

ESTIMATION OF ASTROPHYSICALLY USEFUL PARAMETERS FOR SnF AND ScF MOLECULES

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Abstract. The calculation of Franck-Condon factors and r -centroids are of interest to study the electronic transition between bound molecular states. Franck-Condon factors and r -centroid values estimated using the most reliable numerical integration procedure for the bands of $A^2\Sigma - X^2\Pi_{3/2}$, $A^2\Sigma - X^2\Pi_{1/2}$, $B^2\Sigma - X^2\Pi$, $C^2\Delta - X^2\Pi_{3/2}$, and $C^2\Delta - X^2\Pi_{1/2}$ systems of the astrophysical molecule SnF and $B^2\Sigma - X^2\Pi_{3/2}$, $C\Sigma - X^2\Pi_{1/2}$, and $E^2\Sigma - X^2\Pi$ systems of ScF using a suitable potential.

Key words: astrophysics – molecules SnF and ScF – Franck-Condon factors; r -centroids.

1. INTRODUCTION

The spectral intensity distribution in the electronic states of a molecule requires knowledge of electronic transition probabilities, which are to a good approximation proportional to the Franck-Condon (FC) factors. The FC factors give the molecular information required to evaluate the band intensities in absorption and emission. 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 physical-chemical conditions of the emitting sources.

A precise knowledge of FC factors and r -centroids are essential to understand and to estimate many important aspects of the astrophysical molecules, such as radiative lifetime, variation of electronic transition moment with internuclear separation, vibrational temperature of the source and relative band strengths. The FC factors are useful in studies of radiative transfer in the atmospheres of stellar and other astronomical objects, which contain molecular species (Nicholls et al. 1981).

The molecular spectrum of the SnF molecule and its significance in astrophysics due to its presence in the stellar spectrum were dealt with in detail elsewhere (Singh et al. 1965). The abundances of a number of elements detected in HST GHRS spectra (Hobbs et al. 1993) have clarified the depletion pattern seen in moderately dense interstellar clouds. In addition, the heavy elements Ga, Ge, As, Si, Kr, Sn, Tl and Pb provide probes of nucleosynthetic processes other than those responsible for the lighter elements. Comparison of the depletion properties of Si, Ge, Sn and Pb, all in the same group IV A with similar chemical behaviour, may provide valuable information regarding various processes through to occur on the surfaces of dust grains in the ISM.

The SnF molecule is a diatomic halide of fourth group and having the same structure of SiF, GeF and PbF. Singh and Rai (1965) reported the presence of the SnF molecule in stellar region. The variation of chemical equilibria in stellar atmospheres is still one of the basic obstacles to understanding the atmospheres of cool stars. The atmospheres of cool stars are complicated systems of chemical equilibria in which about a hundred elements are mixed and there are many possible chemical reactions to form molecules. The interstellar matter has different types of molecules wherein the heavy molecules of interest are much denser and so the dust is densest. Especially, the role of the diatomic molecules in stellar atmospheres for various values of H, C, N, O and F with other elements has been limited to the evaluation of some of the equilibrium constants. Peery (1979) reported the presence of SnH molecule in the spectrum of cool carbon stars. Based on the estimates of abundances of Sn, the fluorides of fourth group halides are expected to be present in stellar and cool stars.

The presence of Sc I and Sc II lines has been identified in the stellar spectrum and cool carbon stars (Peery 1979). Angular size and effective temperature for cool carbon stars show a significant elemental abundance for Sc. Schadee (1964) identified that the ScO, TiO and ZrO molecules are to be present in the Sun. Since oxides of Sc are among the most readily formed diatoms in sunspots (Wöhl 1971) and in M-type stars (Nicholls 1977), fluorides of Sc are also expected to be present in these astrophysical objects. Further, Sauval and Tatum (1984) predicted the possible presence of ScF molecules in stellar and cometary spectra. Their relative abundances in the interstellar medium give estimates of stellar activity like nature of stellar wind and the elemental abundances of cool stars.

There has been no report on the FC factors and r -centroids for the band systems $A^2\Sigma - X^2\Pi_{3/2}$, $A^2\Sigma - X^2\Pi_{1/2}$, $B^2\Sigma - X^2\Pi$, $C^2\Delta - X^2\Pi_{3/2}$ and $C^2\Delta - X^2\Pi_{1/2}$ systems of SnF molecule and $B^2\Sigma - X^2\Pi_{3/2}$, $C\Sigma - X^2\Pi_{1/2}$ and $E^2\Sigma - X^2\Pi$ systems of ScF molecule, to our best knowledge, in the literature. Therefore the reliable values of FC factors and r -centroids for these band systems of astrophysically important molecules SnF 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

The wave mechanical formulation of the FC principle leads to: the absorption intensity $I_{\nu'\nu''}$ of a molecular band for a $\nu' - \nu''$ electronic transition is proportional to the product of the number of molecules present in the particular state, the photon energy and the rate of absorption. Thus

$$I_{\nu'\nu''} = DN_{\nu'} E_{\nu'\nu''} R_e^2(\bar{r}_{\nu'\nu''}) q_{\nu'\nu''}, \quad (1)$$

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

The intensities of diatomic molecular bands in absorption are controlled by the square of the overlap integral. The square of the coefficients used in the linear combination tells us about the degree of overlap between the excited state wave function and the ground state wave function. The square of the overlap integral is termed as FC factor:

$$q_{\nu'\nu''} = |\langle \psi_{\nu'} | \psi_{\nu''} \rangle|^2, \quad (2)$$

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

$$\bar{r}_{\nu'\nu''} = \frac{\langle \psi_{\nu'} | r | \psi_{\nu''} \rangle}{\langle \psi_{\nu'} | \psi_{\nu''} \rangle}. \quad (3)$$

Morse's (1929) potential energy curves for diatomic molecules are required in order to evaluate the FC factors, especially for vibrational transition involving between their various low quantum number electronic states (Sri Ramachandran et al. 2004). The computation of the FC factor is made by Bates' (1949) method of numerical integration according to the detailed procedure provided by Partel et al. (2000). Morse wave functions were calculated at intervals of 0.01 Å for the range of r respectively from 1.71 Å to 2.49 Å, from 1.74 Å to 2.37 Å, from 1.69 Å to 2.14 Å, from 1.74 Å to 2.17 Å and from 1.74 Å to 2.11 Å for every observed vibrational level of $A^2\Sigma - X^2\Pi_{3/2}$, $A^2\Sigma - X^2\Pi_{1/2}$, $B^2\Sigma - X^2\Pi$, $C^2\Delta - X^2\Pi_{3/2}$ and $C^2\Delta - X^2\Pi_{1/2}$ states of the SnF molecule and from 1.64 Å to 2.21 Å, from 1.66 Å to 2.36 Å and from 1.69 Å to 2.08 Å for the band $B^2\Sigma - X^2\Pi_{3/2}$, $C\Sigma - X^2\Pi_{1/2}$ and $E^2\Sigma - X^2\Pi$ systems of the ScF molecule, respectively. Once the appropriate wave functions are

obtained, the FC factors can be evaluated by integrating the expression (1). The definition of r -centroids offers a method of computing them directly. Integrals in equations (1) and (2) for the FC factors ($q_{v',v''}$) and r -centroids ($\bar{r}_{v',v''}$) were computed numerically and the results are presented in Tables 1–8 for the respective bands of the SnF and ScF molecules. The wavelengths ($\lambda_{v',v''}$) data (Jenkins and Rochester 1937; McLeod and Weltner 1966) are also included in the tables. The molecular constants used in the present study are collected from the compilations of Huber and Herzberg (1979), and Dai and Balasubramanian (1994).

3. RESULTS AND DISCUSSION

The FC factors of the SnF molecule indicate that the most intense bands are the (1,0), (0,1) and (0,0) for the $A^2\Sigma - X^2\Pi_{3/2}$ and $A^2\Sigma - X^2\Pi_{1/2}$ systems; the (0,0), (2,1), (1,2), (1,0) and (0,1) for the $B^2\Sigma - X^2\Pi$ system; the (0,0), (1,1) and (3,2) for the $C^2\Delta - X^2\Pi_{3/2}$ and $C^2\Delta - X^2\Pi_{1/2}$ systems, whereas all other observed bands are weak.

For $A^2\Sigma - X^2\Pi_{3/2}$ and $A^2\Sigma - X^2\Pi_{1/2}$ band systems of the SnF molecule, it is found that $r'_e > r''_e$ and hence the r -centroid values increase with increasing wavelength, which is expected to be red degraded band system. For $B^2\Sigma - X^2\Pi$, $C^2\Delta - X^2\Pi_{3/2}$ and $C^2\Delta - X^2\Pi_{1/2}$ band systems, it is found that $r'_e < r''_e$ and r -centroid values increase with decreasing wavelength, hence the bands are degraded towards the ultraviolet.

The sequence difference is found to be varying between 0.003 Å to 0.04 Å, and 0.002 to 0.02 for $A-X$ and $C-X$ sub-band systems of the SnF molecule, respectively; hence the potentials are so wide. In the case of the $B-X$ band system, the sequence difference is found to be constant and is about 0.01 Å, which suggests that the potentials are not so wide.

In the case of the $B-X$ system of the ScF molecule, the FC factors imply that the (0,1), (2,0) and (1,0) bands are intense, and other bands are weak. For the $C-X$ system, the FC factors indicate that (0,0) and (1,0) bands are intense. Similarly, in the case of the $E-X$ band system, the (1,0), (2,0), (3,0) and (0,0) bands are intense and all other bands are weak.

The sequence differences for all these band systems ($B-X$, $C-X$ and $E-X$) of the ScF molecule is found to be a constant, and is about 0.01 Å. Further, $r'_e > r''_e$ and hence the r -centroids values increase with an increase in wavelength, which is expected in the red degraded band system.

Table 1

Franck-Condon factors and r -centroids of A-X_{3/2} bands of SnF

		$v''=0$	$v''=1$	$v''=2$	$v''=3$	$v''=4$
$v'=0$	a)	0.300	0.353	0.219	0.092	0.029
	b)	1.990	2.040	2.083	2.126	2.167
	c)	2927.80	2978.17	3029.81		
$v'=1$	a)	0.361	0.013	0.101	0.227	0.179
	b)	1.955	2.025	2.050	2.095	2.137
	c)	2871.36	2919.77	2969.47	3020.18	
$v'=2$	a)	0.219	0.109	0.138		0.112
	b)	1.918	1.962	2.023	*	2.106
	c)	2817.36				3011.34
$v'=3$	a)	0.088	0.235		0.139	0.048
	b)	1.878	1.930	*	2.034	2.078
	c)	2765.96	2810.83			
$v'=4$	a)	0.026	0.179	0.121	0.044	0.057
	b)	1.832	1.892	1.938	2.016	2.044
	c)		2759.93	2804.18	2849.47	2895.74
$v'=5$	a)	0.006	0.081	0.198	0.023	0.099
	b)	1.775	1.849	1.905	1.928	2.021
	c)	2670.45	2711.33	2754.01	2797.64	2841.50
$v'=6$	a)	0.001	0.025	0.141	0.146	0.002
	b)	1.695	1.798	1.865	1.914	2.118
	c)				2748.04	2791.18
$v'=7$	a)	*	0.006	0.061	0.172	0.067
	b)	*	1.729	1.818	1.879	1.917
	c)				2700.4	2742.22
$v'=8$	a)	*	0.001	0.018	0.106	0.160
	b)	*	1.618	1.759	1.837	1.891
	c)					2695.36
$v'=9$	a)	*	*	0.004	0.042	0.142
	b)	*	*	1.670	1.784	1.853
	c)					
$v'=10$	a)	*	*	*	0.011	0.074
	b)	*	*	*	1.710	1.806
	c)					
$v'=11$	a)	*	*	*	*	0.025
	b)	*	*	*	*	1.743
	c)					
$v'=12$	a)	*	*	*	*	0.006
	b)	*	*	*	*	1.644
	c)					
		$v''=5$	$v''=6$	$v''=7$	$v''=8$	$v''=9$
$v'=0$	a)	0.007	0.001			
	b)	2.208	2.249	*	*	*
	c)					

$v' = 1$	a)	0.084	0.028	0.007	0.001	*
	b)	2.178	2.218	2.260	2.302	
	c)					
$v' = 2$	a)	0.194	0.141	0.063	0.020	0.005
	b)	2.148	2.188	2.229	2.270	2.312
	c)					
$v' = 3$	a)	0.019	0.142	0.170	0.104	0.041
	b)	2.117	2.159	2.199	2.240	2.281
	c)	3001.27				
$v' = 4$	a)	0.107	0.003	0.067	0.161	0.139
	b)	2.088	2.130	2.170	2.210	2.250
	c)					
$v' = 5$	a)	0.003	0.106	0.040	0.013	0.119
	b)	2.050	2.099	2.140	2.184	2.221
	c)	2887.95				
$v' = 6$	a)	0.098	0.012	0.061	0.082	0.001
	b)	2.031	2.073	2.110	2.151	2.173
	c)		2880.08			
$v' = 7$	a)	0.036	0.054	0.052	0.015	0.095
	b)	2.022	2.043	2.082	2.120	2.163
	c)	2784.56		2872.37		
$v' = 8$	a)	0.012	0.072	0.011	0.079	*
	b)	1.887	2.024	2.055	2.093	
	c)	2736.42	2778.26			
$v' = 9$	a)	0.113	0.001	0.078	0.001	0.073
	b)	1.899	2.209	2.033	2.058	2.104
	c)	2690.12	2730.61	2771.98		
$v' = 10$	a)	0.156	0.054	0.023	0.054	0.020
	b)	1.867	1.898	2.040	2.045	2.075
	c)		2684.97	2724.85	2765.61	
$v' = 11$	a)	0.109	0.138	0.012	0.051	0.020
	b)	1.825	1.879	1.859	2.034	2.059
	c)			2679.75	2719.18	
$v' = 12$	a)	0.048	0.135	0.098	*	0.063
	b)	1.771	1.842	1.885		2.040
	c)					2713.53

Table 2

Franck-Condon factors and r -centroids of A-X1/2 bands of SnF

		$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$	$v'' = 5$	$v'' = 6$
$v' = 0$	a)	0.315	0.355	0.212	0.086	0.026	0.006	0.001
	b)	1.992	2.042	2.086	2.129	2.171	2.212	2.253
	c)	3141.13	3199.66	3259.90				
$v' = 1$	a)	0.363	0.008	0.115	0.231	0.172	0.078	0.025
	b)	1.956	2.032	2.052	2.097	2.140	2.181	2.222
	c)	3076.22	3132.27	3190.00	3249.29			
$v' = 2$	a)	0.212	0.124	0.130	0.001	0.125	0.195	0.134
	b)	1.917	1.963	2.025	2.044	2.108	2.151	2.192
	c)	3014.59	3068.30		3180.41	3238.5		

$v'=3$	a)	0.082	0.240	0.002	0.145	0.039	0.027	0.151
	b)	1.876	1.929	1.902	2.035	2.081	2.119	2.162
	c)			3060.41			3228.52	
$v'=4$	a)	0.023	0.172	0.135	0.034	0.068	0.101	0.001
	b)	1.828	1.890	1.938	2.020	2.046	2.090	2.138
	c)			3000.15	3052.48			
$v'=5$	a)	0.005	0.074	0.200	0.032	0.094	0.008	0.110
	b)	1.768	1.846	1.903	1.933	2.023	2.053	2.101
	c)						3097.67	
$v'=6$	a)	0.001	0.022	0.133	0.157	*	0.103	0.007
	b)	1.685	1.792	1.862	1.913		2.032	2.077
	c)							3089.06

Table 3

Franck-Condon factors and r -centroids of B-X bands of SnF

		$v''=0$	$v''=1$	$v''=2$
$v'=0$	a)	0.615	0.293	0.076
	b)	1.917	1.863	1.808
	c)	2593.84	2635.64	
$v'=1$	a)	0.303	0.158	0.326
	b)	1.979	1.924	1.872
	c)	2556.45	2595.50	2633.94
$v'=2$	a)	0.071	0.354	0.010
	b)	2.040	1.987	1.926
	c)		2557.98	
$v'=3$	a)	0.010	0.156	0.283
	b)	2.099	2.047	1.995
	c)			2559.68
$v'=4$	a)	0.001	0.034	0.223
	b)	2.160	2.107	2.055
	c)			
$v'=5$	a)		0.005	0.069
	b)	*	2.167	2.114
	c)			
$v'=6$	a)			0.012
	b)	*	*	2.174
	c)			

Table 4

Franck-Condon factors and r -centroids of C-X3/2 bands of SnF

		$v''=0$	$v''=1$	$v''=2$	$v''=3$	$v''=4$
$v'=0$	a)	0.784	0.179	0.032	0.005	*
	b)	1.926	1.841	1.784	1.730	
	c)	2195.34	2223.49	2252.14		
$v'=1$	a)	0.205	0.473	0.240	0.068	0.014
	b)	2.013	1.939	1.842	1.786	1.731
	c)	2163.15		2218.23		

$v' = 2$	a)	0.012	0.322	0.296	0.245	0.095
	b)	2.152	2.024	1.956	1.842	1.788
	c)	2132.67	2158.75			2240.94
$v' = 3$	a)	*	0.027	0.393	0.196	0.226
	b)		2.173	2.036	1.979	1.840
	c)					

Table 5

Franck-Condon factors and r -centroids of C-X1/2 bands of SnF

		$v'' = 0$	$v'' = 1$	$v'' = 2$
$v' = 0$	a)	0.767	0.191	0.036
	b)	1.927	1.846	1.789
	c)	2348.90		
$v' = 1$	a)	0.218	0.438	0.252
	b)	2.011	1.940	1.848
	c)		2344.06	
$v' = 2$	a)	0.015	0.336	0.256
	b)	2.137	2.022	1.957
	c)		2308.37	
$v' = 3$	a)	*	0.033	0.394
	b)		2.156	2.033
	c)			2303.99

Table 6

Franck-Condon factors and r -centroids of B-X bands of ScF

		$v'' = 0$	$v'' = 1$
$v' = 0$	a)	0.114	0.271
	b)	1.853	1.887
	c)	9405.00	
$v' = 1$	a)	0.231	0.155
	b)	1.826	1.858
	c)	8909.00	
$v' = 2$	a)	0.249	0.006
	b)	1.800	1.826
	c)	8468.00	
$v' = 3$	a)	0.191	0.041
	b)	1.775	1.808
	c)	8079.00	8572.49
$v' = 4$	a)	0.115	0.126
	b)	1.750	1.782
	c)	7727.00	
$v' = 5$	a)	0.058	0.149
	b)	1.725	1.757
	c)	7405.00	
$v' = 6$	a)	0.026	0.116
	b)	1.700	1.732
	c)	7111.00	

Table 7

Franck-Condon factors
and r -centroids of C-X bands of ScF

		$v'' = 0$
$v' = 0$	a)	0.1636
	b)	1.848
	c)	6277.50
$v' = 1$	a)	0.275
	b)	1.818
	c)	6010.50
$v' = 2$	a)	0.250
	b)	1.790
	c)	5810.00
$v' = 3$	a)	0.164
	b)	1.763
	c)	5623.50
$v' = 4$	a)	0.086
	b)	1.736
	c)	5450.00
$v' = 5$	a)	0.039
	b)	1.710
	c)	5288.50
$v' = 6$	a)	0.015
	b)	1.6840
	c)	5138.00
$v' = 7$	a)	0.006
	b)	1.658
	c)	4997.50
$v' = 8$	a)	0.002
	b)	1.638
	c)	4864.00

Table 8

Franck-Condon factors
and r -centroids of E-X bands of ScF

		$v'' = 0$
$v' = 0$	a)	0.447
	b)	1.829
	c)	4792.00
$v' = 1$	a)	0.339
	b)	1.785
	c)	4657.00
$v' = 2$	a)	0.145
	b)	1.743
	c)	4531.00
$v' = 3$	a)	0.045
	b)	1.703
	c)	4415.00

The legend: a) = q_{ν^*} ; b) = $\bar{r}_{\nu^*} A^0$; c) = $\lambda_{\nu^*} A^0$; * = $q_{\nu^*} = 0$ is valid for all the above tables.

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Received on 31 July 2006