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Franck-Condon factors and r-centroids for certain band systems of SiD, SiF and SiN molecules of astrophysical interest

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Abstract. The Franck-Condon factors and r-centroids, which are very closely related to relative vibrational transition probabilities, have been computed by the more reliable numerical integration procedure for the bands of $A^2\Delta - X^2\Pi_r$ system of SiD, $D^2\Sigma^+ - X^2\Pi_r$ of SiF and $D^2\Pi_i - A^2\Pi_i$ system of SiN molecules of astrophysical interest, using a suitable potential.

Key words: molecular data — sunspots — stars M-type

1. Introduction

The theoretical prediction of intensity distribution in the spectra of many diatomic molecules which are of interest in astrophysics is necessary for an understanding of the physicochemical conditions of the emitting sources. The intensity distribution of various bands in any band system is mainly governed by the Franck-Condon factors.

The transition probability parameters are required for diagnostic applications in astrophysics and allied subjects. The Franck-Condon (FC) factors and r-centroids are important for determining the variation of electronic transition moment with internuclear separation (Rajamanickam 1985; Rajamanickam et al. 1993).

The SiD molecule is located in sun spots whereas SiF and SiN molecules are found in M-type stars (Nicholls 1977).

There has been no report on the FC factors and r-centroids for the band systems $A^2\Delta - X^2\Pi_r$ of SiD and $D^2\Sigma^+ - X^2\Pi_r$ of SiF, to our best knowledge, in the literature. In the case of $D^2\Pi_i - A^2\Pi_i$ of SiN only partial array of Franck-Condon factors and r-centroids are available (Joshi et al. 1981). Keeping in view of the above facts, we have carried out the calculation of Franck-Condon factors and r-centroids for these systems of astrophysical molecules SiD, SiF and SiN by a more accurate numerical integration procedure using a suitable potential and the complete array of FC factors and r-centroids have been presented.

2. Franck-Condon factors and r-centroids

Mathematically, one can write for the intensity $I_{v'v''}$ of a molecular band for a $v'-v''$ vibronic transition in emission as

$$I_{v'v''} = DN_{v'}E^4_{v'v''}R^2_e(\bar{r}_{v'v''})q_{v'v''} \quad (1)$$

where D is a constant partly depending on the geometry of the apparatus, $N_{v'}$ the population of the level v', $E_{v'v''}$ the energy quantum, $q_{v'v''}$ the FC factors, $r_{v'v''}$ the r-centroid and R_e the electronic transition moment.

The square of the overlap integral $q_{v'v''} = \langle\Psi_{v'}|\Psi_{v''}\rangle$ is termed as FC factor where $\Psi_{v'}$ and $\Psi_{v''}$ are the vibrational wave functions for the upper and lower states respectively. The r-centroid is the unique value of internuclear separation which may be associated with a $v'-v''$ band defined as

$$\bar{r}_{v'v''} = \frac{\langle\Psi_{v'}|r|\Psi_{v''}\rangle}{\langle\Psi_{v'}|\Psi_{v''}\rangle}. \quad (2)$$

The Morse (1929) potential yields accurate FC factors especially for vibrational transition involving low quantum numbers (Rajamanickam 1995; Nagarajan & Rajamanickam 1996). The computation of the FC factors is made by Bates' (1949) method of numerical integration according to the detailed procedure provided by Rajamanickam et al. (1994). The molecular constants used in the present study are collected from the compilation of Huber & Herzberg (1979) for the system $A - X$ of SiD, $D - X$ of SiF and $D - A$ of SiN. Morse wave functions are calculated at intervals of 10^{-2} Å for the range of r respectively from 1.29 Å to 1.91 Å, from 1.38 Å to

Table 1. $q_{v'v''}$ (a) and $r_{v'v''}$ (b, Å) for bands of $A^2\Delta - X^2\Pi_r$ system of SiD

v' \ v''	0	1	2
0	a) 0.994	0.008	0.001
	b) 1.540	2.514	1.731
1	a) 0.008	0.934	0.047
	b) 0.722	1.577	2.135
2	a) 0.000	0.056	0.751
	b) 2.679	1.171	1.611

1.80 Å and from 1.41 Å to 2.25 Å for every observed vibrational levels of A − X, D − X and D − A states of SiD, SiF and SiN molecules. Integrals appearing in the definitions of FC factors ($q_{v'v''}$) and r-centroids ($r_{v'v''}$) are computed numerically and the results are entered respectively in Tables 1, 2 and 3 for the system A − X of SiD, D − X of SiF and D − A of SiN. The wavelength ($\lambda_{v'v''}$) data (Bredohl et al. 1976) for D-A system of SiN molecule is also included in Table 3.

Table 2. $q_{v'v''}$ (a) and $r_{v'v''}$ (b, Å) for bands of $D^2\Sigma^+ - X^2\Pi_r$ system of SiF

v' \ v''	0	1	2	3
0	a) 0.602	0.297	0.082	0.017
	b) 1.576	1.523	1.472	1.420
1	a) 0.314	0.145	0.316	0.163
	b) 1.637	1.585	1.532	1.481
2	a) 0.074	0.363	0.007	0.228
	b) 1.679	1.646	1.597	1.541
3	a) 0.010	0.160	0.293	0.016
	b) 1.762	1.706	1.656	1.599
4	a) 0.000	0.032	0.228	0.188
	b) 1.833	1.771	1.715	1.665

Table 3. $q_{v'v''}$ (a), $r_{v'v''}$ (b, Å) and λ(c, Å) for bands of $D^2\Pi_i - A^2\Pi_i$ system of SiN

v' \ v	0	1	2	3	4	
0	0.0032	0.0220	0.0700	0.1406	0.1971	(a) (i)
	0.0029	0.0193	0.0614	0.1241	—	(ii)
	1.7392	1.7630	1.7871	1.8119	1.8373	(b) (i)
	1.7376	1.7604	—	—	—	(ii)
1	0.0161	0.0733	0.1396	0.1331	0.0514	(a) (i)
	0.0140	0.0647	0.1283	—	—	(ii)
	1.7233	1.7465	1.7699	1.7935	1.8166	(b) (i)
	1.7226	1.7451	—	—	—	(ii)
2	0.0418	0.1206	0.1136	0.0218	0.0135	(a) (i)
	0.0358	0.1093	—	—	—	(ii)
	1.7078	1.7304	1.7530	1.7738	1.8070	(b) (i)
	1.7225	1.7302	1.7528	—	—	(ii)
	—	—	3699	—	—	(c)
3	0.0758	0.1262	0.0356	0.0108	0.0804	(a) (i)
	0.0648	—	—	—	—	(ii)
	1.6927	1.7149	1.7360	1.7660	1.7854	(b) (i)
	1.6940	1.7146	1.7380	1.7604	—	(ii)
	—	3480	3608	3745	—	(c)
4	0.1081	0.0882	0.0000	0.0641	0.0641	(a) (i)
	—	—	—	—	—	(ii)
	1.6780	1.6997	1.1444	1.7464	1.7670	(b) (i)
	—	—	—	—	—	(ii)
	—	3401	3523	3653	—	(c)
5	0.1291	0.0370	0.0252	0.0660	0.0037	(a) (i)
	—	—	—	—	—	(ii)
	1.6637	1.6846	1.7098	1.7299	1.7236	(b) (i)
	—	—	—	—	—	(ii)
	—	3326	3443	—	—	(c)
6	0.1344	0.0046	0.0618	0.0222	0.0255	(a) (i)
	—	—	—	—	—	(ii)
	1.6497	1.6685	1.6941	1.7134	1.7466	(b) (i)
	—	—	—	—	—	(ii)
	—	3255	—	—	—	(c)
7	0.1253	0.0028	0.0678	0.0000	0.0554	(a) (i)
	—	—	—	—	—	(ii)
	1.6359	1.6609	1.6794	1.8205	1.7237	(b) (i)
	—	—	—	—	—	(ii)
	—	3187	—	—	—	(c)
8	0.1065	0.0237	0.0433	0.0188	0.0386	(a) (i)
	—	—	—	—	—	(ii)
	1.6224	1.6448	1.6651	1.6893	1.7080	(b) (i)
	—	—	—	—	—	(ii)
	—	3123	—	—	—	(c)

3. Results and discussion

The FC factors indicate that the $\Delta v = 0$ sequence bands are most intense followed by $\Delta v = \pm 1$ sequence for the A − X system of SiD. The sequence difference for this system is found to be constant and is about 0.035 Å.

In the case of D − X system of SiF, the FC factors indicate that the (0, 0) band is more intense followed by the $\Delta v = \pm 1$ sequence bands. The $\Delta v = 0$ sequence difference vary between 0.002 Å to 0.012 Å but the $\Delta v = \pm 1$ sequence difference is found to be constant and is about 0.009 Å.

In the case of D − A system of SiN, Joshi et al. (1981) have reported FC factors for (0, 0), (0, 1), (0, 2), (0, 3), (1, 0), (1, 1), (1, 2), (2, 0), (2, 1) and (3, 0) bands and r-centroid for (0, 0), (0, 1), (1, 0), (1, 1), (2, 0), (2, 1), (2, 2),

Table 3. continued

v / v'	5	6	7	8	9	
0	0.2070	0.1677	0.1071	0.0546	0.0223	(a) (i)
	—	—	—	—	—	(ii)
	1.8635	1.8907	1.9191	1.9489	1.9803	(b) (i)
	—	—	—	—	—	(ii)
1	0.0000	0.0452	0.1288	0.1627	0.1307	(a) (i)
	—	—	—	—	—	(ii)
	1.7222	1.8751	1.9006	1.9285	1.9581	(b) (i)
	—	—	—	—	—	(ii)
	—	4465	4664	—	—	(c)
2	0.0868	0.0826	0.0126	0.0159	0.0980	(a) (i)
	—	—	—	—	—	(ii)
	1.8276	1.8511	1.8704	1.9163	1.9391	(b) (i)
	—	—	—	—	—	(ii)
	—	—	—	4722	4939	(c)
3	0.0452	0.0011	0.0633	0.0792	0.0135	(a) (i)
	—	—	—	—	—	(ii)
	1.8068	1.8605	1.8622	1.8856	1.9044	(b) (i)
	—	—	—	—	—	(ii)
4	0.0024	0.0645	0.0407	0.0019	0.0647	(a) (i)
	—	—	—	—	—	(ii)
	1.8071	1.8179	1.8386	1.8935	1.8969	(b) (i)
	—	—	—	—	—	(ii)
	3937	—	—	4439	4631	(c)
5	0.0522	0.0352	0.0057	0.0635	0.0244	(a) (i)
	—	—	—	—	—	(ii)
	1.7776	1.7972	1.8361	1.8501	1.8691	(b) (i)
	—	—	—	—	—	(ii)
6	0.0482	0.0009	0.0547	0.0166	0.0196	(a) (i)
	—	—	—	—	—	(ii)
	1.7596	1.8081	1.8083	1.8253	1.8637	(b) (i)
	—	—	—	—	—	(ii)
7	0.0054	0.0387	0.0259	0.0125	0.0510	(a) (i)
	—	—	—	—	—	(ii)
	1.7381	1.7701	1.7878	1.8223	1.8384	(b) (i)
	—	—	—	—	—	(ii)
8	0.0093	0.0441	0.0010	0.0477	0.0038	(a) (i)
	—	—	—	—	—	(ii)
	1.7359	1.7523	1.7995	1.7991	1.8071	(b) (i)
	—	—	—	—	—	(ii)

(a) $a_{v'v''}$ (i) Present study; (ii) Joshi et al. (1981)
(b) $r_{v'v''}$ (Å) (i) Present study; (ii) Joshi et al. (1981).

(3, 0), (3, 1), (3, 2) and (3, 3) bands. They have used the approximate analytical method proposed by Fraser & Jarmain (1953). However Bredohl et al. (1976) have observed experimentally the following 19 bands (8, 1), (7, 1), (6, 1), (5, 1), (4, 1), (3, 1), (5, 2), (4, 2), (3, 2), (2, 2), (4, 3), (3, 3), (4, 5), (4, 8), (1, 6), (4, 9), (1, 7), (2, 8), (2, 9).

In the present study the complete array of FC factors and r-centroids have been presented and the calculations are carried out by the most accurate numerical integration procedure.

The $\Delta v = 0$ sequence difference for this system vary between 0.001 Å to 0.01 Å and the $\Delta v = \pm 1$ sequence difference vary between 0.04 Å to 0.128 Å.

References

Bates D.R., 1949, Proc. Roy. Soc. A196, 217

Bredohl H., Dubois I., Houbrechts Y., 1976, Can. J. Phys. 54, 680

Fraser P.A., Jarmain W.R., 1953, Proc. Phys. Soc. A66, 1145

Huber K.P., Herzberg G., 1979, Molecular Spectra and Molecular Structure, Vol. IV, Constants of Diatomic Molecules, Van Nostrand Reinhold, New York

Joshi V.C., Mamtajoshi., Singh R.N., 1981, Indian J. Phys. 55B, 335

Morse P.M., 1929, Phys. Rev. 34, 57

Nagarajan K., Rajamanickam, 1996, Acta Phys. Slov. 46, 645

Nicholls R.W., 1977, ARA&A 15, 197

Rajamanickam N., 1985, Pramana 25, 179

Rajamanickam N., Fernandez Gomez M., Lopez Gonzalez J.J., 1993, Collect. Czech. Chem. Commun. 58, 748

Rajamanickam N., Kannan K., Jaganathan C., 1994, Opt. Pura Aplic. 27, 209

Rajamanickam N., Karthikeyan G., Jaganathan S., 1995, Ap&SS 225, 271