Serb. Astron. J. № 175 (2007), 25 - 32 **UDC 52-355.3 : 524.327**
DOI: 10.2298/SAJ0775025K Original scientific paper

ON THE FRANCK-CONDON FACTORS AND R-CENTROIDS OF THE ASTROPHYSICALLY INTERESTING MOLECULE CS

B. Karthikeyan[1], V. Raja[2], N. Rajamanickam[1] and S. P. Bagare[3]

[1]*Physics Research Centre, V.H.N.S.N College, Virudhunagar - 626 001*

[2]*Kalasalingam University, Krishnankoil - 626 190*

[3]*Indian Institute of Astrophysics, Kodaikanal & Bangalore - 560 034*

(Received: February 21, 2007; Accepted: August 23, 2007)

SUMMARY: In molecular astrophysics, the Franck-Condon (FC) factors and r-centroids are essential for the interpretation of spectral intensities in terms of emitting astrophysical source conditions. They have been evaluated for the band systems a $^3\Pi_r$ - X $^1\Sigma^+$, d $^3\Delta_i^n$ - X $^1\Sigma^+$, e $^3\Sigma^-$ - X $^1\Sigma^+$, A′ $^1\Sigma^+$ - X $^1\Sigma^+$ and d $^3\Delta_i^n$ - a $^3\Pi_r$ of astrophysical molecule CS. The physical and astrophysical significances of our evaluated FC factors and r-centroids are discussed. The FC factor values of a - X system have been compared with the values of FC factors reported by Reddy et al. (2003).

Key words. Molecular data - Methods: numerical - Sun: abundances - Stars: abundances.

1. INTRODUCTION

Carbon monosulphide (CS) is the first molecule containing sulphur that has been detected in interstellar space (e.g. Jefferts et al. 1971). It has been found in molecular clouds (e.g. Williams et al. 1998), planetary nebulae (e.g. Woods et al. 2005), circumstellar envelope of C-type stars (e.g. Nyman 1992, Woods et al. 2003), solar photosphere (e.g. Singh et al. 1987, Sinha 1978), other galaxies (e.g. Martin et al. 2005) and its production was also observed in the collision of Comet Shoemaker-Levy 9 with Jupiter (e.g. Kaiser et al. 1998). With the help of IUE satellite, the (0,0) band of CS at 2576Å has been observed in many comets (e.g. Yeomans 1991). The radical CS also has been clearly identified in cometary ices (e.g. Crovision et al. 2000).

In the field of atmospheric and space physics, CS molecule plays a vital role in the atmospheric reactions. For instance, in the production of atmospheric carbonyl sulphide (OCS), CS may be a possible source for the stratospheric sulphate aerosol layer which influences the earth's climate (Deutscher et al. 2006).

Reliable molecular data on the diatomic molecules of astrophysical interest are required for the models of photon-driven physical and chemical processes and for the models of the steady state properties of astronomical objects that absorb or emit photons. In this way, the molecular parameters like dissociation energies, potential energy curves, Franck-Condon (FC) factors and r-centroids etc., are essential for estimating the molecular abundances and for understanding the physicochemical conditions of the emitting sources. Particularly, the concept of r-centroid has been much

used since then in the interpretation of intensity measurements on many band systems of importance in astrophysics, atmospheric physics, space physics and chemical physics to determine the variation of electronic transition moment with internuclear separation, and thereby to derive band strengths, and other molecular transition probability parameters (Nicholls et al. 2001). Hence, the evaluation of FC factors and r-centroids of astrophysically significant diatomic molecules is very important.

Up to the present, there has been no report in the literature on the FC factors and r-centroids for d - X, e - X, A′ - X and d - a band systems of CS molecule. For the a - X system of CS molecule, Reddy et al. (2003) have already reported the FC factors. However, their reported values were evaluated by an unsafe method and therefore, we have evaluated the FC factors and r-centroids for the a - X system too.

2. THEORY

The integrated intensity of each band in a system corresponding to transitions between two electronic states of a diatomic molecule is proportional to the square of an integral of wave functions of vibrational states, simply called FC factor ($q_{v'v''}$).

$$q_{v'v''} = |\langle\psi_{v\prime}|\psi_{v''}\rangle|^2 \qquad (1)$$

where v' and v'' are the upper and lower vibrational quantum numbers, $\psi_{v'}$ and $\psi_{v''}$ are the vibrational wave functions of the upper and lower vibrational level respectively.

The r-centroid ($\bar{r}_{v'v''}$) is the most likely value of internuclear separation at which the $v' - v''$ transition will occur. It is also defined as the weighted average with respect to $\psi_{v'}\psi_{v''}$ of the range of values experienced by the molecule in both states of the $v' - v''$ transition. The form of r-centroid is

$$\bar{r}_{v'v''} = \frac{\langle\psi_{v'}|r|\psi_{v''}\rangle}{\langle\psi_{v'}|\psi_{v''}\rangle} \qquad (2)$$

As widely known, the electronic transition moment is given by

$$R_e = |\langle\psi_{e'}|\mu|\psi_{e''}\rangle| \qquad (3)$$

where μ is the electronic transition dipole moment, $\psi_{e'}$ and $\psi_{e''}$ are the electronic wave functions of the states. As already mentioned in the introduction, the r-centroids are useful in the determination of variation of electronic transition moment $R_e(r)$ which can be determined by fitting a straight line between $(IE^{-4}/q)^{1/2}_{v'v''}$ and $\bar{r}_{v'v''}$, where $I_{v'v''}$ is the intensity of the band, E is the energy quantum. The band strengths then can be obtained using the formula

$$p_{v'v''} = R_e^2(\bar{r}_{v'v''})q_{v'v''} \qquad (4)$$

By calculating the relative band strengths, one can measure the vibrational temperature of the emitting source (e.g. Rajamanickam 1987 and 1988). In this way, one could find the vibrational temperature of the astrophysical object with the help of $q_{v'v''}$ and $\bar{r}_{v'v''}$ along with other parameters like wavelengths and intensities of the bands and classify the object according to temperature sequence (Straughan and Walker 1976). Keeping the above required theory and necessary equations in view, the FC factors and r-centroids for some electronic band systems of CS molecule could be evaluated according to the procedure described below.

3. EVALUATION PROCEDURE

In order to evaluate $q_{v'v''}$ and $\bar{r}_{v'v''}$, one should have a suitable potential energy curve such that the curve shows maximum closeness to the experimental potential energy curve like Rydberg-Klein-Rees (RKR) curve. We have constructed both Morse (1929) and RKR potential curve (Vanderslice et al. 1960) and compared them. It is found that the Morse function represents the potential for all the states of CS molecule quite adequately, since the RKR curves coincide with the Morse's. Therefore, we can obtain quite satisfactory values of $q_{v'v''}$ and $\bar{r}_{v'v''}$ using Morse wave functions for all the states involved in the present study.

The Morse wave functions are calculated at the intervals of 0.01 Å for the values of r ranging from 1.31 to 2.07 Å, 1.32 to 2.27 Å, 1.31 to 2.28 Å, 1.30 to 2.60 Å and 1.43 to 2.24 Å for every observed vibrational level of each state of a $^3\Pi_r$ - X $^1\Sigma^+$, d $^3\Delta_i^n$ - X $^1\Sigma^+$, e $^3\Sigma^-$ - X $^1\Sigma^+$, A′ $^1\Sigma^+$ - X $^1\Sigma^+$ and d $^3\Delta_i^n$ - a $^3\Pi_r$ systems of CS molecule. Once the appropriate wave functions are obtained, the FC factors and r-centroids can be evaluated by performing the integration in equations (1) and (2). The computation of FC factors is made by Bates (1949) method of numerical integration according to the detailed procedure provided by Partal Urena et al. (2000). The definition of r-centroid offers a method of computing r-centroids directly.

The FC factors and r-centroids for the band systems a - X, d - X, e - X, A′ - X and d - a connecting states from $v' = 0$-13 to $v'' = 0$-7, from $v' = 0$-13 to $v'' = 0$-9 , from $v' = 0$-12 to $v'' = 0$-11, from $v' = 0$-9 to $v'' = 0$-12 and from $v' = 0$-12 to $v'' = 0$-2 respectively, are evaluated. The results are presented in Tables 1 to 5. For comparison, we have also presented the Reddy et al. (2003) values of FC factors for a - X system in Table 1. The available wavelengths ($\lambda_{v'v''}$) data are taken from Tewarson et al. (1968) and Bell et al. (1972) for the systems a - X and A′ - X respectively. Note that we have entered only the available wavelengths from the literature, into the corresponding tables. The molecular constants collected from the compilation of Huber and Herzberg (1979), are used in the present study.

4. RESULTS AND DISCUSSION

Reddy et al. (2003) reported the partial array of FC factors of a - X system by an approximate analytical integration method of average 'α' Morse constant given by Fraser and Jarmain (1953), considering the approximation $\alpha = (\alpha_1+\alpha_2)/2$ where α_1 and α_2 are the Morse constants for the two potentials involved in the transition. The two difficulties with the application of formulae provided by Fraser and Jarmain (1953) are: (i) the limited reliability of the results when $|(\alpha_1-\alpha_2)/(\alpha_1+\alpha_2)| = |\delta\alpha/\alpha|$ is large, say $\geq$5%, (ii) the limitation on the extent of a table of overlaps due to the large cancellation originating from the polynomial used in finding the wave functions. For larger $|\delta\alpha/\alpha|$, the results are only satisfactory or, at worst, indicative of trends (Jarmain and Fraser 1953) and hence the analytical integration method is not safe (James 1966).

In general, the fundamental theorem of calculus gives us an exact formula for computing an integral, provided we can find an antiderivative for that integral. This method of evaluating definite integrals is called the analytic method. Since the analytic method is infeasible and unsatisfactory in large number of instances, it is usually good enough to find a numerical solution for the given integral. Even though all the numerical methods are approximations, the truncation error associated with the approximation can be made smaller by making the increments smaller yielding more accurate solution of the integral. In the present study, the increment for the r value is very small, that is 0.01 Å, for the integral in Eq. (1). Therefore, we may consider our FC factors calculated by numerical integration method as reliable and more satisfactory than those evaluated by the analytical method followed by Reddy et al. (2003).

Also, Reddy et al. (2003) have not reported the FC factor values for the bands (5,7), (8,6) and (9,7), likely to be intense, whose FC factors calculated by us are 0.205, 0.219 and 0.223, respectively.

On comparing of present and previously reported $q_{v'v''}$ values, we may observe that the percentage of deviation between two sets of values lies within 4 percent, except for the band (0,0) where it is about 71 percent. While analyzing such large deviation of FC factor value for the (0,0) band, in view of Condon parabola, it is clear that the origin of the parabola lies on the (0,0) band having the highest value 0.830. So, it is not possible to have the lower value of FC factor for (0,0) band. Further, $\Delta v = 0$ sequence bands are intense and the (0,0) band is the most intense one. Therefore, the FC factor value of (0,0) band (that is 0.232) obtained by Reddy et al. (2003) is definitely an erroneous value. While performing the analytical integration for (0,0) band, such a large error would have occurred.

The FC factors of a - X system evaluated by us indicate that the $\Delta v = 0, \pm1, \pm2$ bands are intense compared to others. The FC factors of d - X divulge that (0,3), (0,4), (0,5), (0,6), (0,7), (1,2), (1,3), (1,8), (1,9), (2,1), (2,2), (3,1), (4,0), (5,0), (6,0), (7,0) and (8,0) bands should be more intense. From the FC factors of e - X band system, we may observe that the bands (0,4), (0,5), (0,6), (0,7), (0,8), (1,3), (1,4), (1,9), (1,10), (1,11), (2,2), (3,1), (4,1), (6,0), (7,0), (8,0) and (9,0) are relatively intense. In the case of A' - X system, (0,11), (0,12), (1,9), (1,10), (1,11), (1,12), (2,8) and (2,9) bands would be more intense compared to others. The bands (0,1), (0,2), (1,1), (1,2), (2,0), (2,1), (3,0), (4,0), (5,0) and (6,0) of d - a system should be more intense.

In the case of a - X system, a narrow parabola, centered along the main diagonal ($v' = v''$), results. This parabola is shown in Table 1 by underlining the respective FCF values. In three dimensions, this FCF surface looks like a diagonal mountain ridge originating at a high point at (0,0) with the FCF value 0.830. The ridge starts to separate into two ridges, which run down the $\Delta v = \pm1$ sequences at the (1,2) and (2,1) bands. Outside the immediate regions of the bands on the $\Delta v = \pm1$ sequences, very few bands are strongly excited.

It is worth mentioning that in the case of a - X and A' - X systems, the r-centroid values are found to increase linearly with the corresponding wavelength following $r_{e'} > r_{e''}$ and hence the bands are red degraded as expected.

Since the sequence differences of r-centroids for the system d - X, e - X, A' - X and d - a are found to be constants amounting to about 0.01 Å, we may conclude that the potentials involved in these transitions are not so wide. But, the situation is somewhat different in a - X system in which the sequence difference varies from 0.01 to 0.04 Å.

The presence of the intense bands of above mentioned systems in the spectrum will be an excellent diagnostic for the presence of CS molecule in the observed astrophysical source. Even though the CS molecule has been well established in the field of astrophysics, the analysis of these band systems will be of renewed interest in the identification of CS molecules in sunspots, since their possible occurrence in solar photosphere has already been predicted and mentioned (e.g. Singh et al. 1987, Sinha 1978), but their identification in sunspots has still not been confirmed by now. Further, the wavelengths of the CS transitions in the UV region are not found in the sources mentioned in the introduction, although CS exists there. So, this is a first step towards the search of UV bands of CS in such sources and the identification of CS molecule in sunspots using the rotational line wavelengths data, which is a proposed work by the authors in due course.

Table 1. Franck-Condon factors and r-centroids of a - X system

$v'\backslash v''$		0	1	2	3	4	5	6	7
	a) i)	0.830	0.156	0.015	0.001	*	*	*	*
	ii)	0.232	0.156	0.013	-				
0	b)	1.556	1.654	1.293	1.317				
	c)	3622.27	3796.94						
	a) i)	0.155	0.535	0.265	0.043	0.004	*	*	*
	ii)	0.151	0.549	0.257	0.040	-			
1	b)	1.469	1.564	1.662	1.744	1.818			
	c)	3481.05	3642.99	3817.23					
	a) i)	0.016	0.260	0.308	0.327	0.080	0.010	0.001	*
	ii)	0.014	0.252	0.337	-	-	-	-	
2	b)	1.373	1.482	1.572	1.671	1.752	1.825	1.896	
	c)		3501.65	3662.60					
	a) i)	0.001	0.045	0.317	0.147	0.346	0.123	0.020	0.002
	ii)	-	0.041	0.252	-	-	-	-	-
3	b)	1.263	1.389	1.494	1.578	1.679	1.759	1.832	1.902
	c)		3522.99						
	a) i)	*	0.005	0.083	0.330	0.049	0.329	0.166	0.035
	ii)		0.005	-	-	-	-	-	-
4	b)		1.284	1.405	1.506	1.577	1.688	1.767	1.839
	c)				3543.96				
	a) i)	*	0.004	0.012	0.126	0.306	0.005	0.284	0.205
	ii)		0.006	-	-	-	-	-	-
5	b)		1.161	1.305	1.421	1.517	1.534	1.697	1.775
	c)					3566.08			
	a) i)	*	*	0.001	0.025	0.167	0.255	0.004	0.221
	ii)			-	-	-	-	-	-
6	b)			1.188	1.325	1.436	1.528	1.713	1.705
	c)						3588.86		
	a) i)	*	*	*	0.003	0.042	0.199	0.190	0.031
	ii)				-	-	-	-	-
7	b)				1.215	1.345	1.451	1.539	1.665
	c)							3609.59	3782.29
	a) i)	*	*	*	*	0.007	0.065	0.219	0.122
	ii)					-	-	-	-
8	b)					1.240	1.364	1.466	1.547
	c)								
	a) i)	*	*	*	*	0.001	0.013	0.091	0.223
	ii)					-	-	-	-
9	b)					1.119	1.265	1.383	1.480
	c)								
	a) i)	*	*	*	*	*	0.002	0.022	0.118
	ii)						-	-	-
10	b)						1.151	1.289	1.401
	c)								
	a) i)	*	*	*	*	*	*	0.004	0.035
	ii)							-	-
11	b)							1.181	1.312
	c)								
	a) i)	*	*	*	*	*	*	0.001	0.007
	ii)							-	-
12	b)							1.058	1.210
	c)								
	a) i)	*	*	*	*	*	*	*	0.001
	ii)								-
13	b)								1.095
	c)								

a) $q_{v'v''}$ - FC factors (i) Present Study (ii) Reddy et al. (2003); b) $\bar{r}_{v'v''}$ - r-centroids (in Å); c) $\lambda_{v'v''}$ - Wavelengths (in Å); $*q_{v'v''} \approx 0$

Table 2. Franck-Condon factors and r-centroids of d - X system

$v'\backslash v''$		0	1	2	3	4	5	6	7	8	9
0	a)	0.004	0.023	0.067	0.129	0.180	0.193	0.166	0.116	0.068	0.034
	b)	1.628	1.651	1.674	1.697	1.721	1.745	1.769	1.793	1.818	1.844
1	a)	0.018	0.075	0.135	0.129	0.057	0.002	0.024	0.093	0.140	0.136
	b)	1.613	1.636	1.659	1.682	1.705	1.722	1.755	1.778	1.802	1.827
2	a)	0.046	0.121	0.110	0.023	0.008	0.073	0.088	0.031	0.001	0.046
	b)	1.599	1.622	1.645	1.666	1.694	1.715	1.737	1.759	1.806	1.813
3	a)	0.082	0.124	0.033	0.009	0.074	0.054	0.001	0.038	0.081	0.043
	b)	1.586	1.608	1.630	1.656	1.677	1.699	1.706	1.748	1.770	1.792
4	a)	0.114	0.083	*	0.061	0.050	*	0.050	0.056	0.003	0.028
	b)	1.572	1.595		1.640	1.662		1.709	1.730	1.746	1.781
5	a)	0.134	0.032	0.027	0.066	0.002	0.043	0.047	*	0.044	0.051
	b)	1.559	1.581	1.605	1.626	1.643	1.672	1.693		1.741	1.762
6	a)	0.136	0.003	0.063	0.023	0.021	0.053	0.001	0.041	0.037	0.001
	b)	1.546	1.569	1.591	1.612	1.637	1.657	1.666	1.704	1.724	1.769
7	a)	0.124	0.005	0.067	*	0.053	0.011	0.026	0.040	*	0.045
	b)	1.533	1.555	1.578		1.622	1.642	1.668	1.688		1.735
8	a)	0.103	0.029	0.041	0.018	0.042	0.004	0.047	0.002	0.036	0.024
	b)	1.520	1.542	1.565	1.588	1.609	1.634	1.653	1.667	1.699	1.718
9	a)	0.080	0.057	0.012	0.046	0.010	0.034	0.019	0.017	0.036	0.002
	b)	1.507	1.530	1.553	1.575	1.596	1.619	1.639	1.664	1.683	1.717
10	a)	0.058	0.076	*	0.053	0.001	0.044	*	0.041	0.002	0.033
	b)	1.495	1.517		1.562	1.586	1.606		1.650	1.664	1.694
11	a)	0.039	0.082	0.009	0.035	0.020	0.022	0.019	0.023	0.012	0.030
	b)	1.482	1.505	1.526	1.550	1.572	1.593	1.616	1.636	1.661	1.679
12	a)	0.026	0.077	0.029	0.012	0.041	0.002	0.038	0.001	0.035	0.003
	b)	1.470	1.492	1.514	1.539	1.560	1.581	1.603	1.618	1.646	1.661
13	a)	0.016	0.064	0.050	*	0.043	0.005	0.030	0.009	0.025	0.009
	b)	1.457	1.480	1.502		1.548	1.570	1.591	1.614	1.633	1.658

a) $q_{v'v''}$ - FC factors; b) $\bar{r}_{v'v''}$ - r-centroids (in Å); $*q_{v'v''} \approx 0$

Table 3. Franck-Condon factors and r-centroids of e - X system

$v'\backslash v''$		0	1	2	3	4	5	6	7	8	9	10	11
0	a)	0.001	0.009	0.031	0.073	0.125	0.166	0.178	0.157	0.117	0.074	0.040	0.019
	b)	1.636	1.658	1.680	1.702	1.724	1.746	1.768	1.791	1.814	1.838	1.862	1.887
1	a)	0.007	0.036	0.090	0.129	0.110	0.048	0.002	0.018	0.075	0.124	0.132	0.106
	b)	1.623	1.645	1.666	1.688	1.710	1.731	1.748	1.779	1.801	1.824	1.847	1.871
2	a)	0.020	0.077	0.118	0.079	0.011	0.011	0.067	0.083	0.037	*	0.026	0.085
	b)	1.611	1.632	1.654	1.675	1.695	1.721	1.741	1.763	1.784		1.835	1.857
3	a)	0.043	0.108	0.085	0.010	0.019	0.071	0.047	0.001	0.028	0.073	0.054	0.007
	b)	1.598	1.620	1.641	1.661	1.686	1.706	1.727	1.739	1.774	1.795	1.816	1.835
4	a)	0.070	0.108	0.028	0.010	0.065	0.037	0.001	0.045	0.056	0.008	0.014	0.062
	b)	1.586	1.608	1.628	1.652	1.672	1.692	1.728	1.737	1.758	1.776	1.807	1.827
5	a)	0.096	0.079	*	0.050	0.045	*	0.043	0.043	*	0.033	0.054	0.010
	b)	1.574	1.596		1.639	1.659		1.703	1.723		1.769	1.789	1.807
6	a)	0.114	0.039	0.015	0.061	0.005	0.030	0.044	*	0.035	0.040	*	0.032
	b)	1.562	1.584	1.606	1.626	1.645	1.669	1.689		1.733	1.753		1.800
7	a)	0.121	0.009	0.046	0.033	0.008	0.049	0.004	0.027	0.038	*	0.0360	0.034
	b)	1.551	1.573	1.594	1.614	1.637	1.657	1.674	1.700	1.719		1.764	1.783
8	a)	0.117	*	0.061	0.004	0.038	0.023	0.010	0.042	0.001	0.030	0.029	0.001
	b)	1.539		1.582	1.603	1.624	1.644	1.668	1.686	1.699	1.730	1.749	1.787
9	a)	0.104	0.011	0.051	0.004	0.046	*	0.038	0.012	0.017	0.034	*	0.035
	b)	1.528	1.548	1.571	1.592	1.613		1.655	1.673	1.698	1.716		1.760
10	a)	0.086	0.033	0.028	0.025	0.026	0.013	0.033	0.002	0.037	0.003	0.026	0.022
	b)	1.516	1.537	1.560	1.581	1.602	1.623	1.643	1.669	1.684	1.698	1.727	1.745
11	a)	0.068	0.054	0.007	0.044	0.004	0.035	0.008	0.025	0.017	0.011	0.030	*
	b)	1.505	1.526	1.550	1.570	1.591	1.612	1.630	1.653	1.671	1.696	1.713	
12	a)	0.050	0.068	*	0.045	0.002	0.036	0.001	0.034	*	0.032	0.004	0.024
	b)	1.494	1.516		1.559	1.579	1.601	1.624	1.641		1.682	1.697	1.724

a) $q_{v'v''}$ - FC factors; b) $\bar{r}_{v'v''}$ - r-centroids (in Å); $*q_{v'v''} \approx 0$

Table 4. Franck-Condon factors and r-centroids of A′ - X system

$v'\backslash v''$		0	1	2	3	4	5	6	7	8	9	10	11	12
0	a)	*	*	*	*	*	0.001	0.002	0.006	0.012	0.023	0.039	0.058	0.079
	b)						1.771	1.789	1.806	1.824	1.842	1.860	1.878	1.896
	c)											2275.20	2335.97	
1	a)	*	*	*	*	0.001	0.004	0.011	0.023	0.039	0.058	0.073	0.076	0.066
	b)					1.747	1.765	1.782	1.800	1.817	1.835	1.852	1.870	1.888
	c)									2140.22	2195.14	2252.29	2311.84	2373.89
2	a)	*	*	*	0.001	0.005	0.013	0.027	0.045	0.060	0.064	0.052	0.028	0.006
	b)				1.724	1.741	1.758	1.776	1.793	1.810	1.828	1.845	1.863	1.879
	c)							2018.95	2068.86	2120.71	2174.61	2230.65		
3	a)	*	*	0.001	0.004	0.011	0.025	0.043	0.056	0.055	0.036	0.011	*	0.011
	b)			1.701	1.718	1.735	1.752	1.769	1.787	1.804	1.821	1.838		1.876
	c)						1954.96	2002.35	2051.44	2102.43	2155.40			
4	a)	*	*	0.002	0.008	0.020	0.038	0.051	0.049	0.029	0.006	0.001	0.018	0.036
	b)			1.695	1.712	1.729	1.746	1.764	1.781	1.798	1.814	1.838	1.852	1.869
	c)					1895.47	1940.35	1986.94	2035.25	2085.43				
5	a)	*	0.001	0.004	0.014	0.030	0.046	0.047	0.029	0.006	0.001	0.019	0.034	0.026
	b)		1.673	1.690	1.707	1.724	1.741	1.758	1.775	1.791	1.814	1.828	1.845	1.862
	c)			1798.63	1839.88	1882.60	1926.85	1972.80						
6	a)	*	0.002	0.007	0.020	0.038	0.046	0.033	0.009	*	0.015	0.031	0.023	0.004
	b)		1.668	1.685	1.702	1.719	1.735	1.752	1.769		1.805	1.822	1.838	1.856
	c)		1748.50	1788.07	1828.80	1871.01	1914.77							
7	a)	*	0.003	0.011	0.027	0.041	0.038	0.016	*	0.009	0.027	0.023	0.005	0.002
	b)		1.663	1.680	1.697	1.714	1.730	1.747		1.783	1.799	1.816	1.831	1.854
	c)		1739.88	1778.85	1819.22	1860.93	1904.18							
8	a)	0.001	0.004	0.015	0.032	0.040	0.026	0.005	0.003	0.020	0.025	0.008	0.001	0.016
	b)	1.641	1.658	1.675	1.692	1.709	1.725	1.741	1.762	1.777	1.794	1.809	1.835	1.846
	c)	1695.16	1732.52	1771.15	1811.11	1852.46								
9	a)	0.001	0.006	0.019	0.035	0.035	0.014	*	0.011	0.024	0.014	*	0.010	0.022
	b)	1.637	1.654	1.671	1.687	1.704	1.720		1.756	1.772	1.788		1.824	1.840
	c)		1726.38	1764.77	1804.47	1845.48								

a) $q_{v'v''}$ - FC factors; b) $\bar{r}_{v'v''}$ - r-centroids (in Å); c) $\lambda_{v'v''}$ - Wavelengths (in Å); $*q_{v'v''} \approx 0$

Table 5. Franck-Condon factors and r-centroids of d - a system

$v'\backslash v''$		0	1	2
0	a)	0.026	0.108	0.210
	b)	1.652	1.681	1.710
1	a)	0.083	0.181	0.124
	b)	1.632	1.660	1.687
2	a)	0.142	0.131	0.003
	b)	1.613	1.639	1.656
3	a)	0.173	0.040	0.038
	b)	1.595	1.619	1.651
4	a)	0.170	*	0.092
	b)	1.577		1.630
5	a)	0.141	0.022	0.072
	b)	1.559	1.587	1.611
6	a)	0.104	0.066	0.021
	b)	1.542	1.569	1.592
7	a)	0.069	0.095	*
	b)	1.525	1.551	
8	a)	0.043	0.100	0.019
	b)	1.509	1.535	1.561
9	a)	0.025	0.086	0.051
	b)	1.493	1.518	1.544
10	a)	0.013	0.065	0.074
	b)	1.477	1.502	1.528
11	a)	0.007	0.044	0.078
	b)	1.461	1.487	1.512
12	a)	0.004	0.028	0.069
	b)	1.445	1.471	1.496

a) $q_{v'v''}$ - FC factors; b) $\bar{r}_{v'v''}$ - r-centroids (in Å); $*q_{v'v''} \approx 0$

Acknowledgements – The authors thank the referee for his critical comments and valuable suggestions. One of the authors (BK) thanks the University Grants Commission, New Delhi for the award of a project fellowship.

REFERENCES

Bagare, S.P., Balachandra Kumar, K. and Rajamanickam, N.: 2006, *Solar Phys.*, **234**, 1.
Bates, D.R.: 1949, *Proc. Roy. Soc.*, **A196**, 217.
Bell, S., Ng, T.L. and Suggitt, C.: 1972, *J. Mol. Spectros.*, **44**, 267.
Crovision, J. and Encrenaz, T.: 2000, *Comet Science*, Cambridge University Press, Cambridge.
Deutscher, N.M., Jones, N.B., Griffith, D.W.T., Wood, S.W. and Murcray, F.J.: 2006, *Atmos. Chem. Phys. Discuss*, **6**, 1619.
Fraser, P.A. and Jarmain, W.R.: 1953, *Proc. Phys. Soc.*, **A66**, 1145.
James, T.C.: 1966, *J. Mol. Spectr.*, **20**, 77.
Jarmain, W.R. and Fraser, P.A.: 1953, *Proc. Phys. Soc.*, **A66**, 1153.
Jefferts, K.B., Penzias, A.A. Wilson, R.W. and Solomon, P.M.: 1971, *Astrophys. J.*, **168**, L111.
Huber, K.P. and Herzberg, G.: 1979, Molecular Spectra and Molecular Structure - Vol. IV, Constants of Diatomic Molecules, Van Nostrand Reinhold, NewYork.
Kaiser, R.I., Ochsenfeld, C., Head-Gordon, M. and Lee, Y.T.: 1998, *Science*, **279**, 1181.
Martin, S., Martin-Pintado, J., Manersberger, R., Henkel, C. and Garcia-Burillo, S.: 2005, *Astrophys. J.*, **620**, 210.
Morse, P.M.: 1929, *Phys. Rev.*, **34**, 57.
Nicholls, R.W., Amani, M. and Mandelman, M.: 2001, *Can. J. Phys.*, **79**, 611.
Nyman, L.Å.: 1992, *IAU Symp.*, **150**, 401.
Partal Urena, F., Fernandez Gomez, M., Lopez Gonzalez, J.J. and Rajamanickam, N.: 2000, *Astrophys. Space Sci.*, **272**, 345.
Rajamanickam, N.: 1987, *J. Quant. Spectrosc. Radiat. Transf.*, **37**, 207.
Rajamanickam, N.: 1988, *Acta Phys. Hung.*, **63**, 341.
Reddy, R.R., Nazeer Ahammed, Y., Rama Gopal, K. and Baba Basha, D.: 2003, *Astrophys. Space Sci.*, **286**, 419.
Singh, M. and Chaturvedi, J.P.: 1987, *Astrophys. Space Sci.*, **135**, 1.
Sinha, K.: 1978, Molecules in Solar Atmosphere, Ph.D. Thesis, University of Gorakhpur, Gorakhpur, India.
Straughan, B.P. and Walker, S.: 1976, Spectroscopy - Vol.3, Chapman & Hall, London.
Tewarson, A. and Palmer, H.B.: 1968, *J. Mol. Spectros.*, **27**, 246.
Vanderslice, J.T., Mason, E.A., Maisch, W.G. and Lippincott, E.R.: 1960, *J. Chem. Phys.*, **33**, 614.
Williams, J.P. and Blitz, L.: 1998, *Astrophys. J.*, **494**, 657.
Woods, P.M., Schoier, F.L., Nyman, L.A. and Olofsson, H.: 2003, *Astron. Astrophys.*, **402**, 617.
Woods, P.M. and Nyman, L.A.: 2005, *IAU Symp.*, **231**, Cambridge University Press, Cambridge.
Yeomans, D.K.: 1991, Comets, Wiley Science Edition, New York.

ФРЕНК-КОНДОН ФАКТОРИ И R-ЦЕНТРОИДИ УГЉЕНИК СУЛФИДА (CS), ЈЕДНОГ АСТРОФИЗИЧКИ ИНТЕРЕСАНТНОГ ЈЕДИЊЕЊА

B. Karthikeyan[1], V. Raja[2], N. Rajamanickam[1] and S. P. Bagare[3]

[1]*Physics Research Centre, V.H.N.S.N College, Virudhunagar - 626 001*

[2]*Kalasalingam University, Krishnankoil - 626 190*

[3]*Indian Institute of Astrophysics, Kodaikanal & Bangalore - 560 034*

УДК 52-355.3 : 524.327
Оригинални научни рад

За интерпретацију интензитета спектралног зрачења у молекулској астрофизици познавање вредности Френк-Кондонових (FC) фактора и величине r-центроида је од суштинске важности. У овом раду су израчунате вредности FC фактора и r-центроида за CS стања и прелазе a $^3\Pi_r$ - X $^1\Sigma^+$, d $^3\Delta_i^n$ - X $^1\Sigma^+$, e $^3\Sigma^-$ - X $^1\Sigma^+$, A′ $^1\Sigma^+$ - X $^1\Sigma^+$ и d $^3\Delta_i^n$ - a $^3\Pi_r$ и дискутован њихов значај у астрофизичком и физичком смислу. Вредности FC фактора за a-X систем су упоређене за већ израчунатим вредностима које су дате у раду Reddy et al. (2003).