Franck-Condon factors and r-centroids for the B, C, D – X and d-b band systems of astrophysical molecule BF

V. Raja and N. Rajamanickam

Physics Research Centre, V.H.N.S.N. College, Virudhunagar 626 001, India

Abstract. The Franck-Condon factors and r-centroids, which are very closely related to transition probabilities, have been evaluated by the reliable numerical integration procedure for the bands of $B^1\Sigma^+ - X^1\Sigma^+$, $C^1\Sigma^+ - X^1\Sigma^+$ $D^1\pi - X^1\Sigma^+$ and $d^3\pi - b^3\Sigma^+$ systems of astrophysical molecule BF, using Morse potential.

Key words : Franck - Condon factors and r-centroids – B,C,D $\rightarrow$ X and d-b band systems - BF molecule.

1. Introduction

The theoretical prediction of intensity distribution in the band system requires knowledge of vibrational transition probabilities which are to a good approximation proportional to the Frank - Condon (FC) factors. A precise knowledge of FC factors and related quantities are required for diagnostic applications in astronomy, astrophysics and allied subjects. The FC factors and r-centroids play an important role to arrive at the variation of electronic transition moment and vibrational temperature of the source.

Dealing with 300 diatomic molecules of known or of possible astrophysical interest, Sauval and Tatum (1984) report polynomial expressions of partition functions and equilibrium constants for the molecule BF also.

There has been no report on the FC factors and r – centroids for the band systems $B^1\Sigma^+ - X^1\Sigma^+$, $C^1\Sigma^+ - X^1\Sigma^+$, $D^1\pi - X^1\Sigma^+$ and $d^3\pi - b^3\Sigma^+$ of astrophysical molecule BF (Huber and Herzberg, 1979). Therefore the reliable values of FC factors and r – centroids for these band systems of the BF molecule have been determined by the numerical integration procedure, using the Most potential.

2. Franck-Condon Factors and r-centroids

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

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

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 Franck-Condon factor, $\bar{r}_{v'v''}$ the r-centroid and R_e the electronic transition moment.

The square of the overlap integral is termed as FC factor

$$q_{v'v''} = | \langle \Psi_{v'} | \Psi_{v''} \rangle |^2 \tag{2}$$

where $\Psi_{v'}$ and $\Psi_{v''}$ are the vibrational wave functions for the upper and lower states, respectively. The r-centroid is a unique value of internuclear separation associated with a $v' - v''$ band and defined as

$$\bar{r}_{v'v''} = \frac{\langle \Psi_{v'} | r | \Psi_{v''} \rangle}{\langle \Psi_{v'} | \Psi_{v''} \rangle} \tag{3}$$

For a proper understanding of the intensity distribution in the band systems of the molecules, it is necessary to choose a suitable potential. The Morse (1929) potential yields accurate FC factors especially for vibrational transition involving low quantum numbers (Anandaraj et al. 1992, Nagarajan and Rajamanickam 1998, Raja and Rajamanickam 2000). The computation of the FC factor is made by Bates's (1949) method of numerical integration according to the procedure detailed in Nagarajan et al. 1998, Partal et al. (2000) and Rajamanickam et al. (2000). Morse wave functions are calculated at intervals of 0.01Å for the range of r respectively from 1.06 Å to 1.59 Å, from 1.05 Å to 1.57 Å, from 1.08 Å to 1.48 Å and from 1.05 Å to 1.45 Å for every observed (in laboratory) vibrational level of B-X, C-X, D-X and d-b states of BF molecule. Integrals in the equations (2) and (3) for the FC factors ($q_{v'v''}$) and r-centroids ($\bar{r}_{v'v''}$) are computed numerically and the results are presented respectively in Tables 1, 2, 3 and 4 for the systems B-X, C-X, D-X and d-b of BF molecule. The wavelengths ($\lambda_{v'v''}$) data (Maltsev 1960, Caton and Dougles 1970) are also entered in the respective tables for all systems. The molecular constants used in the present study are collected from the compilation of Huber and Herzberg (1979).

3. Results and Discussion

Tables 1 to 4 clearly show that the (0,0) bands of each considered transition are the most intense ones followed by the $\Delta v = \pm 1$ and the $\Delta v = \pm 2$ sequences in that order. In the case of the d-b system, only those bands that correspond to $\Delta v = 0$ sequence are the bright ones.

Since $r'_e < r''_e$ for all the band systems of BF molecule, the r – centroid values increase with the decrease in wavelength which is expected in the violet degraded band system. For BF molecule, the sequence differences for all these band systems are found to be constant and is about 0.01Å which suggests that the potentials are not wide. The r – centroid values for all the (0,0) transitions are slightly greater than $(r'_e + r''_e)/2$ and hence the potentials are not very anharmonic.

Table 1. $q_{v'v''}$ and $\bar{r}_{v'v''}$ for B-X system of BF.

v',v''	$\lambda_{v'v''}$(Å)	$q_{v'v''}$	$\bar{r}_{v'v''}$(Å)
0,0	1527.1	0.611	1.239
0,1	1559.9	0.291	1.187
0,2	1593.6	0.080	1.137
0,3	1628.1	0.017	1.086
0,4	1663.6	0.003	1.032
1,0	1489.2	0.310	1.301
1,1	1520.4	0.153	1.249
1,2	1552.3	0.313	1.198
1,3	1585.1	0.161	1.149
1,4	1618.7	0.050	1.099
1,5	1653.1	0.012	1.047
1,6	1688.4	0.002	0.991
2,0	1453.7	0.071	1.362
2,1	1483.4	0.365	1.311
2,3	1544.9	0.223	1.209
2,4	1576.8	0.206	1.160
2,5	1609.4	0.092	1.112
2,6	1642.8	0.028	1.062
2,7	1677.1	0.007	1.008
3,1	1448.7	0.159	1.372
3,2	1477.6	0.295	1.322
3,4	1537.6	0.114	1.220
3,5	1568.6	0.205	1.172
3,7	1632.8	0.051	1.076

Table 2. $q_{v'v''}$ and $\bar{r}_{v'v''}$ for C-X system of BF.

v',v''	$\lambda_{v'v''}$(Å)	$q_{v'v''}$	$\bar{r}_{v'v''}$(Å)
0,0	1446.9	0.760	1.246
0,1	1476.3	0.203	1.175
0,2	1506.4	0.034	1.106
0,3	1537.2	0.004	1.035
1,0	1414.6	0.216	1.329
1,1	1442.6	0.400	1.258
1,2	1471.3	0.290	1.185
1,3	1500.7	0.080	1.117
1,4	1530.7	0.014	1.048
2,0	1384.3	0.025	1.413
2,1	1411.0	0.331	1.340
2,2	1438.4	0.183	1.271
2,3	1466.5	0.303	1.195
2,4	1495.2	0.124	1.128
3,2	1407.6	0.378	1.353
3,4	1461.8	0.274	1.206
3,5	1489.8	0.159	1.139
4,3	1404.3	0.379	1.365
4,5	1457.3	0.224	1.216
5,4	1401.0	0.353	1.379

Table 3. $q_{v'v''}$ and $\bar{r}_{v'v''}$ for D-X system of BF.

v',v''	$\lambda_{v'v''}$(Å)	$q_{v'v''}$	$\bar{r}_{v'v''}$(Å)
0,0	1383.8	0.733	1.245
0,1	1410.7	0.224	1.179
1,0	1352.7	0.231	1.322
1,1	1378.4	0.338	1.255
1,2	1404.5	0.316	1.191
2,0	1323.5	0.035	1.393
2,1	1348.0	0.337	1.333
2,2	1373.0	0.114	1.263
2,3	1398.5	0.315	1.203
3,2	1343.3	0.353	1.344

Table 4. $q_{v'v''}$ and $\bar{r}_{v'v''}$ for d-b system of BF.

v',v''	$\lambda_{v'v''}$(Å)	$q_{v'v''}$	$\bar{r}_{v'v''}$(Å)
0,0	10293.9	0.993	1.218
1,1	10199.5	0.964	1.230
2,2	10084.2	0.904	1.241
3,3	9939.8	0.806	1.252
4,4	9757.0	0.665	1.262

Acknowledgements

References

Anandaraj R. et al., 1992, Bull. Astr. Soc. India, 20, 279.

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

Caton R.B., Douglas A.E., 1970, Can. J. Phys., 48, 432.

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

Maltes A.A., 1960, Optics & Spectrosc., 9, 225.

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

Nagarajan K., Rajamanickam N., 1998, Astrophys. Space Sci., 259, 421.

Nagarajan K.; et al., 1998, Astron. Astrophys. Suppl. Ser., 129, 157.

Partal F. et al., 2000, Astrophys. Space Sci., 272, 345.

Raja V., Rajamanickam N., 2000, Astrophys. Space Sci., 271, 59.

Rajamanickam N. et al., 2000, Astrophys. Space Sci., in press.

Sauval A.J., Tatum J.B., 1984, Astrophys. J. Suppl. Ser., 56, 193.