# FRANCK-CONDON FACTORS AND *r*-CENTROIDS FOR CERTAIN BAND SYSTEMS OF ASTROPHYSICAL MOLECULES SrF AND ScF

P. SRI RAMACHANDRAN[1], N. RAJAMANICKAM[1], S.P. BAGARE[2,3] and BALA CHANDRA KUMAR[1]

[1]*Physics Research Centre, V.H.N.S.N. College, Virudhunagar, India*
[2]*Indian Institute of Astrophysics, Kodaikanal, Tamil Nadu, India*
[3]*Indian Institute of Astrophysics, Koramangala, Bangalore, India*
*E-mail: dkbaldr@rediffmail.com*

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**Abstract.** The Franck-Condon factors and *r*-centroids, which are very closely related to vibrational transition probabilities, have been evaluated by the more reliable numerical integration procedure for the bands of $B^2\sum^+ - X^2\sum^+$, $F^2\sum^+ - X^2\sum^+$ systems of SrF and $C^1\sum^+ - X^1\sum^+$, $G^1\Pi - X^1\sum^+$ systems of ScF molecules of astrophysical interest, using a suitable potential.

**Keywords:** Franck-Condon factors, *r*-centroids, sunspot spectra

## 1. Introduction

The Franck-Condon (FC) factor of a molecular band plays a controlling role in the determination of the relative band intensity. 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 physico-chemical conditions of the emitting sources.

The transition probability parameters are required for diagnostic applications in astronomy, astrophysics and allied subjects. To a good approximation, the FC factors are proportional to these transition probabilities. A precise knowledge of the FC factors and related quantities are essential to understand and to calculate many important aspects of the astrophysical molecules, such as radiative life times, vibrational temperatures and kinetics of the energy transfer.

Nicholls (1977) and Singh and Charturvedi (1987) reported the presence of SrF molecule in sunspot spectra. Based on the estimates of abundances of Sr and Sn, the flourides of these second row transition metals are expected to be present in stars. Since oxides of Sc are present in sunspots (Wohl, 1971) and in M-type stars (Nicholls, 1977), fluorides of Sc are also expected to be present in these celestial objects. Further, Sauval and Tatum (1984) predicted the possible presence of SrF and ScF molecules in stellar and cometary spectra. The estimates of relative abundances of these metallic species are important for understanding the evolutionary phases of the stars observed and are also the essential inputs in modeling the stellar

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atmospheres of the late type stars. Their relative abundances in interstellar medium give estimates of stellar activity like supernovae in the region observed. Similarly, their abundance variations in cometary spectra can be used to study the interaction of solar wind with cometary material. Also, the relative abundances of these metallic species are useful in studying the cosmic recipe in these pristine objects.

To the best of our knowledge, there has been no report on the FC factors and $r$-centroids for the band systems B–X and F–X of SrF and C–X and G–X of ScF in the literature. Therefore the reliable values of the FC factors and $r$-centroids for these band systems of the astrophysically important molecules SrF and ScF have been determined in this study by using a numerical integration procedure adopting a suitable potential.

## 2. Franck-Condon Factors and $r$-Centroids

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

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

where $D$ is a constant depending partly on the geometry of the apparatus, $N_{\nu'}$ the population of the level $\nu'$, $E_{\nu'\nu''}$ the energy quantum, $q_{\nu'\nu''}$ the Franck-Condon factor, $\bar{r}_{\nu'\nu''}$ the $r$-centroid and $R_{\mathrm{e}}$ the electronic transition moment.

The square of the overlap integral is termed as FC factor

$$q_{\nu'\nu''} = |\langle \psi_{\nu'} \mid \psi_{\nu''} \rangle|^2 \tag{2}$$

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

$$\bar{r}_{\nu'\nu''} = \frac{\langle \psi_{\nu'} | r | \psi_{\nu''} \rangle}{\langle \psi_{\nu'} \mid \psi_{\nu''} \rangle} \tag{3}$$

The Morse (1929) potential function yields the accurate FC factors especially for vibrational transition involving low quantum numbers (Rajamanickam et al., 2000; Partal et al., 2000; Prithivikumaran et al., 2002). The computation of the FC factor is made by Bates's (1949) method of numerical integration according to the detailed procedure provided by Rajamanickam et al. (2000, 2002). The Morse wave functions are calculated at intervals of 0.01 Å for the range of $r$, respectively, from 1.16 to 1.63, 1.8 to 2.32 and 1.65 to 2.16 Å, from 1.63 to 2.06 Å for every observed vibrational level of B–X, F–X and C–X, G–X of SrF and ScF molecules. Integrals in Eqs. (2) and (3) for the FC factors ($q_{\nu'\nu''}$) and $r$-centroids ($\bar{r}_{\nu'\nu''}$) are computed numerically and the results are presented, respectively, in Tables I–IV

TABLE I
Franck-Condon factors and $r$-centroids of B–X bands of SrF

| | $\nu''$ | | | | | | |
|---|---|---|---|---|---|---|---|
| | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| $\nu' = 0$ | | | | | | | |
| (a) | 0.998 | 0.003 | * | * | * | * | * |
| (b) | 2.083 | 2.982 | | | | | |
| (c) | – | – | | | | | |
| $\nu' = 1$ | | | | | | | |
| (a) | 0.003 | 0.992 | 0.006 | * | * | * | * |
| (b) | 1.195 | 2.092 | 2.972 | | | | |
| (c) | 5623.3 | – | – | | | | |
| $\nu' = 2$ | | | | | | | |
| (a) | * | 0.006 | 0.986 | 0.009 | * | * | * |
| (b) | | 1.227 | 2.102 | 2.964 | | | |
| (c) | | 5627.1 | – | – | | | |
| $\nu' = 3$ | | | | | | | |
| (a) | * | * | 0.009 | 0.979 | 0.013 | * | * |
| (b) | | | 1.257 | 2.112 | 2.956 | | |
| (c) | | | 5630.8 | – | – | | |
| $\nu' = 4$ | | | | | | | |
| (a) | * | * | * | 0.013 | 0.972 | 0.016 | * |
| (b) | | | | 1.287 | 2.121 | 2.948 | |
| (c) | | | | 5634.5 | – | – | |
| $\nu' = 5$ | | | | | | | |
| (a) | * | * | * | * | 0.016 | 0.964 | 0.021 |
| (b) | | | | | 1.317 | 2.131 | 2.941 |
| (c) | | | | | 5638.3 | – | – |
| $\nu' = 6$ | | | | | | | |
| (a) | * | * | * | * | * | 0.020 | 0.954 |
| (b) | | | | | | 1.345 | 2.142 |
| (c) | | | | | | 5642.1 | – |
| $\nu' = 7$ | | | | | | | |
| (a) | * | * | * | * | * | * | 0.025 |
| (b) | | | | | | | 1.373 |
| (c) | | | | | | | 5645.9 |

(a) $q_{\nu'\nu''}$, (b) $\bar{r}_{\nu'\nu''}$ Å, (c) $\lambda_{\nu'\nu''}$ Å, $^*q_{\nu'\nu''} = 0$.

TABLE II
Franck-Condon factors and $r$-centroids of F–X bands of SrF

| | $\nu''$ | | | | |
|---|---|---|---|---|---|
| | 0 | 1 | 2 | 3 | 4 |
| $\nu' = 0$ | | | | | |
| (a) | 0.4951 | 0.3375 | 0.1262 | 0.0337 | 0.0071 |
| (b) | 2.0405 | 1.9917 | 1.9438 | 1.8952 | 1.8437 |
| (c) | 3041.5 | 3088.3 | – | – | – |
| $\nu' = 1$ | | | | | |
| (a) | 0.3613 | 0.0454 | 0.2695 | 0.2081 | 0.0857 |
| (b) | 2.0986 | 2.0513 | 2.0003 | 1.9525 | 1.9044 |
| (c) | 2987.8 | – | – | – | – |
| $\nu' = 2$ | | | | | |
| (a) | 0.1192 | 0.3217 | 0.0098 | 0.1313 | 0.2178 |
| (b) | 2.1568 | 2.1091 | 2.0534 | 2.0085 | 1.9608 |
| (c) | – | 2978.1 | – | – | – |
| $\nu' = 3$ | | | | | |
| (a) | 0.0225 | 0.2216 | 0.1871 | 0.0784 | 0.0364 |
| (b) | 2.2192 | 2.1669 | 2.1207 | 2.0660 | 2.0154 |
| (c) | – | 2929.6 | – | – | – |
| $\nu' = 4$ | | | | | |
| (a) | 0.0026 | 0.0639 | 0.2698 | 0.0749 | 0.1352 |
| (b) | 2.2892 | 2.2295 | 2.1773 | 2.1350 | 2.0761 |
| (c) | – | – | – | – | – |
| $\nu' = 5$ | | | | | |
| (a) | * | 0.0098 | 0.1135 | 0.2676 | 0.0146 |
| (b) | | 2.3002 | 2.2398 | 2.1879 | 2.1601 |
| (c) | | – | – | – | – |
| $\nu' = 6$ | | | | | |
| (a) | * | * | 0.0223 | 0.1603 | 0.2297 |
| (b) | | | 2.3112 | 2.2501 | 2.1983 |
| (c) | | | – | – | – |

(a) $q_{\nu'\nu''}$, (b) $\bar{r}_{\nu'\nu''}$ Å, (c) $\lambda_{\nu'\nu''}$ Å, $^*q_{\nu'\nu''} = 0$.

for the systems B–X and F–X of SrF and C–X and G–X of ScF molecules. The wavelengths ($\lambda_{\nu'\nu''}$) data (Donald McLeod and William Weltner, 1966; Gurvich and Shenyavskaya, 1963; Harvey, 1931) are also included in the respective tables. The molecular constants used in the present study are collected from the compilation of Huber and Herzberg (1979).

TABLE III
Franck-Condon factors and $r$-centroids of C–X bands of ScF

| | $v''$ | | |
|---|---|---|---|
| | 0 | 1 | 2 |
| $v' = 0$ | | | |
| (a) | 0.160 | 0.316 | 0.287 |
| (b) | 1.848 | 1.884 | 1.921 |
| (c) | 6219.0 | 6510.5 | 6828.5 |
| $v' = 1$ | | | |
| (a) | 0.272 | 0.110 | 0.010 |
| (b) | 1.819 | 1.853 | 1.901 |
| (c) | 6000.5 | – | – |
| $v' = 2$ | | | |
| (a) | 0.250 | 0.001 | 0.154 |
| (b) | 1.791 | 1.843 | 1.862 |
| (c) | 5801.0 | – | – |
| $v' = 3$ | | | |
| (a) | 0.165 | 0.086 | 0.073 |
| (b) | 1.763 | 1.799 | 1.831 |
| (c) | 5617.0 | – | – |
| $v' = 4$ | | | |
| (a) | 0.088 | 0.156 | * |
| (b) | 1.737 | 1.771 | |
| (c) | 5446.0 | – | |

(a) $q_{v'v''}$, (b) $\bar{r}_{v'v''}$ Å, (c) $\lambda_{v'v''}$ Å, $^*q_{v'v''} = 0$.

## 3. Results and Discussion

In the case of B–X system of SrF molecule, the FC factors imply that $\Delta v = 0$ sequence bands should be more intense. For the F–X system, the FC factors indicate that the following (0, 0), (0, 1), (0, 2), (1, 0), (1, 2), (1, 3), (2, 0), (2, 1), (2, 3), (2, 4), (3, 1), (3, 2), (4, 2), (4, 4), (5, 4), (5, 3), (6, 3) and (6, 4) bands are intense. These bands should therefore be readily observable in sunspot and other astrophysical sources where the molecule is expected to be present under favorable physical conditions of temperature and abundance. Similarly in the case of G–X band system of ScF, the (0, 0) and (1, 1) bands of $\Delta v = 0$ sequence must be strong due to the FC factor values. Other prominent bands are (3, 2), (2, 1), (2, 3), (1, 2), (1, 0), (0, 1) and (2, 2). For the C–X band system of ScF, the FC factors indicate that the (0, 1), (0, 2), (1, 0),

TABLE IV
Franck-Condon factors and $r$-centroids of G–X bands of ScF

| | $v''$ | | | |
|---|---|---|---|---|
| | 0 | 1 | 2 | 3 |
| $v' = 0$ | | | | |
| (a) | 0.795 | 0.173 | 0.029 | 0.004 |
| (b) | 1.811 | 1.914 | 1.968 | 2.022 |
| (c) | 2862.3 | 2923.2 | – | – |
| $v' = 1$ | | | | |
| (a) | 0.187 | 0.437 | 0.275 | 0.083 |
| (b) | 1.731 | 1.819 | 1.924 | 1.979 |
| (c) | 2816.3 | – | 2936.0 | 2949.5 |
| $v' = 2$ | | | | |
| (a) | 0.019 | 0.321 | 0.170 | 0.291 |
| (b) | 1.614 | 1.751 | 1.818 | 1.934 |
| (c) | – | 2829.8 | – | – |
| $v' = 3$ | | | | |
| (a) | 0.001 | 0.064 | 0.370 | 0.027 |
| (b) | 1.380 | 1.653 | 1.769 | 1.774 |
| (c) | – | – | 2843.4 | – |

(a) $q_{v'v''}$, (b) $\bar{r}_{v'v''}$ Å, (c) $\lambda_{v'v''}$ Å.

(2, 0), (3, 0), (0, 0), (4, 1), (2, 2) and (1, 1) bands should be more intense than the other bands.

The sequence differences for all these systems B–X, F–X of SrF and C–X, G–X of ScF are found to be varying from 0.007 to 0.03, 0.002 to 0.03 and 0.005 to 0.02 Å, from 0.001 to 0.04 Å, respectively. Further, $r'_e > r''_e$ and hence the $r$-centroid values increase with an increase in wavelength, which is expected in the red degraded band system.

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