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Einstein A-coefficients for rotational transitions in the ground vibrational state of $^{28}SiC_2$, $^{29}SiC_2$ and $^{30}SiC_2$

S. Chandra and Rashmi

School of Sciences, Indira Gandhi National Open University, New Delhi 110 068, India

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Abstract. Einstein A-coefficients for the electric dipole transitions in Silicon Dicarbide molecule and its isotopomers between rotational levels of the ground vibrational state up to 51 cm^{-1} are calculated. These coefficients are used for computing radiative life times of the levels. The A-coefficients are one of the important input parameters for the radiative transfer calculations[1].

Key words: molecular data — ISM: molecules — radio lines: stars — stars: IRC + 10216

1. Introduction

Spectral lines from astronomical objects at 95.579 GHz, 115.383 GHz and 140.918 GHz could not be assigned to any of the known molecular species for several years. Besides these lines some more spectral lines at 93.065 GHz, 94.245 GHz, 137.180 GHz, 141.751 GHz, 141.755 GHz and 170.742 GHz from cosmic objects, were identified as generated due to the transitions between the rotational levels in the cyclic molecule SiC_2 ($^{28}SiC_2$) by Thaddeus et al. (1984). Thaddeus et al. (1984) assigned 9 lines in the molecular envelope of the evolved carbon star IRC +10216 to SiC_2 and determined its rotational and lower order centrifugal distortion constants with sufficient accuracy to enable Snyder et al. (1985) to detect lowest lying $1_{0,1} \rightarrow 0_{0,0}$ transition. Till now over 30 transitions of SiC_2 are known in IRC +10216. In order to provide accurate frequencies, Bogey et al. (1991) recorded the rotational spectrum of SiC_2 in the ground and vibrationally excited ν_3 states.

The IRC +10216 (=CW Leo) is a cool carbon star with a rich molecular chemistry. A number of molecules are detected in the envelope of the star. Some of these molecules have been detected even in vibrationally excited states. In some cases scientists were not successful detecting molecules in vibrationally excited states. On the basis of these negative results it has been concluded that the excitation mechanisms in the envelope of IRC +10216 are rather complex. In order to learn more about these excitation mechanisms, one should search for the vibrationally excited states of other abundant molecules, already detected in IRC +10216 in the ground vibrational state. Among these molecules, SiC_2 is of special interest as it has already been detected in the ground vibrational state in IRC +10216 (Thaddeus et al. 1984; Gensheimer et al. 1992).

For analysing a spectrum, Einstein A-values for the transitions are one of the required data. Therefore, Einstein A-coefficients for rotational transitions in the vibrationally excited ν_3 state have been reported by Chandra & Sahu (1993). (In the paper of Chandra & Sahu (1993), ortho and para states may please be read with interchange. Further, the results for the para states (earlier reported ortho states) may please be treated as cancelled because the para states in the molecules are missing as the carbon nuclei do not posses any nuclear spin). Since one would like to study SiC_2 in the ground and vibrationally excited ν_3 states for the same physical conditions in the atmosphere of an astronomical object. Thus, in the present investigation, we have calculated the Einstein A-values for the rotational transitions between the levels up to 51 cm^{-1} in the ground vibrational state of SiC_2. Since $^{29}SiC_2$ and $^{30}SiC_2$ isotopomers of Silicon Dicarbide have been observed (Cernicharo et al. 1986), therefore, Einstein A-coefficients for rotational transitions in the ground vibrational state of these isotopomers are also calculated. Einstein A-values are used for calculating the radiative life times of the levels.

2. Silicon dicarbide molecule

High resolution spectroscopy has shown that Silicon Dicarbide is a three membered ring molecule with

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[1] Tables 2 to 5 are only available in electronic form at the CDS via anonymous ftp (135.79.128.5) or via http://cdsweb.u-strasbg.fr/Abstract.html

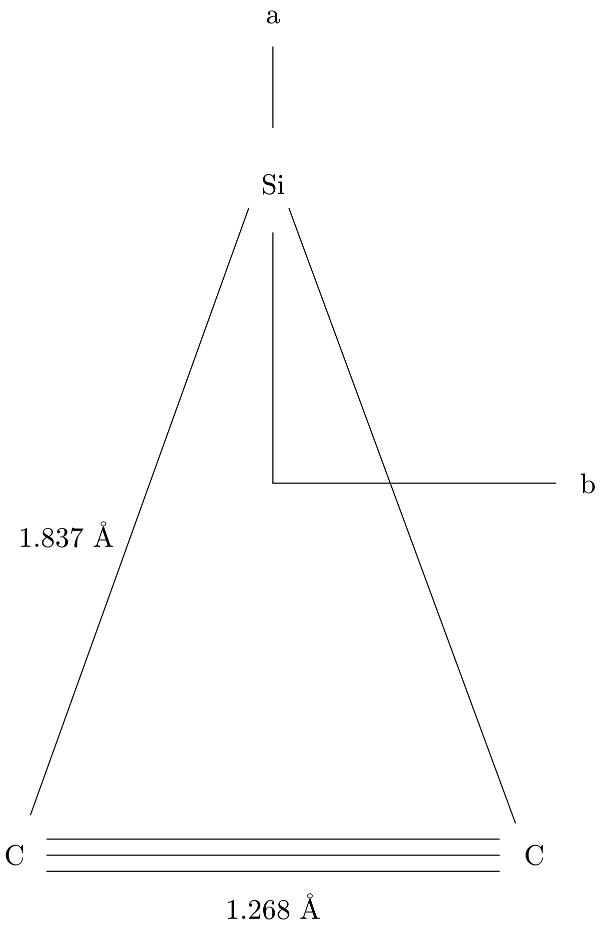

Fig. 1. The geometry of the ^{28}SiC$_2$ molecule

equivalent carbon atoms (Michalopoulos et al. 1984). Its linear isomer is less stable than the ring structure (Grev & Schaefer 1984). The bond length of Si-C and C-C are 1.837 Å and 1.268 Å, respectively. The geometry of Silicon Dicarbide molecule is shown in Fig. 1.

The Silicon Dicarbide molecule is an *a*-type asymmetric top molecule with dipole moment $\mu = 2.393$ D (Suenram et al. 1989). SiC$_2$ has three fundamental vibrational modes at $\nu_1 = 1742$ cm^{-1}, $\nu_2 = 837$ cm^{-1}, and $\nu_3 = 177$ cm^{-1} (Shepherd & Graham 1985, 1988; Gottlieb et al. 1989). The wavefunction of an asymmetric top molecule can be expressed as linear combination of wave functions for a symmetric top molecule (Chandra & Sahu 1993)

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

where α, β, γ are the Eulerian angles specifying the orientation of the molecule, J the rotational quantum number, $g^J_{\tau K}$ the expansion coefficient, D^J_{MK} the Wigner D-function.

The rotational transitions are governed by the selection rules

Table 1. Molecular constants used in the calculations

Constants	^{28}SiC$_2$	^{29}SiC$_2$	^{30}SiC$_2$
A(MHz)	52473.66(64)	52390.0	52390.0
B(MHz)	13158.654(26)	12947.1	12752.2
C(MHz)	10441.619(28)	10314.0	10189.1
Δ_J(MHz)	0.013115(52)	0.013115(52)	0.013115(52)
Δ_{JK}(MHz)	1.53689(34)	1.53689(34)	1.53689(34)
Δ_K(MHz)	−1.53(24)	−1.53(24)	−1.53(24)
δ_J(MHz)	0.002360(54)	0.002360(54)	0.002360(54)
δ_K(MHz)	0.850(10)	0.850(10)	0.850(10)
Φ_J(KHz)	−0.00026(21)	−0.00026(21)	−0.00026(21)
Φ_{JK}(KHz)	−0.141(21)	−0.141(21)	−0.141(21)
Φ_{KJ}(KHz)	0.665(73)	0.665(73)	0.665(73)
Φ_K(KHz)	−42.(21)	−42.(21)	−42.(21)
ϕ_J(KHz)	−0.000200(96)	−0.000200(96)	−0.000200(96)
ϕ_{JK}(KHz)	−0.037(15)	−0.037(15)	−0.037(15)
ϕ_K(KHz)	−1.73(96)	−1.73(96)	−1.73(96)

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

$$\begin{aligned} K_\mathrm{a}, K_\mathrm{c}: \quad & \text{odd, even} \longleftrightarrow \text{odd, odd} \quad (\text{para} - \text{transition}) \\ & \text{even, odd} \longleftrightarrow \text{even, even} \, (\text{ortho} - \text{transition}) \end{aligned}$$

K_a and K_c are sub-quantum numbers and each of them can assume the values ranging from 0 to J. On the basis of the selection rules, the rotational energy levels are grouped into two sets of transitions behaving as if they belong to two independent species. These species are referred to as para- and ortho-species, respectively.

3. Einstein *A*-coefficients

In a representation in which the axis of quantization is along *a*-axis of inertia, the expression for the line strength for *a*-type molecule is given by

$$S(J'_{\tau'} \to J_\tau) = \mu^2 (2J+1) \Big[\sum_{K=-J}^{J} g^J_{\tau K} g^{J'}_{\tau' K} C^{J'K}_{JK10} \Big]^2 \qquad (2)$$

where the C′s are Clebsch-Gordan coefficients. The transition probabilities follow directly from the line strength (Chandra & Sahu 1993)

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

where ν corresponds to the energy difference of the two levels. The rotational constants and quartic and sextic centrifugal distortion coefficients taken for Silicon Dicarbide from Bogey et al. (1984) are presented in Table 1. Table 1 carries also the constants for ^{29}SiC$_2$ and ^{30}SiC$_2$ isotopomers. The distortional constants for ^{29}SiC$_2$ and ^{30}SiC$_2$ are the same as for ^{28}SiC$_2$ (Cernicharo et al. 1986). The computed value of Einstein *A*-coefficients between the levels up to 51 cm^{-1} are given in Tables 2, 3 and 4 for ^{28}SiC$_2$ (Silicon Dicarbide), ^{29}SiC$_2$ and ^{30}SiC$_2$, respectively for ortho-rotational transitions in the ground vibrational state. Here, the primed parameters correspond to the upper level of the transition whereas the unprimed correspond to the lower level of transition. Table 5 shows the radiative life times of the levels which are calculated by using Einstein *A*-coefficients.

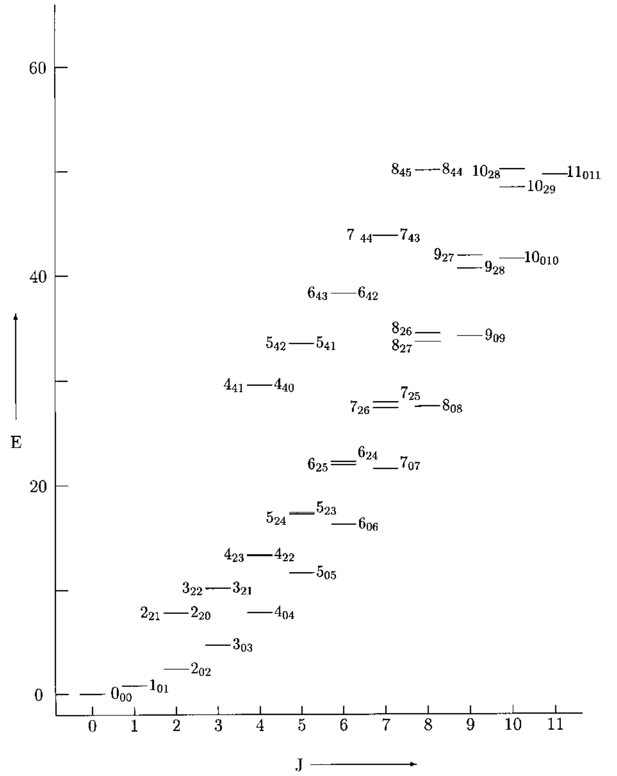

Fig. 2. Energy level diagram if rotationl levels in the ground vibrational state of $^{28}SiC_2$

4. Discussion

In the circumstellar envelope of IRC +10216 a number of molecules in the vibrationally excited state have been observed. Since the scientists are optimistic to detect SiC_2 in the vibrationally excited state at 177 cm^{-1} above the ground state, therefore Chandra & Sahu (1993) calculated Einstein A-coefficients for rotational transitions in the ν_3 vibrationally excited state of SiC_2. Their belief has a strong support since a number of molecules observed in the vibrationally excited state(s) in the envelope of IRC +10216 have the excited state(s) at quite high energies above the ground state. However, for the detailed study one has to account for both the ground and vibrationally excited states for the same physical conditions in the atmosphere. Therefore, Einstein A-coefficients for the rotational transitions in the ground vibrational state are also needed. Besides $^{28}SiC_2$, Einstein A-coefficients for rotational transitions in the ground vibrational state of $^{29}SiC_2$ and $^{30}SiC_2$ are also calculated.

After the careful survey of the energy level diagram in the ground vibrational state of $^{28}SiC_2$ (Silicon Dicarbide) (Fig. 2), we predict that the transition between the backbone levels 2_{02}, 3_{03}, 4_{04}, 5_{05} ... are of specific interest. Furthermore the ratios of the radiative lifetime of upper level to that of the lower level for the transitions $3_{03} \rightarrow 2_{02}, 4_{04} \rightarrow 3_{03}, 5_{05} \rightarrow 4_{04}, 6_{06} \rightarrow 5_{05}, 7_{07} \rightarrow 6_{06}, 8_{08} \rightarrow 7_{07}, 9_{09} \rightarrow 8_{08}$ are 0.281, 0.415, 0.514, 0.586, 0.642, 0.683, 0.716, respecively. This trend of increasing the value of the ratio of radiative lifetimes with the quantum number J reflects the probability for the detection of transition between the levels with higher values of J. However, the population of the levels decreases with the increase of J. Thus, in the ground vibrational state a compromising state may come around the transition $6_{06} \rightarrow 5_{05}$. Hence, in the ground vibrational state, the rotational transition $6_{06} \rightarrow 5_{05}$ may play an important role regarding the conclusions to be drawn about the excitation mechanism in the envelope of IRC +10216. However, a detailed analysis of radiative transfer for the three cases

(i) For rotational transitions in the ground vibrational state.

(ii) For rotational transitions in the vibrationally excited ν_3 state.

(iii) For the rotational and vib-rotational transitions in the ground and vibrationally excited state

are to be carried out. In the further work, we intend to investigate the radiative transfer calculations.

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