

EVALUATION OF TRANSITION PROBABILITY PARAMETERS FOR GAS-PHASE DIATOMIC TIN HALIDES: SnF AND SnCl

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The Franck–Condon factors and r -centroids are defined through elementary integrals that involve vibrational wave functions on which they depend in a sensitive manner. The Franck–Condon factors are more useful for the interpretation of astronomical molecular spectra. These factors, which are very closely related to transition probabilities, have been evaluated by the reliable numerical integration procedure for the band systems $A^1\Sigma \rightarrow X^2\Pi_{3/2}$, $A^1\Sigma \rightarrow X^2\Pi_{1/2}$, $B^2\Sigma \rightarrow X^2\Pi_{1/2}$, and $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ of SnF molecule and $A'^2\Sigma \rightarrow X^2\Pi_{1/2}$ of SnCl molecule using an adequate potential. The Franck–Condon factors, r -centroids, and the available data on wavelengths are given in the respective tables.

for band systems are required for the astrophysical determination of stellar abundances and excitation temperatures [2].

Group IV halides have received the significant attention for several decades. Knowledge of the spectral characteristics of the stellar medium is of vital value in the studies of stellar evolution and nucleosynthesis. Dealing with 300 diatomic molecules of known or possible astrophysical interest, Sauval and Tatum [3] have reported polynomial expressions of the partition functions and the equilibrium constants for the tin halides. The chemistry of fluorine-bearing molecules in the interstellar medium has been the subject of a recent theoretical study [4]. The elemental abundance of fluorine is of particular interest, because it is produced in asymptotic giant branch stars [5, 6]. The abundances of a number of elements detected in HST GHRS spectra [7] 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. The relative elemental abundances of Na, K, Si, Mg, Ca, Al, Ti, Cl, and S which are astrophysically effective have been arranged in [8]. Based on the estimation of the abundances of tin, tin halides are also expected to be present in stellar and cool stars.

1. Introduction

Molecular bands of many diatoms are found in the spectra of stellar radiation. The molecules in their excited states provide a valuable information about the physical conditions prevailing near star-forming regions and in the circumstellar envelopes of late-type stars. The theoretical prediction of the intensity distribution in the spectra of many diatomic molecules, which are of interest in astrophysics, is necessary for the understanding of physico-chemical conditions of the emitting sources. The interpretation of the spectral intensity distribution in the electronic states of a molecule requires to know the electronic transition probabilities which are, in a good approximation, proportional to the Franck–Condon (FC) factors. The FC factors and r -centroids are essential to understand and to estimate many important aspects of the astrophysical molecules such as the radiative lifetime, variation of the electronic transition moment with internuclear separation, vibrational temperature of the source and relative band strengths, among other applications. The FC factors are useful in studies of the radiative transfer in the atmospheres of stellar and other astronomical objects which contain molecular species [1]. The values of FC factors and r -centroids

To the best of our knowledge, there has been no report so far in the literature on the FC factors and r -centroids for the band systems $A'^2\Sigma \rightarrow X^2\Pi_{1/2}$ of SnCl molecule and $B^2\Sigma \rightarrow X^2\Pi_{1/2}$ and $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ of SnF molecule. Therefore, we have taken up the evaluation of reliable FC factors and r -centroid values for these systems. In the case of $A^1\Sigma \rightarrow X^2\Pi_{3/2}$ and $A^1\Sigma \rightarrow X^2\Pi_{1/2}$ system of SnF molecule, Singh *et al.* [9] reported the partial array of FC factors by an approximate analytical method. Hence, we have evaluated numerically FC factors and r -centroids for

Table 1. Franck–Condon factors and r -centroids for the $A \rightarrow X_{3/2}$ band system of SnF molecule

		$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$	$v'' = 5$	$v'' = 6$	
$v' = 0$	a)	i)	0.286	0.351	0.226	0.098	0.031	0.008	*
		ii)	0.1793	0.2027	0.1218	0.0509			
	b)	i)	1.989	2.038	2.081	2.122	2.164	2.204	
		ii)	1.9930	2.0404	2.0840	2.1284			
	c)		5635.91	5827.52	6032.59	6242.99	–	–	
	$v' = 1$	a)	i)	0.356	0.019	0.089	0.222	0.184	0.090
ii)			0.2077	0.0057		0.0660			
b)		i)	1.955	2.018	2.048	2.092	2.134	2.174	2.215
		ii)	1.9560	2.0068		2.0524			
c)			5506.78	5688.71	–	6087.72	6301.02	–	–
$v' = 2$		a)	i)	0.226	0.094	0.145	0.001	0.100	0.192
	ii)		0.1227	0.0694	0.0772				
	b)	i)	1.919	1.962	2.021	2.090	2.103	2.145	2.185
		ii)	1.9152	1.9708	2.0196				
	c)		5384.84	5554.83	5745.92	–	6144.63	–	–
	$v' = 3$	a)	i)	0.095	0.227	*	0.132	0.058	0.013
ii)									
b)		i)	1.880	1.930		2.031	2.075	2.114	2.156
		ii)							
c)			5270.36	5436.70		–	–	–	–
$v' = 4$		a)	i)	0.030	0.184	0.104	0.054	0.046	0.112
	ii)								
	b)	i)	1.836	1.894	1.937	2.011	2.042	2.086	2.126
		ii)							
	c)		–	5319.61	–	–	–	–	–
	$v' = 5$	a)	i)	0.007	0.089	0.193	0.014	0.105	*
ii)									
b)		i)	1.783	1.852	1.906	1.921	2.018		2.097
		ii)							
c)			–	5209.66	5371.50	–	–	–	–
$v' = 6$		a)	i)	0.001	0.030	0.147	0.130	0.006	0.093
	ii)								
	b)	i)	1.712	1.804	1.868	1.915	2.047	2.028	2.070
		ii)							
	c)		–	5108.28	5260.05	–	–	–	–
	$v' = 7$	a)	i)	*	0.007	0.069	0.171	0.051	0.046
ii)									
b)		i)		1.742	1.823	1.881	1.916	2.014	2.039
		ii)							
c)			–	–	–	–	–	–	–

i) Present study, ii) Singh *et al.* (1970).

the experimentally observed vibrational levels using the molecular constants from [10].

2. Theory and Method of Calculations

Mathematically, the intensity $I_{v'v''}$ of a molecular band for an electronic transition in emission ($v' \rightarrow v''$) can be written as [11]

$$I_{v'v''} = DN_{v'}E_{v'v''}^4 R_e^2(\bar{r}_{v'v''})q_{v'v''}, \quad (1)$$

where D is a constant partly depending on the geometry of the apparatus, $N_{v'}$ is the population of the level v' , $E_{v'v''}$ is the quantum energy which is the difference between the energies of upper vibrational level v' and lower vibrational level v'' , R_e is the electronic transition moment, $q_{v'v''}$ is the FC factor, and $\bar{r}_{v'v''}$ is the r -centroid for the transition $v' - v''$.

One of the parameters which determines the intensity distribution in the emission of molecular bands is the FC factor which is the square of the overlap integral between

the upper state wave function and the lower state wave function:

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

Here, $\psi_{v'}$ and $\psi_{v''}$ are the vibrational wave functions for the upper and lower electronic states, respectively, between which the transition takes place. The r -centroid is a unique value of internuclear separation which can be associated with the $v' - v''$ band and is defined as

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

For a proper understanding of the intensity distribution in the band systems of molecules, it is necessary to choose a suitable potential. The potential energy curves for the appropriate electronic states of SnCl and SnF have been constructed by using the Morse function [12] and by the Rydberg–Klein–Rees (RKR) procedure modified in [13, 14]. It is found that the Morse function represents the potential for the states of SnCl

T a b l e 2. Franck–Condon factors and r -centroids for the $A \rightarrow X_{1/2}$ band system of SnF molecule

		$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$	$v'' = 5$	$v'' = 6$	
$v' = 0$	a)	i)	0.315	0.355	0.212	0.086	0.026	0.006	*
		ii)	0.2841	0.3499	0.2282	0.1022			
	b)	i)	1.992	2.042	2.086	2.130	2.171	2.212	
		ii)	1.9912	2.0372	2.0808	2.1232			
	c)		4985.58	5132.63	5287.55	5451.65	–	–	
	$v' = 1$	a)	i)	0.363	0.008	0.0115	0.231	0.173	0.078
ii)			0.3559	0.0219	0.0801	0.1995	0.1321		
b)		i)	1.956	2.022	2.052	2.097	2.140	2.181	2.222
		ii)	1.9548	2.0044	2.0496	2.0924	2.1348		
c)			4883.32	5025.21	5174.20	5331.70	5497.52	56680.29	–
$v' = 2$		a)	i)	0.212	0.124	0.130	0.001	0.125	0.195
	ii)		0.2281	0.0827	0.0779				
	b)	i)	1.918	1.963	2.025	2.044	2.108	2.151	2.192
		ii)	1.9164	1.9700	2.0172				
	c)		4786.43	4922.41	5067.00	–	5375.26	5537.93	5714.00
	$v' = 3$	a)	i)	0.082	0.240	*	0.145	0.039	0.027
ii)			1.876	1.929		2.035	2.081	2.119	2.162
b)		i)	1.876	1.929		2.035	2.081	2.119	2.162
		ii)	1.876	1.929		2.035	2.081	2.119	2.162
c)			4696.03	4826.70		–	–	–	–
$v' = 4$		a)	i)	0.023	0.172	0.135	0.034	0.068	0.101
	ii)		1.828	1.890	1.938	2.020	2.046	2.090	
	b)	i)	1.828	1.890	1.938	2.020	2.046	2.090	
		ii)	1.828	1.890	1.938	2.020	2.046	2.090	
	c)		4609.47	4734.89	4866.65	–	–	–	–
	$v' = 5$	a)	i)	0.005	0.074	0.200	0.032	0.094	0.008
ii)			1.769	1.846	1.903	1.933	2.023	2.053	2.101
b)		i)	1.769	1.846	1.903	1.933	2.023	2.053	2.101
		ii)	1.769	1.846	1.903	1.933	2.023	2.053	2.101
c)			–	4647.44	4774.61	–	–	–	–
$v' = 6$		a)	i)	*	0.022	0.133	0.157	*	0.103
	ii)		1.792	1.862	1.913	1.913	2.032	2.077	
	b)	i)	1.792	1.862	1.913	1.913	2.032	2.077	
		ii)	1.792	1.862	1.913	1.913	2.032	2.077	
	c)		5108.28	5260.05	–	–	–	–	–
	$v' = 7$	a)	i)	*	0.005	0.055	0.170	0.081	0.028
ii)			1.721	1.813	1.877	1.877	1.918	2.027	2.043
b)		i)	1.721	1.813	1.877	1.877	1.918	2.027	2.043
		ii)	1.721	1.813	1.877	1.877	1.918	2.027	2.043
c)			–	4599.11	4721.64	–	–	–	–

i) Present study, ii) Singh *et al.* (1970).

and SnF quite adequately, since the experimental (RKR) curves are coincident with the Morse ones. The Morse wave functions were calculated at intervals of 0.01 Å for the range, respectively, from 2.10 to 2.92 Å for the observed band $A^2\Sigma \rightarrow X^2\Pi_{1/2}$ system of SnCl molecule and from 1.73 to 2.42 Å, from 1.74 to 2.42 Å, from 1.73 to 2.11 Å, and from 1.75 to 2.07 Å for observed vibrational band $A^1\Sigma \rightarrow X^2\Pi_{3/2}$, $A^1\Sigma \rightarrow X^2\Pi_{1/2}$, $B^2\Sigma \rightarrow X^2\Pi_{1/2}$, and $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ systems of SnF molecule. The computation of the Franck–Condon factor is made by the Bates method [15] of numerical integration according to the detailed procedure provided in [16]. The integrals in Eqs. (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 in Tables 1 to 5 for the respective band systems of SnF and SnCl molecules. The available wavelengths ($\lambda_{v'v''}$) data [17–19] are also included in the respective Tables. The necessary molecular constants are collected from the compilation in [10].

T a b l e 3. Franck–Condon factors and r -centroids for the $B \rightarrow X_{1/2}$ band system of SnF molecule

		$v'' = 0$	$v'' = 1$	$v'' = 2$
$v' = 0$	a)	0.394	0.348	0.171
	b)	1.907	1.868	1.831
	c)	2927.90	2978.20	3020.70
$v' = 1$	a)	0.383	0.002	0.178
	b)	1.953	1.934	1.877
	c)	2871.40	–	2964.4
$v' = 2$	a)	0.169	0.235	0.075
	b)	2.000	1.961	1.918
	c)	2817.60	–	–

T a b l e 4. Franck–Condon factors and r -centroids for the $B \rightarrow X_{3/2}$ band system of SnF molecule

		$v'' = 0$	$v'' = 1$
$v' = 0$	a)	0.430	0.344
	b)	1.905	1.865
	c)	3141.20	3199.70
$v' = 1$	a)	0.378	0.010
	b)	1.953	1.921
	c)	3076.20	–

Table 5. Franck–Condon factors and r -centroids for the $A' \rightarrow X_{1/2}$ band system of SnCl molecule

		$v'' = 0$	$v'' = 1$	$v'' = 2$	$v'' = 3$	$v'' = 4$	$v'' = 5$
$v' = 0$	a)	0.001	0.004	0.017	0.045	0.088	0.132
	b)	2.477	2.498	2.519	2.540	2.561	2.582
	c)	5165.10	5259.60	5356.50	5457.10	5561.10	5668.30
$v' = 1$	a)	0.004	0.022	0.063	0.109	0.123	0.085
	b)	2.463	2.484	2.505	2.525	2.546	2.567
	c)	5106.50	5196.10	5290.90	5389.00	5490.40	5595.20
$v' = 2$	a)	0.122	0.055	0.106	0.103	0.041	*
	b)	2.450	2.470	2.491	2.511	2.531	
	c)	5045.30	5134.90	5227.50	5323.20	5422.30	
$v' = 3$	a)	0.029	0.092	0.103	0.035	0.001	0.047
	b)	2.436	2.457	2.477	2.497	2.523	2.539
	c)	4988.20	5075.40	—	—	—	—
$v' = 4$	a)	0.054	0.110	0.055	*	0.045	0.060
	b)	2.423	2.443	2.464		2.505	2.525
	c)	4932.40	5018.30	5104.50		—	—
$v' = 5$	a)	0.082	0.097	0.009	0.028	0.010	0.017
	b)	2.410	2.430	2.450	2.471	2.491	2.510
	c)	4878.50	4962.30	—	—	—	—
		$v'' = 6$	$v'' = 7$	$v'' = 8$	$v'' = 9$	$v'' = 10$	$v'' = 11$
$v' = 0$	a)	0.161	0.164	0.142	0.106	0.068	0.039
	b)	2.603	2.624	2.646	2.668	2.691	2.713
	c)	5779.30	5893.90	6013.10	6136.40	6264.60	6398.10
$v' = 1$	a)	0.027	*	0.024	0.076	0.115	0.121
	b)	2.587		2.633	2.654	2.676	2.698
	c)	5703.10		5930.90	6050.10	6175.20	6305.10
$v' = 2$	a)	0.029	0.076	0.071	0.025	*	0.027
	b)	2.575	2.595	2.616	2.636		2.684
	c)	—	5739.10	5850.70	—	—	—
$v' = 3$	a)	0.069	0.025	0.001	0.040	0.070	0.044
	b)	2.560	2.579	2.611	2.624	2.645	2.665
	c)	—	—	—	—	—	—
$v' = 4$	a)	0.009	0.013	0.057	0.040	0.001	0.022
	b)	2.543	2.568	2.588	2.608	2.620	2.653
	c)	—	—	—	—	—	—
$v' = 5$	a)	0.017	0.055	0.019	0.005	0.047	0.042
	b)	2.533	2.553	2.572	2.599	2.616	2.636
	c)	—	—	—	—	—	—

In all the above Tables a) FC factors $q_{v'v''}$, b) r -centroids $\bar{r}_{v'v''}$ (in Å), c) wavelengths $\lambda_{v'v''}$ (in Å), * $q_{v'v''} \simeq 0$.

3. Results and Discussion

In the case of the $A'^2\Sigma \rightarrow X^2\Pi_{1/2}$ band system of SnCl molecule, the FC factors indicate that (0,5), (0,6), (0,7), (0,8), (0,9), (1,3), (1,4), (1,10), (1,11), (2,0), (2,2), (2,3), (3,2), and (4,1) bands are more intense than the all other observed bands. For the $A^1\Sigma \rightarrow X^2\Pi_{3/2}$ band system of SnF, the FC factors indicate that (0,0), (0,1), (0,2), (1,0), (1,2), (1,3), (1,4), (2,0), (2,1), (2,2), (2,4), (2,5), (2,6), (3,1), (3,3), (3,6), (4,1), (4,2), (4,5), (5,2), (5,6), (6,2), (6,3), (6,5), and (7,3) bands are more intense, and all other observed bands are with feeble intensity. In the case of the $A^1\Sigma \rightarrow X^2\Pi_{1/2}$ band system of SnF molecule, the FC factors signify that (0,0), (0,1), (0,2), (1,0), (1,3),

(1,4), (2,0), (2,2), (2,4), (2,5), (2,6), (3,1), (3,3), (3,6), (4,1), (4,2), (4,5), (5,2), (5,6), (6,2), (6,3), and (7,3) bands are intense, and all other bands are weak. For the $B^2\Sigma \rightarrow X^2\Pi_{1/2}$ band system of SnF molecule, the FC factors manifest that all the bands are intense except (1,1) and (2,2) bands. The FC factor for the $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ band system of SnF molecule indicates that all the observed bands are intense except (1,1) band.

Singh *et al.* [9] reported a partial array of the FC factors of the $A^1\Sigma \rightarrow X^2\Pi_{3/2}$ and $A^1\Sigma \rightarrow X^2\Pi_{1/2}$ band systems of SnF molecule by a simplified procedure of calculations (commonly known as the α -averaging method) described in [20]. The results are generally, only indicative of trends [21], and hence the method is not safe

[22]. For that reason, we may consider our FC factors and r -centroids calculated by the numerical integration method as reliable and satisfactory. On comparing the present FC factors and those reported in [9], it is estimated that the percentage of the deviation between two sets of values lies within 15%.

For a given $r_{e'}$ and $r_{e''}$, the r -centroid values depend only on the difference between v' and v'' , but not on their values taken individually. The sequence difference $\Delta\bar{r}_{v'v''} = \bar{r}_{v'+1,v''+1} - \bar{r}_{v',v''}$ was found to be approximately constant ($\approx 0.01 \text{ \AA}$) for a given sequence, indicating that the potential curves are not wide [23]. In our discussed systems of SnF and SnCl molecules, the sequence difference of an r -centroid is found to be nearly a constant and is about 0.01 \AA , which suggests that the potentials are not wide.

Since $r'_e > r''_e$ in the $A'^2\Sigma \rightarrow X^2\Pi_{1/2}$ band system of SnCl molecule, the estimates of r -centroids are expected to increase linearly with the corresponding wavelength which is the trend observed in a red-degraded band system.

In the case of SnF molecule, for the $A^1\Sigma \rightarrow X^2\Pi_{3/2}$ and $A^1\Sigma \rightarrow X^2\Pi_{1/2}$ band systems, the present data show that the r -centroid values increase with the wavelength, which suggests that these bands are degraded to longer wavelengths. For the band $B^2\Sigma \rightarrow X^2\Pi_{1/2}$ and $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ systems of SnF molecule, since $r'_e < r''_e$, the r -centroid value increases with decrease in the wavelength, which is expected in a violet-degraded band system. These variations are of the expected nature, and the decrease or increase is found to be linear.

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ОЦІНКА ПАРАМЕТРІВ ІМОВІРНОСТІ ПЕРЕХОДІВ ДЛЯ ДВОХАТОМНИХ ГАЛОЇДІВ ОЛОВА В ГАЗОВІЙ ФАЗІ: SnF ТА SnCl

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Фактори Франка – Кондона та r -центроїди визначено через елементарні інтеграли, в які суттєвим чином входять осциляторні хвильові функції. Фактори Франка – Кондона найбільш корисні для інтерпретації молекулярних спектрів в астрономії і тісно пов'язані з імовірностями переходів. Фактори Франка – Кондона оцінено за допомогою процедури чисельного інтегрування полос $A^1\Sigma \rightarrow X^2\Pi_{3/2}$, $A^1\Sigma \rightarrow X^2\Pi_{1/2}$, $B^2\Sigma \rightarrow X^2\Pi_{1/2}$ та $B^2\Sigma \rightarrow X^2\Pi_{3/2}$ для молекули SnF і $A'^2\Sigma \rightarrow X^2\Pi_{1/2}$ для молекули SnCl з використанням відповідних потенціалів. Величини факторів Франка – Кондона та r -центроїдів наведено у таблицях.