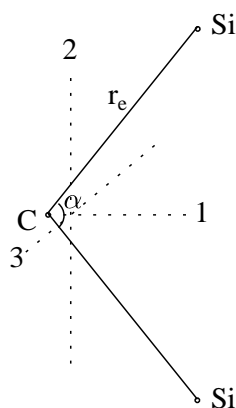


Figure 1. Geometry of Si<sub>2</sub>C molecule.

Table 1. Molecular parameters.

	S (cm <sup>-1</sup> )	B (cm <sup>-1</sup> )
$A$	2.0390911	2.13131
$B$	0.1461906	0.14281
$C$	0.1364001	0.13384
$\Delta_J$	$0.273212 \times 10^{-6}$	$0.2889 \times 10^{-6}$
$\Delta_{JK}$	$-0.2072262 \times 10^{-4}$	$-25.3641 \times 10^{-6}$
$\Delta_K$	$0.4909885 \times 10^{-3}$	$675.1668 \times 10^{-6}$
$\delta_J$	$0.4275785 \times 10^{-7}$	$-0.0446 \times 10^{-6}$
$\delta_K$	$0.1080399 \times 10^{-5}$	$-0.0007 \times 10^{-6}$
$\mu$	0.904 D	0.85 D

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

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

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

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 quite distinct from each other. Einstein  $A$ -coefficients for the 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 as *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<sub>2</sub> 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]

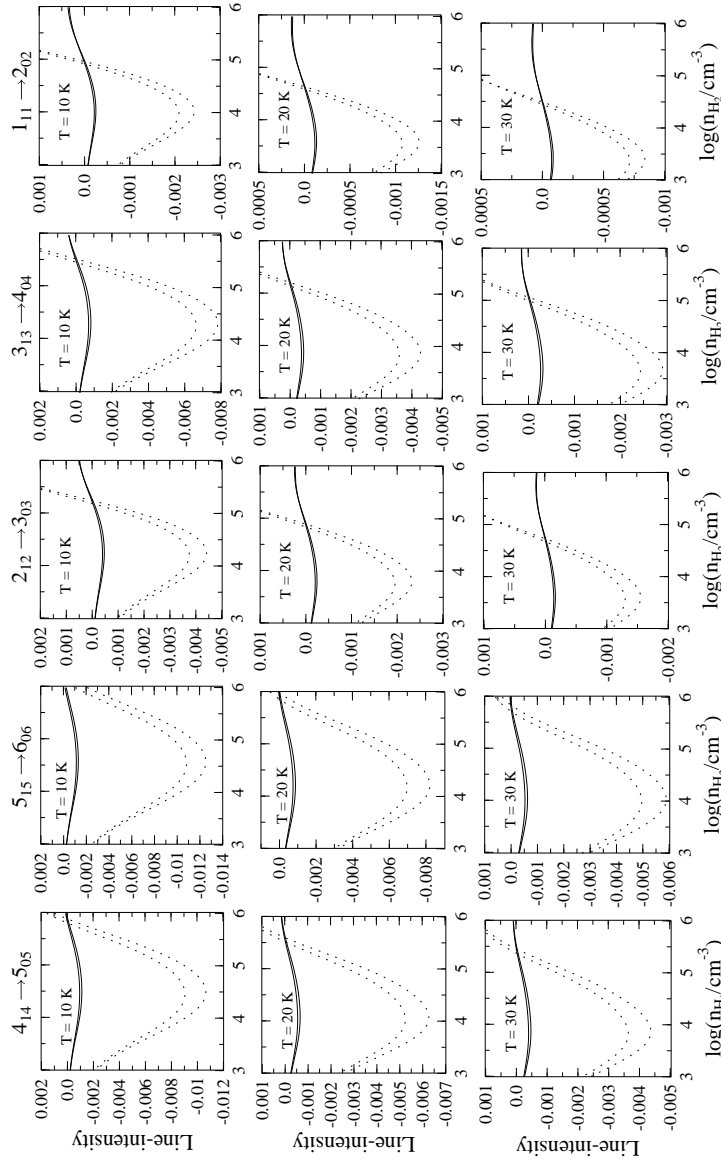
$$C(J'k'_ak'_c \rightarrow Jk_ak_c) = \frac{1 \times 10^{-11}}{2J' + 1} \sqrt{\frac{T}{30}}.$$

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<sub>2</sub>C may be found, numerical calculations are carried out for wide ranges for physical parameters. The molecular hydrogen density  $n_{\text{H}_2}$  has been varied over the range  $10^3 \text{ cm}^{-3}$  to  $10^6 \text{ cm}^{-3}$ , and calculations are performed for three kinetic temperatures 10, 20, and 30 K. In the calculations, free parameters are the hydrogen density  $n_{\text{H}_2}$  and  $\gamma \equiv n_{\text{mol}}/(dv_r/dr)$ , where  $n_{\text{mol}}$  is the density of the molecule and  $dv_r/dr$  is the velocity gradient.

A number of lines of Si<sub>2</sub>C 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



**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  $T$  (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 Spielfield [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].

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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.,  $(I_\nu - I_{\nu,\text{bg}})/B_\nu(T)$ , for three kinetic temperatures 10, 20, and 30 K is shown in figure 2 for the lines of Si<sub>2</sub>C, 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 top curve is 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  $5_{1,5} \rightarrow 6_{0,6}$  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 an important role for identification of Si<sub>2</sub>C in astronomical objects in a region having low temperature.

## Acknowledgements

The author is grateful to J V Narlikar, S A Suryawanshi, and W H Kegel for encouragement. Thanks are due to H O Vats for his help.

## References

- [1] P Thaddeus, S E Cummins and R A Linke, *Astrophys. J.* **283**, L45 (1984)
- [2] L E Snyder, C Henkel, J M Hollis and F G Lovas, *Astrophys. J.* **290**, L29 (1985)
- [3] J Cernicharo, C A Gottlieb, M Guelin, P Thaddeus and J M Vrtilek, *Astrophys. J.* **341**, L25 (1989)
- [4] J Cernicharo, C Kahane, J Gomez-Gonzalez and M Guelin, *Astron. Astrophys.* **167**, L9 (1986)
- [5] S Chandra and Rashmi, *Astron. Astrophys. Suppl.* **131**, 137 (1998)
- [6] S Chandra and A Sahu, *Astron. Astrophys.* **272**, 700 (1993)
- [7] W Weltner Jr. and D McLeod Jr., *J. Chem. Phys.* **41**, 235 (1964)
- [8] G H F Dierksen, N E Grüner, J Oddershede and J R Sabin, *Chem. Phys. Lett.* **117**, 29 (1985)
- [9] A Spielfiedel (1998) (private communication)
- [10] V Barone, P Jensen and C Minichino, *J. Mol. Spectrosc.* **154**, 252 (1992)
- [11] S Chandra, D A Varshalovich and W H Kegel, *Astron. Astrophys. Suppl.* **55**, 51 (1984)
- [12] S Chandra, *Indian J. Phys.* **B76**, 649 (2002)
- [13] E Rausch, W H Kegel, T Tsuji and G Piehler, *Astron. Astrophys.* **315**, 533 (1996)
- [14] A K Sharma and S Chandra, *Astron. Astrophys.* **376**, 333 (2001)