Indian J. Phys. **76B** (5), 649–655 (2002)

I J P B
— an international journal

Einstein *A*-coefficients for rotational transitions in the ground vibrational state of Si_2C molecule

Suresh Chandra
School of Physical Sciences, S R T M University, Nanded-431 606, Maharashtra, India
E-mail : sch@iucaa.ernet.in

Received 19 April 2000, accepted 5 June 2002

Abstract : We have calculated Einstein *A*-coefficients for rotational transitions in the ground vibrational state of the Si_2C molecule between the rotational energy levels up to 21 cm^{-1}. The coefficients are used to calculate the mean radiative lifetime of the levels. These *A*-coefficients may be used as input parameters for analyzing the spectra of Si_2C, as and when it would be observed in an astronomical object The transitions $7_{07} \rightarrow 6_{16}$ (5.34 GHz) and $8_{08} \rightarrow 7_{17}$ (14.74 GHz) may play important role for the search of the Si_2C molecule in astronomical objects.

Keywords . Si_2C molecule, Einstein *A*-coefficients

PACS Nos. : 33.20.Bx, 33.20.Ea, 33 70 -w

1. Introduction

Two molecules, SiC and SiC_2, comprising silicon and carbon atoms have already been observed in astronomical objects [1–4]. SiC_2 is an *a*-type asymmetric top molecule. Einstein *A*-coefficients for rotational transitions in the ground vibrational state, and in the vibrationally excited ν_3 state of SiC_2 have been 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. As per speculations [7,8] some of these lines may come from Si_2C, Si_2C_3, Si_3 or Si_4 molecules. Very little information about these molecules is known. Theoretical studies of Si_2C have, however, been carried out by a number of authors [9–12].

Since the temperature in astronomical objects, in general, is rather low, the probability of observation of Si_2C through its rotational transitions is larger than that through its vib-rotational ones. In the event of the observation of Si_2C in an astronomical object, Einstein *A*-coefficients for rotational transitions in the ground vibrational state of the molecule would be one of the input parameters required for analyzing the spectra. Therefore, in the present investigation, we have calculated Einstein *A*-coefficients for rotational transitions in the ground vibrational state of Si_2C molecule.

2. The Si_2C molecule –asymmetric rotor

Geometry of the Si_2C molecule is shown in Figure 1 where the angle α is obtuse. The axis of symmetry for the molecule, lying in its plane, 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 and passing through

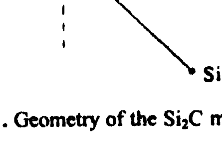

Figure 1. Geometry of the Si_2C molecule.

Inordinate delay in the acceptance of this manuscript is due to long time taken by the author for revision.

the centre of mass. The moments of inertia about these three (principal inertial) axes are

$$I_1 = 56r^2 \sin^2 \alpha/2,$$

$$I_2 = \frac{168}{17} r^2 \cos^2 \alpha/2,$$

$$I_3 = 56r^2 \left[1 - \frac{14}{17} \cos^2 \alpha/2 \right].$$

Since α is an obtuse angle, therefore $I_2 < I_1 < I_3$. As per convention, the three principal inertial axes are named a, b and c in a manner such that the moments of inertia about them, I_a, I_b and I_c repectively, satisfy the condition $I_a \le I_b \le I_c$. Thus, obviously, the electric dipole moment ($\mu = 0.904$ Debye) of the Si_2C is along the b-axis of inertia. Further, all the three moments of inertia are different, $I_a \ne I_b \ne I_c$. Hence, it is a b-type asymmetric top molecule. The molecular constants A, B and C are given by

$$A = \frac{\hbar^2}{2I_a}, \quad B = \frac{\hbar^2}{2I_b} \quad \text{and} \quad C = \frac{\hbar^2}{2I_c}.$$

Energy of a rigid rotor is given by

$$E(A,B,C) = \frac{P_a^2}{2I_a} + \frac{P_b^2}{2I_b} + \frac{P_c^2}{2I_c}$$

$$= \frac{AP_a^2 + BP_b^2 + CP_c^2}{\hbar^2}, \qquad (1)$$

where P_a, P_b and P_c are components of angular momentum, so that

$$P^2 = P_a^2 + P_b^2 + P_c^2 = J(J+1)\hbar^2,$$

where J is rotational quantum number.

For a spherical top molecule, $A = B = C$, and the energy of a rotational level with quantum number J is given by

$$E(J) = J(J+1)B.$$

Here, rotational energy levels have $(2J+1)$-fold degeneracy.

For a prolate symmetric top molecule $A \ne B = C$ (the axis of symmetry is the a-axis), and the energy of the rotational level, denoted by J_{K_a}, is given by

$$E(J_{K_a}) = J(J+1)B + K_a^2(A - C),$$

where K_a is the projection of J on the axis of symmetry a, and it can assume $(2J+1)$ values. For a given J, the level with $K_a = 0$ is the lowest one. Further, all the levels with $K_a \ne 0$ have a two-fold degeneracy as the energy does not depend on the sign of K_a.

For an oblate symmetric top molecule $A = B \ne C$ (the axis of symmetry is the c-axis), and the energy of the rotational level, denoted by J_{K_c}, is given by

$$E(J_{K_c}) = J(J+1)B - K_c^2(A - C),$$

where K_c is the projection of J on the axis of symmetry, c, and it can assume $(2J+1)$ values. For a given J, the level with $K_c = 0$ is the highest one. Further, all the levels with $K_c \ne 0$ have a two-fold degeneracy as the energy does not depend on the sign of K_c.

For asymmetric top molecule, unlike symmetric top molecules (prolate and oblate), there is no preferential axis, and the molecular intertial axes, a, b and c may be identified with the space-fixed axes, x, y and z in six ways (Table 1).

Table 1. The six representations of molecular fixed axes a, b and c identified with the space fixed axes x, y, and z and the parameters F, G, and H for the representations.

	I^r	I^l	II^r	II^l	III^r	III^l
x	b	c	c	a	a	b
y	c	b	a	c	b	a
z	a	a	b	b	c	c
F	$(\kappa - 1)/2$	$(\kappa - 1)/2$	0	0	$(\kappa + 1)/2$	$(\kappa + 1)/2$
G	1	1	κ	κ	-1	-1
H	$-(\kappa + 1)/2$	$(\kappa + 1)/2$	1	-1	$(\kappa - 1)/2$	$-(\kappa - 1)/2$

For two scalars σ and ρ, eq. (1) gives

$$E(\sigma A + \rho, \sigma B + \rho, \sigma C + \rho) = \sigma E(A,B,C) + \rho J(J+1). \qquad (2)$$

Now, we choose

$$\sigma = \frac{2}{A - C} \quad \text{and} \quad \rho = -\frac{A + C}{A - C},$$

so that

$$\sigma A + \rho = 1, \quad \sigma B + \rho = \frac{2B - A - C}{A - C} = \kappa,$$

and $\sigma C + \rho = -1$,

where κ is known as Ray asymmetry parameter, which is -1 for prolate top molecule, and $+1$ for oblate top molecule.

Energy levels for an asymmetric top molecule are denoted by J_{K_a,K_c} or J_τ, where a pseudo quantum number τ, given by $\tau = K_a - K_c$, can assume $(2J+1)$ values ranging from $-J$ to J. For a given J, the lowest level corresponds to $\tau = -J$. It shows that the level J_{K_a,K_c} lies in between the prolate level J_{K_a} and the oblate level J_{K_c}, depending on the value of κ. Thus, from eq. (2), we have

$$E(1,\kappa,-1) = E(\kappa) = \frac{2}{A - C} E(A,B,C)$$

$$- \frac{A + C}{A - C} J(J+1)$$

and thus energy of an asymmetric rotor is given by

$$E(A,B,C) = E(J_\tau) = \frac{A + C}{2} J(J+1)$$

$$+ \frac{A - C}{2} E(\kappa).$$

For computation of $E(\kappa)$, the matrix elements may be written as [13,14]

$$E_{KK} = FJ(J+1) - (F-G)K^2,$$

$$E_{KK\pm2} = 0.5H\left[J(J+1) - K(K\pm1)\right]^{1/2} \times \left[J(J+1) - (K\pm1)(K\pm2)\right]^{1/2},$$

where K is projection of J on the molecular fixed axis of quantization. Values of the parameters F, G, and H, which depend on the representation, are given in Table 1.

3. Symmetry properties of wavefunctions of asymmetric rotor

The ellipsoid of inertia for an asymmetric rotor has a four-group $V(a, b, c)$ symmetry with character table for the species A, B_a, B_b and B_c given in Table 2. Wavefunctions for rotational energy levels of an asymmetric top molecule can be expressed as [13–15] :

Table 2. Character table of $V(a, b, c)$ group, and evenness (e) and oddness (o) of K_a and K_c for the symmetry species

Symmetry species	E	C_2^a	C_2^b	C_2^c	K_a	K_c
A	1	1	1	1	e	e
B_a	1	1	−1	−1	e	o
B_b	1	−1	1	−1	o	o
B_c	1	−1	−1	1	o	e

$$A_{JK_aK_cM} = A_{J_\tau M} = \sum_K a_K^{J_\tau} \psi_{JKM\gamma},$$

where $\Psi_{JKM\gamma} = \frac{1}{\sqrt{2}}\left[\phi_{JKM} + (-1)^\gamma \phi_{J-KM}\right]$, for $K \neq 0$,

$= \phi_{J0M}$ for $K = 0$,

where γ is 0 or 1, ϕ_{JKM}'s the wavefunctions for symmetric top molecule and $a_K^{J_\tau}$ are expansion coefficients.

The wavefunctions $\Psi_{JKM\gamma}$ have the following characteristics with respect to the four group $V(x, y, z)$:

$$E : \psi_{JKM\gamma} \rightarrow \psi_{JKM\gamma},$$

$$C_2^x : \psi_{JKM\gamma} \rightarrow (-1)^{J+K+\gamma} \psi_{JKM\gamma},$$

$$C_2^y : \psi_{JKM\gamma} \rightarrow (-1)^{J+\gamma} \psi_{JKM\gamma},$$

$$C_2^z : \psi_{JKM\gamma} \rightarrow (-1)^{K} \psi_{JKM\gamma}.$$

These relations help in assigning the symmetry species of $V(x, y, z)$ for even and odd values of K and γ as given in Table 3. With the help of Tables 2 and 3, the energy levels and the energy matrix may be divided into four sub-matrices E^+, E^-, O^+ and O^-. E and O refer to the even and odd values of K, and the prefices + and – correspond to the even and odd (0 and 1) values of γ, respectively. The sub-matrices are given by [13–16]

Table 3. Assignment of space symmetry species with the sub-matrices.

Sub-matrix	K	γ	$J+\gamma$		Symmetry species	
			J_{even}	J_{odd}	J_{even}	J_{odd}
E^+	e	e	e	o	A	B_z
E^-	e	o	o	e	B_z	A
O^+	o	e	e	o	B_y	B_x
O^-	o	o	o	e	B_x	B_y

$$E^+(\kappa) = \begin{vmatrix} E_{00} & \sqrt{2}E_{02} & 0 & \cdots \\ \sqrt{2}E_{02} & E_{22} & E_{24} & \cdots \\ 0 & E_{24} & E_{44} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix}$$

$$E^-(\kappa) = \begin{vmatrix} E_{22} & E_{24} & \cdots \\ E_{24} & E_{44} & \cdots \\ \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots \end{vmatrix}$$

$$O^+(\kappa) = \begin{vmatrix} E_{11} + E_{-11} & E_{13} & 0 & \cdots \\ E_{13} & E_{33} & E_{35} & \cdots \\ 0 & E_{35} & E_{55} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix}$$

$$O^-(\kappa) = \begin{vmatrix} E_{11} - E_{-11} & E_{13} & 0 & \cdots \\ E_{13} & E_{33} & E_{35} & \cdots \\ 0 & E_{35} & E_{55} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{vmatrix}$$

and the division of the levels for J up to 3, for example, are given in Table 4. Energy of a rigid asymmetric rotor does

Table 4. Division of energy levels into four sub-groups, E^+, E , O^+, and O for the six representations

J	K_a	K_c	τ	I^r	I^l	II^r	II^l	III^r	III^l
0	0	0	0	E^+	E^+	E^+	E^+	E^+	E^+
1	0	1	−1	E^+	E^+	O^-	O^+	O^+	O^-
	1	1	0	O^+	O^-	E^+	E^+	O^-	O^+
	1	0	1	O^-	O^+	O^+	O	E^+	E^+
2	0	2	−2	E^+	E^+	E^+	E^+	E^+	E^+
	1	2	−1	O^+	O	O^-	O^+	E^-	E^-
	1	1	0	O^-	O^+	E^-	E^-	O^+	O^-
	2	1	1	E^-	E^-	O^+	O^-	O	O^+
	2	0	2	E^+	E^+	E^+	E^+	E^+	E^+
3	0	3	−3	E^+	E^+	O^-	O^+	O^+	O
	1	3	−2	O^+	O^-	E^+	E^+	O^-	O^+
	1	2	−1	O^-	O^+	O^+	O^-	E^+	E^+
	2	2	0	E^-	E^-	E^-	E^-	E^-	E^-
	2	1	1	E^+	E^+	O^-	O^+	O^+	O^-
	3	1	2	O^+	O^-	E^+	E^+	O^-	O^+
	3	0	3	O	O^+	O^+	O^-	E^+	E^+

not depend on the representation. However, the wavefunctions (expansion coefficients) depend strongly on the representation. This division into sub-matrices helps in the way that for a given J we have not to find out eigenvalues and eigenfunctions of a square matrix of order $(2J + 1)$, but to solve four sub-matrices, E^+, E , O^+ and O of orders given in Table 5.

Table 5. Order of submatrices

Submatrix	J even	J odd
E^+	$\frac{1}{2}(J + 2)$	$\frac{1}{2}(J + 1)$
E^-	$\frac{1}{2}J$	$\frac{1}{2}(J - 1)$
O^+	$\frac{1}{2}J$	$\frac{1}{2}(J + 1)$
O^-	$\frac{1}{2}J$	$\frac{1}{2}(J + 1)$

4. Eigenvalues and eigenfunctions of energy sub-matrices

For a given J, eigenvalues and eigenfunctions (*i.e.*, the coefficinets $a_K^{J\tau}$) of sub-matrices are calculated. For example, for $J = 3$, there are 2, 1, 2, and 2 levels belonging to E^+, E , O', and O sub-matrices, respectively. Thus, orders of sub-matrices E^+, E , O', and O for $J = 3$ are 2, 1, 2, and 2, respectively. Sub-matrices of orders 1 and 2 can be solved analytically also. The eigenvalues do not depend on the representation, and their values for J up to 3 is given in Table 6.

Table 6. Eigenvalues for the level.

J	K_a	K_c	Eigenvalue
0	0	0	0
1	0	1	$\kappa - 1$
	1	1	0
	1	0	$\kappa + 1$
2	0	2	$2[\kappa - (\kappa^2 + 3)^{1/2}]$
	1	2	$\kappa - 3$
	1	1	4κ
	2	1	$\kappa + 3$
	2	0	$2[\kappa + (\kappa^2 + 3)^{1/2}]$
3	0	3	$5\kappa - 3 - 2[4\kappa^2 + 6\kappa + 6]^{1/2}$
	1	3	$2[\kappa - (\kappa^2 + 15)^{1/2}]$
	1	2	$5\kappa + 3 - 2[4\kappa^2 - 6\kappa + 6]^{1/2}$
	2	2	4κ
	2	1	$5\kappa - 3 + 2[4\kappa^2 + 6\kappa + 6]^{1/2}$
	3	1	$2[\kappa + (\kappa^2 + 15)^{1/2}]$
	3	0	$5\kappa + 3 + 2[4\kappa^2 - 6\kappa + 6]^{1/2}$

Eigenfunctions depend on the representation and analytical expressions for the expenasion coefficients up to $J = 3$ are given below [15] :

$J = 0$ $\quad E^+ \quad a_0^{\lambda_1} = 1.$

$J = 1$ $\quad E^+ \quad a_0^{\lambda_1} = 1,$

$O^+ \quad a_1^{\lambda_1} = 1,$

$O^- \quad a_1^{\lambda_1} = 1.$

$J = 2$ $\quad E^- \quad a_0^{\lambda_1} = 1,$

$O^+ \quad a_1^{\lambda_1} = 1,$

$O^- \quad a_1^{\lambda_1} = 1,$

$$E^+ \quad a_0^{\lambda_1} = \frac{\left[\sqrt{(G-F)^2+3H^2}+(G-F)\right]^{1/2}}{\sqrt{2}\left[(G-F)^2+3H^2\right]^{1/4}},$$

$$a_2^{\lambda_1} = -\frac{|H|\left[\sqrt{(G-F)^2+3H^2}-(G-F)\right]^{1/2}}{H\sqrt{2}\left[(G-F)^2+3H^2\right]^{1/4}},$$

$$a_0^{\lambda_2} = \frac{\left[\sqrt{(G-F)^2+3H^2}-(G-F)\right]^{1/2}}{\sqrt{2}\left[(G-F)^2+3H^2\right]^{1/4}},$$

$$a_2^{\lambda_2} = \frac{|H|\left[\sqrt{(G-F)^2+3H^2}+(G-F)\right]^{1/2}}{H\sqrt{2}\left[(G-F)^2+3H^2\right]^{1/4}}.$$

$J = 3$

$$E^+ \quad a_0^{\lambda_1} = \frac{\left[\sqrt{(G-F)^2+15H^2}+(G-F)\right]^{1/2}}{\sqrt{2}\left[(G-F)^2+15H^2\right]^{1/4}},$$

$$a_2^{\lambda_1} = -\frac{|H|\left[\sqrt{(G-F)^2+15H^2}-(G-F)\right]^{1/2}}{H\sqrt{2}\left[(G-F)^2+15H^2\right]^{1/4}},$$

$$a_0^{\lambda_2} = \frac{\left[\sqrt{(G-F)^2+15H^2}-(G-F)\right]^{1/2}}{\sqrt{2}\left[(G-F)^2+15H^2\right]^{1/4}},$$

$$a_2^{\lambda_2} = \frac{|H|\left[\sqrt{(G-F)^2+15H^2}+(G-F)\right]^{1/2}}{H\sqrt{2}\left[(G-F)^2+15H^2\right]^{1/4}},$$

O^+

$$a_1^{\lambda_1} = \frac{\left[2\sqrt{4(G-F)^2+6(H^2+FH-GH)}+(4G-4F-3H)\right]^{1/2}}{2\left[4(G-F)^2+6(H^2+FH-GH)\right]^{1/4}},$$

$$a_3^{\lambda_1} = -\frac{|H|\left[2\sqrt{4(G-F)^2+6(H^2+FH-GH)}-(4G-4F-3H)\right]^{1/2}}{H2\left[4(G-F)^2+6(H^2+FH-GH)\right]^{1/4}},$$

$a_1^{\lambda_2} =$

$$\frac{\left[2\sqrt{4(G-F)^2+6(H^2+FH-GH)}-(4G-4F-3H)\right]^{1/2}}{2\left[4(G-F)^2+6(H^2+FH-GH)\right]^{1/4}},$$

$a_3^{\lambda_2} =$

$$\frac{|H|\left[2\sqrt{4(G-F)^2+6(H^2+FH-GH)}+(4G-4F-3H)\right]^{1/2}}{H2\left[4(G-F)^2+6(H^2+FH-GH)\right]}$$

() $a_1^{\lambda_1} =$

$$\frac{2\sqrt{4(G-F)^2+6(H^2-FH+GH)}+(4G-4F+3H)}{2\left[4(G-F)^2+6(H^2-FH+GH)\right]^{1/4}}$$

$$-\frac{|H|\left[2\sqrt{4(G-F)^2+6(H^2-FH+GH)}-(4G-4F+3H)\right]}{H2\left[4(G-F)^2+6(H^2-FH+GH)\right]^{1/4}}$$

$$\frac{\left[2\sqrt{4(G-F)^2+6(H^2-FH+GH)}-(4G-4F+3H)\right]^{1/2}}{2\left[4(G-F)^2+6(H^2-FH+GH)\right]^{1/4}}$$

$a_3^{\lambda_2} =$

$$\frac{|H|\left[2\sqrt{4(G-F)^2+6(H^2-FH+GH)}+(4G-4F+3H)\right]}{H2\left[4(G-F)^2+6(H^2-FH+GH)\right]^{1/4}}$$

Finally, the wavefunctions for asymmetric top molecules can be written as [17,18]

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

where α, β, γ are the Eulerian angles specifying the orientation of the molecule, D^J_{MK} is the Wigner D-function and the expansion coefficients $g^J_{\tau,K}$ are given as

$$g^J_{\tau,K}=\frac{1}{\sqrt{2}}a_K^{J\tau} \qquad \text{for } K>0,$$

$$=(-1)^{\gamma}\frac{1}{\sqrt{2}}a_K^{J\tau} \qquad \text{for } K<0,$$

$$=a_K^{J\tau} \qquad \text{for } K=0.$$

5. Distortional effects

Treatment of asymmetric top molecules discussed so far is for the rigid rotor case. However, owing to the rotational motion, the molecule is distorted and the energy levels are affected [19]. Energy of the level J_τ is therefore given by

$$E_{J\tau}=E^{(0)}_{J\tau}+E^{(1)}_{J\tau}+E^{(2)}_{J\tau}+E^{(3)}_{J\tau}+E^{(4)}_{J\tau},$$

where $E^{(0)}_{J\tau}$ is energy of the rigid molecule, and $E^{(1)}_{J\tau}$, $E^{(2)}_{J\tau}$, $E^{(3)}_{J\tau}$, $E^{(4)}_{J\tau}$ are various order corrections :

$$E^{(1)}_{J\tau}=-\Delta_J J^2(J+1)^2-\Delta_{JK}J(J+1)\langle P_z^2\rangle-\Delta_K\langle P_z^4\rangle$$

$$-2\delta_J\sigma J(J+1)\left[W_{J\tau}-\langle P_z^2\rangle\right]-2\delta_K\sigma\left[W_{J\tau}\langle P_z^2\rangle-\langle P_z^4\rangle\right],$$

$$E^{(2)}_{J\tau}=L_J J^3(J+1)^3+H_{JK}J^2(J+1)^2\langle P_z^2\rangle$$

$$+H_{KJ}J(J+1)\langle P_z^4\rangle+H_K\langle P_z^6\rangle+2h_J\sigma J^2(J+1)^2$$

$$\times\left[W_{J\tau}-\langle P_z^2\rangle\right]+2h_{JK}\sigma J(J+1)\left[W_{J\tau}\langle P_z^2\rangle-\langle P_z^4\rangle\right]$$

$$+2h_K\sigma\left[W_{J\tau}\langle P_z^4\rangle-\langle P_z^6\rangle\right],$$

$$E^{(3)}_{J\tau}=L_{JK}J^2(J+1)^2\langle P_z^4\rangle+L_{KJ}J(J+1)\langle P_z^6\rangle$$

$$+L_K\langle P_z^8\rangle+2l_K\sigma\left[W_{J\tau}\langle P_z^6\rangle-\langle P_z^8\rangle\right],$$

$$E^{(4)}_{J\tau}=P_K\langle P_z^{10}\rangle+2\sigma p_K\left[W_{J\tau}\langle P_z^8\rangle-\langle P_z^{10}\rangle\right],$$

where $\sigma=\frac{2A-B-C}{B-C}$; $W_{J\tau}=\frac{2E^{(0)}_{J\tau}-(B+C)J(J+1)}{2A-B-C}$.

$$\langle P_z^r\rangle=\sum_{K=-J}^{J}\left(g^J_{\tau,K}\right)^2K^r.$$

The distortional constants Δ_J, Δ_{JK}, Δ_K, δ_J, δ_K, H_J, H_{JK}, H_{KJ}, H_K, h_J, h_{JK}, h_K, L_{JK}, L_{KJ}, L_K, l_K, P_K, and p_K are derived form the observed spectra of the molecule. Values of rotational and some distortional constants for Si_2C molecule, received from Spielfiedel [20], are given in Table 7. (The distortional constants which are not given in the Table are zero.)

Table 7. Rotational and distortional constants of Si_2C in MHz.

Parameter	Value
A	61130.41277
B	4382.68308
C	4089.17195
Δ_J	0.00819
Δ_{JK}	−0.62125
Δ_K	14.71947
δ_J	0.00128
δ_K	0.03239

6. Selection rules for radiative transitions and probabilities for the allowed transitions

From the symmetries discussed in Section 3, for b-type asymmetric top molecule (e.g., Si_2C molecule), radiatively allowed transitions are governed by the selection rules [17,18] :

$J : \Delta J = 0, \pm 1,$

k_a, k_c : even, odd ↔ odd, even (ortho-transitions,)

even, even ↔ odd, odd (para-transitions.)

Thus, the molecule is divided into two independent species, called ortho and para. For radiative transitions between the rotational levels given by $A_{J\tau M}$ and $A_{J'\tau' M}$ the dipole moment matrix elements are

$$\langle \mu_x \rangle = \int A_{J'\tau' M} \mu \theta_x A_{J\tau M} d\Omega ,$$

$$\langle \mu_y \rangle = \int A_{J'\tau' M} \mu \theta_y A_{J\tau M} d\Omega ,$$

$$\langle \mu_z \rangle = \int A_{J'\tau' M} \mu \theta_z A_{J\tau M} d\Omega ,$$

where μ is the electric dipole moment of the molecule, and θ_x, θ_y and θ_z are direction cosines of the electric dipole moment.

In the first right (I^r) representation, where the axis of quantization is along the *a*-axis of inertia. For the transition $J'_{\tau'} - J_\tau$, the line strength $S(J'_{\tau'} - J_\tau)$ is given by

$$S(J'_{\tau'} - J_\tau) = \langle \mu_x \rangle^2 + \langle \mu_y \rangle^2 + \langle \mu_z \rangle^2 = \frac{\mu^2 (2J+1)}{2}$$

$$\times \left[\sum_{K=-J}^{J} g^{J}_{\tau K} \left\{ g^{J'}_{\tau' K+1} C^{J'K+1}_{JK1,1} + g^{J'}_{\tau' K-1} C^{J'K-1}_{JK1,-1} \right\} \right]^2 ,$$

where *C*'s are the Clebsch-Gordan coefficients [21]. Einstein *A*-coefficient for the transition $J'_{\tau'} \rightarrow J_\tau$ is given by

$$A(J'_{\tau'} \rightarrow J_\tau) = \frac{64 \pi^4 \nu^3 S(J'_{\tau'} - J_\tau)}{3hc^3 (2J'+1)} ,$$

where ν is the frequency of the transition, *h* the Planck's constant, and *c* the speed of light.

7. Results for Si$_2$C and discussion

The required values for the molecular constants and distortional constants for Si$_2$C molecule have been provided by Spielfiedel [20] and are given in Table 7. The value of electric dipole moment μ = 0.904 Debye has been obtained from Spielfiedel [20].

The computed value of the Einstein *A*-coefficients for rotational transitions between the levels up to 21 cm^{-1} are give in Tables 8 and 9 for ortho and para species, respectively. The Einstein *A*-coefficients are used for computing the mean radiative lifetime of the level :

$$T_{J'_{\tau'}} = \frac{1}{\sum_{J_\tau} A(J'_{\tau'} \rightarrow J_\tau)} . \qquad (3)$$

Table 8. Einstein *A*-coefficients for rotational transitions in ortho-Si$_2$C

J'	τ'	J	τ	A (s^{-1})	J'	τ'	J	τ	A (s^{-1})
1	1	1	–1	9.95×10^{-7}	2	–1	1	–1	1.23×10^{-6}
2	1	1	1	2.08×10^{-5}	2	1	2	–1	8.91×10^{-6}
2	–1	3	–3	7.29×10^{-8}	2	1	3	–1	1.32×10^{-6}
3	1	2	–1	1.88×10^{-5}	3	3	2	1	1.11×10^{-4}
3	–1	3	–3	6.26×10^{-7}	3	1	3	–1	1.28×10^{-5}
3	3	3	–3	1.11×10^{-9}	3	3	3	1	3.05×10^{-5}
3	1	4	–3	1.54×10^{-6}	3	3	4	–1	3.03×10^{-6}
4	–3	3	–3	2.03×10^{-6}	4	–1	3	–1	2.09×10^{-5}
4	1	3	–3	3.13×10^{-9}	4	1	3	1	9.80×10^{-5}
4	–1	4	–3	1.22×10^{-5}	4	1	4	–1	4.28×10^{-5}
4	–3	5	–5	8.71×10^{-9}	4	–1	5	–3	1.52×10^{-6}
4	1	5	–5	1.62×10^{-9}	4	1	5	–1	5.13×10^{-6}
5	–1	4	–3	1.90×10^{-5}	5	–3	5	–5	1.08×10^{-6}
5	–1	5	–3	1.23×10^{-5}	5	–1	6	–5	1.56×10^{-6}
6	–5	5	–5	3.07×10^{-6}	6	–3	5	–3	1.77×10^{-5}
6	–3	6	–5	1.17×10^{-5}	6	–3	7	–5	9.93×10^{-7}
7	–7	6	–5	3.03×10^{-10}	7	–3	6	–5	1.97×10^{-5}
7	–5	7	–7	1.05×10^{-6}	7	–3	7	–5	1.12×10^{-5}
7	–3	8	–7	9.95×10^{-7}	8	–7	7	–7	4.41×10^{-6}
8	–5	7	–5	2.04×10^{-5}	8	–5	8	–7	1.23×10^{-5}
8	–5	9	–7	6.15×10^{-7}	9	–9	8	–7	3.06×10^{-8}
9	–5	8	–7	2.27×10^{-5}	9	–7	9	–9	1.17×10^{-6}
9	–5	9	–7	1.13×10^{-5}	9	–5	10	–9	6.89×10^{-7}
10	–9	9	–9	6.25×10^{-6}	11	–11	10	–9	1.88×10^{-7}
11	–9	11	–11	1.33×10^{-6}					

Table 9. Einstein *A*-coefficients for rotational transitions in para-Si$_2$C

J'	τ'	J	τ	A (s^{-1})	J'	τ'	J	τ	A (s^{-1})
1	0	0	0	9.73×10^{-7}	1	0	2	–2	1.21×10^{-7}
2	2	1	0	2.09×10^{-5}	2	0	2	–2	1.01×10^{-6}
2	2	2	0	8.84×10^{-6}	2	2	3	–2	1.13×10^{-6}
3	–2	2	–2	1.59×10^{-6}	3	0	2	0	1.87×10^{-5}
3	2	2	–2	7.32×10^{-10}	3	2	2	2	1.11×10^{-4}
3	0	3	–2	1.12×10^{-5}	3	2	3	0	3.05×10^{-5}
3	–2	4	–4	3.20×10^{-8}	3	0	4	–2	1.49×10^{-6}
3	2	4	–4	3.93×10^{-10}	3	2	4	0	3.03×10^{-6}
4	0	3	–2	1.85×10^{-5}	4	2	3	0	9.80×10^{-5}
4	–2	4	–4	1.04×10^{-6}	4	0	4	–2	1.19×10^{-5}
4	2	4	–4	4.68×10^{-9}	4	2	4	0	4.28×10^{-5}
4	0	5	–4	1.62×10^{-6}	4	2	5	–2	5.13×10^{-6}
5	–4	4	–4	2.53×10^{-6}	5	–2	4	–2	1.88×10^{-5}
5	–2	5	–4	1.28×10^{-5}	5	–4	6	–6	2.90×10^{-11}
5	–2	6	–4	1.43×10^{-6}	6	–2	5	–4	1.82×10^{-5}
6	–4	6	–6	1.00×10^{-6}	6	–2	6	–4	1.11×10^{-5}
6	–2	7	–6	1.15×10^{-6}	7	–6	6	–6	3.65×10^{-6}
7	–4	6	–4	1.91×10^{-5}	7	–4	7	–6	1.20×10^{-5}
7	–4	8	–6	8.01×10^{-7}	8	–8	7	–6	6.64×10^{-9}
8	–4	7	–6	2.11×10^{-5}	8	–6	8	–8	1.10×10^{-6}
8	–4	8	–6	1.12×10^{-5}	8	–4	9	–8	8.37×10^{-7}
9	–8	8	–8	5.28×10^{-6}	9	–6	8	–6	2.19×10^{-5}
9	–6	9	–8	1.26×10^{-5}	9	–6	10	–8	4.49×10^{-7}
10	–10	9	–8	8.64×10^{-8}	10	–8	10	–10	1.23×10^{-6}
11	–10	10	–10	7.32×10^{-6}					

The calculated values of the mean radiative lifetime of the levels are given in Table 10. It is interesting to note down that there are no downward radiative transitions from the 2_{02}, 3_{03}, 4_{04}, 5_{05} and 6_{06} levels. Further, the lifetime of the levels 7_{07}, 8_{08}, 9_{09}, $10_{0,10}$ and $11_{0,11}$ is larger than that of the adjacent levels. The Einstein *A*-coefficients for rotational transitions $7_{07} \rightarrow 6_{16}$ (5.34 GHz) and $8_{08} \rightarrow 7_{17}$ (14.74 GHz) are 3.0×10^{-10} s^{-1} and 6.6×10^{-9} s^{-1}, respectively. These two transitions, particularly in the low density regions, may play an important role for the search of the Si_2C molecule in astronomical objects.

Table **10.** Energy and mean radiative lifetimes of the rotational levels

J	τ'	$E(\mathrm{cm}^{-1})$	T(s)	J	τ'	$E(\mathrm{cm}^{-1})$	T(s)
1	-1	0.28	-	0	0	0.00	-
3	-3	1.68	-	2	-2	0.84	-
1	1	2.26	1.01×10^6	1	0	2.25	9.14×10^5
2	-1	2.80	7.67×10^5	4	-4	2.80	-
3	-1	3.38	1.60×10^6	2	0	2.83	9.93×10^5
5	-5	4.20	-	3	-2	3.63	6.16×10^5
4	-3	4.73	4.91×10^5	4	-2	4.82	9.58×10^5
5	-3	6.25	9.23×10^5	6	-6	5.93	-
6	-5	7.73	3.26×10^5	5	-4	6.10	3.95×10^5
7	7	7.91	3.30×10^9	6	-4	7.93	9.97×10^7
2	1	8.73	3.22×10^4	2	2	8.73	3.24×10^4
3	1	9.57	3.02×10^4	3	0	9.57	3.19×10^4
7	-5	9.95	9.54×10^5	7	-6	9.67	2.74×10^5
4	-1	10.69	2.89×10^4	8	-8	10.16	1.51×10^8
8	-7	11.89	2.27×10^5	4	0	10.69	3.12×10^4
5	-1	12.09	3.04×10^4	5	-2	12.09	3.03×10^4
9	-9	12.70	3.27×10^7	8	-6	12.24	9.07×10^5
6	-3	13.52	3.28×10^4	6	-2	13.52	3.29×10^4
9	-7	14.83	8.58×10^5	9	-8	14.39	1.90×10^5
7	-3	15.50	3.14×10^4	7	-4	15.50	3.13×10^4
10	-9	17.17	1.60×10^5	10	-10	15.52	1.16×10^7
8	-5	17.76	3.00×10^4	10	-8	17.70	8.11×10^5
11	-11	18.62	5.31×10^6	8	-4	17.77	3.01×10^4
3	3	19.40	6.91×10^3	3	2	19.40	6.91×10^3
9	-5	20.32	2.89×10^4	11	-10	20.23	1.37×10^5
4	1	20.52	6.86×10^3	9	-6	20.30	2.86×10^4
11	-9	20.86	7.54×10^5	4	2	20.52	6.86×10^3

Acknowledgements

We are grateful to Professor J V Narlikar, IUCAA, Pune for encouragement. Thanks are due to Dr. A Spielfiedel for supplying the values of the molecular constants.

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 Kahane, J Gomez-Gonzalez and M Guelin *Astron Astrophys.* **167** L9 (1986)

[4] J Cernicharo, C A Gottlieb, M Guelin, P Thaddeus and J M Vrtilek *Astrophys J* **341** L25 (1989)

[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 L Mcleod (Jr.) *J Chem Phys* **41** 235 (1964)

[8] G H F Diercksen, N E Grüner, J Oddershede and J R Sabin *Chem Phys. Lett.* **117** 29 (1985)

[9] R S Grev and H F Schaefer III *J Chem Phys* **82** 4126 (1985)

[10] J R Sabin, J Oddershede, G H F Diercksen and N E Grüner *J. Chem Phys* **84** 354 (1986)

[11] C M L Rittby *J Chem Phys.* **95** 5609 (1991)

[12] A Spielfiedel, S Caeter, N Feautrier, G Chambaud and P Rosmus *J Phys Chem* **100** 10055 (1996)

[13] H C Allen and P C Cross *Molecular Vib-rotors* (New York : John Wiley) (1963)

[14] G W King, R M Hainer and P C Cross *J Chem Phys* **11** 27 (1943)

[15] S Chandra *Astrophys Space Sci.* **138** 221 (1987)

[16] W Gardy and R L Cook *Microwave Molecular Spectra* (New York Interscience) (1970)

[17] S Chandra, D A Varshalovich and W H Kegel *Astron Astrophys. Suppl. (France)* **55** 51 (1984)

[18] S Chandra, D A Varshalovich and W H Kegel *Pramāna* **25** 557 (1985)

[19] J K G Watson *J. Chem. Phys* **46** 1935 (1957)

[20] A Spielfiedel (private communication)

[21] A R Edmonds *Angular Momentum in Quantum Mechanics* (Princeton : Princeton Press) (1957)