Franck-Condon Factors and r -Centroids For Several Systems of CoF Molecule

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ABSTRACT. Franck–Condon factors and r -centroids have been calculated for the $G^3\Phi_4 - X^3\Phi_4$, $K^3\Phi_4 - X^3\Phi_4$, $L^3\Phi_4 - X^3\Phi_4$, $[20.6]^3\Gamma_5 - X^3\Phi_4$ and $[34.7]^3\Gamma_5 - X^3\Phi_4$ bands of Cobalt monofluoride $^{59}\text{Co}^{19}\text{F}$ from the best available molecular constants using Morse and Rydberg–Klein–Rees (RKR) methods. The reliability of the obtained values was verified by comparing the results of five different programs. Based on the calculated Franck–Condon factors values, the appearance of the bands in these systems are discussed and the relationship between the r -centroids and the band-origin wavenumbers and wavelengths are also determined along with accuracy factors.

1. INTRODUCTION

Franck–Condon factors (FCFs) are important parameters for every molecular band system, since they are involved in the calculation of the relative band intensities, the determination of the molecular structure, population of the levels in the upper electronic state involved in transition and the calculation of radiative lifetimes, vibrational temperature, kinetics of energy transfer, etc [1]. The FCFs are also useful in the studies of radiative transfer in the atmospheres of stellar and other astronomical objects, which contain molecular species [2]. On the other hand, the r -centroid [3-5] also has been found of much importance as it is used in the interpretation of intensity measurements of many band systems of astrophysically important molecules and, to determine the variation of the electronic transition moment with inter-nuclear separation, and thereby to derive band strengths, and other molecular transition probability parameters [6].

“The properties of transition metal compounds have fascinated physicists and chemists for a long time. These compounds have an enormous potential for future applications of solar energy conversion, information storage systems, chemical or biochemical sensors, low dimensional semiconductors, supramolecular systems, chemical synthesis, etc”[7]. In astrophysics it is the transition-metal-containing compounds are very important [8-10]. More over the presence of transition metal elements in cool stars has been known for some time [11].

In recent years, enough progress has been made in an understanding of the electronic structure of transition metal oxides and hydrides. Metal fluorides are also potential stellar and interstellar molecules, although Fluorine has relatively small cosmic abundance. Metal fluorides also have strong bonds, which favor their formation in stellar atmospheres [12]. In this paper, the FCFs and r -centroids for the bands of the $G^3\Phi_4 - X^3\Phi_4$, $K^3\Phi_4 - X^3\Phi_4$, $L^3\Phi_4 - X^3\Phi_4$, $[20.6]^3\Gamma_5 - X^3\Phi_4$ and $[34.7]^3\Gamma_5 - X^3\Phi_4$ systems of the $^{59}\text{Co}^{19}\text{F}$ molecule are reported. To the best of our knowledge, such information is not available in the literature. Therefore the reliable values of FCFs and r -centroids for these band systems have been determined using more accurate numerical integration procedure and suitable potentials. The required molecular constants are taken from the works of [8- 12].

2. FRANCK CONDON FACTORS AND R-CENTROID

Within the framework of the Born-Oppenheimer approximation, the expression for band intensities in emission is given in as [13]:

$$I_{em}(v'v'') = \frac{64}{3} \pi^4 C N_{v'} v^4 \overline{R_e(r)}^2 \left[\int \psi_{v'}(r) \psi_{v''}(r) dr \right]^2 \quad (1)$$

Where C is velocity of light, $N_{v'}$ is number of molecules in v' th level, v is the wave number of radiation of the $v' \rightarrow v''$ vibronic transition; and $\overline{R_e(r)}$ is the average transition moment, which is commonly represented as a function of internuclear distance r . $\psi_{v'}(r)$ and $\psi_{v''}(r)$ are the wave functions which correspond to the rotationless ($J = 0$) vibrational levels in the upper and lower electronic states, respectively. They satisfy the time-independent Schrödinger radial wave equation:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) \right] \psi_v(r) = E_v \psi_v(r) \quad (2)$$

In which r is the inter-nuclear distance, $\hbar$ is Planck's constant, μ is the reduced mass of the two atoms forming the molecule and $V(r)$ is the potential energy.

For many band systems, $R_e(r)$ can be well approximated by a constant or a linear function of r . Since the wave-mechanical formulation of the Franck-Condon principle rests on the assumption that this variation is slow. In such a situation, the r -centroid approximation can be employed. The quantity in the square bracket appearing in eq. (1) is the square of overlap integral known as Franck-Condon factor which is usually denoted by $q_{v'v''}$ and determines how the intensity is distributed among the vibrational bands of a band system. It is expressed as,

$$q_{v'v''} = \left[\int \psi_{v'}(r) \psi_{v''}(r) dr \right]^2 \quad (3)$$

r -Centroid is the r -coordinate of the centroid of the area represented by the overlap integral and defined as:

$$\bar{r}_{v'v''} = \frac{\int \psi_{v'}(r) r \psi_{v''}(r) dr}{\int \psi_{v'}(r) \psi_{v''}(r) dr} \quad (4)$$

In the above equation $\bar{r}$ is the r -centroid which is the weighted average with respect to $\psi_{v'}$ $\psi_{v''}$ of the range of internuclear separation r values experienced by the molecule in both states of the $v' \rightarrow v''$ transition [11] or may be looked upon as an effective value of r for the band in much the same way as the v of eqn.(1) constitutes its effective wave number [14]. The r -centroid is the most practical method for calculation of the band strengths of the observed transitions in diatomic molecules. Since it is an approximation, there are limits to its use. According to [9] the approximation is good to the n th order if:

$$\bar{r}_{v'v''}^n = \int \psi_{v'}(r) r^n \psi_{v''}(r) dr / \int \psi_{v'}(r) r^{n-1} \psi_{v''}(r) dr \quad (5)$$

and its accuracy factor that indicates the degree of its applicability given by Drake [15].

$$Y_{v'v''}^{(n)} = \bar{r}_{v'v''}^n / (\bar{r}_{v'v''})^n \int \psi_{v'}(r) r^n \psi_{v''}(r) dr / (\bar{r}_{v'v''})^n \int \psi_{v'}(r) \psi_{v''}(r) dr \cong 1 \quad (6)$$

When $Y_{v'v''}^{(n)}$ is unity the approximation implied in equations (4) and (6) is exact. Deviation from unity for ($n \geq 2$) is a measure of the error in the approximation.

The accuracy of the calculated FCFs and r -centroids depend on knowledge of the potential energy function of the lower and upper electronic states, which are used to solve the radial Schrödinger

equation for rotationless vibrational wavefunctions $\psi_{v'}(r)$ and $\psi_{v''}(r)$. The commonly used potentials are Morse [16] and Rydberg–Klein–Rees (RKR) [17-19].

3. COMPUTATIONAL METHOD

In the present work we use the same computational methods as described in our previous work [20], where the results are given for each method by mentioning the name of the author in the following order: (1) Le Roy[21-22], (2) Telle[23], (3) Espy[24], (4) Jarman and McCallum[25] referred as Jarman and (5) Felenbok[26].

4. RESULTS AND DISCUSSION

Using above mentioned approaches, FCFs and r -centroids arrays have been computed for the following Systems: G-X, K-X, L-X, [20.6] $^3\Gamma_5$ -X and [34.7] $^3\Gamma_5$ -X of cobalt monofluoride. Tables 2, 3, 4, 5 and 6, show the results obtained using the approach based on Espy RKR/FCF computer programmes along with the wave number, wavelengths and accuracy factor of r -centroids for $n = 3$. The Comparison of the FCFs and r -centroids calculated using the five approaches for G-X system is presented in Table 7 and 8. In these tables the values are calculated for many bands which were not experimentally observed.

The $\Delta r_e = r'_e - r''_e$ for the band systems G-X, K-X, L-X, [20.6] $^3\Gamma_5$ -X and [34.7] $^3\Gamma_5$ -X are: 0.088, 0.027, 0.026, 0.045 and 0.016 respectively. These small values indicate that the minima of the potential energy curves involved in K-X, L-X, and [34.7] $^3\Gamma_5$ -X transitions lie one above the other (Fig.1) and their Condon parabola is very narrow, appear to lie along the main diagonal $v' = v''$ in the Deslandres table and has its maximum value at the (0,0) band. In a three dimensional representation, the FCFs surface looks like a diagonal ridge along $v' = v''$. The situation is somewhat different for [20.6] $^3\Gamma_5$ -X band system in which Δr_e is a little larger (~ 0.05 Å), the ridge widens into a very narrow parabolic ridge with an axial valley. For G-X band system Δr_e is relatively larger and the Condon parabola widens and its vertex moves right the prime diagonal away from (0,0) in accordance with the observations of Nicholls [27]. Condon parabola is a locus of intense bands in v'' progressions which often pass through (0,0) and are not completely symmetric about $v' = v''$ unless the ω'_e and ω''_e are very close together [28]. FCFs of such bands are shown in bold figures in corresponding tables.

The FCFs of G-X show that the (0,1), (0,0) and (1,0) bands are the strongest of all the observed bands. Some bands are found to be roughly equal in magnitude such as [(0,2), (2,0), (3,1)] and [(2,1), (4,1), (5,2)] bands which indicate that these bands of comparable intensities. FCFs for the bands (1,2), (3,3), (3,5), (4,4), (4,6), (6,2) and (6,3) are likely to be intense, hence one expects that these bands may be observed experimentally where as other bands, having small FCFs may not be observed experimentally. Refer to Fig.2. The FCFs of K-X, L-X, [20.6] $^3\Gamma_5$ -X and [34.7] $^3\Gamma_5$ -X systems show that the (0, 0) is the strongest of all the observed bands. The $\Delta v = 0, \pm 1$ bands are intense compared to others, suggesting their presence in the observed spectrum.

The FCFs generated using Morse potential show deviations with those generated by RKR potentials for most of the transitions even for low vibrational levels and these differences for most intense observed bands in G-X, K-X, L-X, [20.6] $^3\Gamma_5$ -X and [34.7] $^3\Gamma_5$ -X are as follows : 1.74×10^{-2} , 1.29×10^{-2} , 6.97×10^{-3} , 2.07×10^{-2} and 6.16×10^{-3} respectively (approximately 0.01 Å). In case of r -centroids, these differences are: 2.66×10^{-3} , 8.00×10^{-4} , 1.16×10^{-3} , 6.80×10^{-4} and 9.20×10^{-4} respectively or approximately 0.001(Å). These differences increase for higher levels in a v'' or v' progression. The FCFs differences may be explained in terms of deviation of theoretical value of rotational constant α , computed using Pekeris relation [29] from corresponding experimental value.

The percentage error (deviation) between the experimental and computed values of the rotational constant α for X, G, K, L, $[20.6]^3\Gamma_5$ and $[34.7]^3\Gamma_5$ systems are: 46 %, 15 %, 4 %, 19 %, 15 % and 8 % respectively. This suggests that the lower part of the potential energy curves of the excited states may be described by a simple Morse function but it cannot describe the ground state properly. The r-centroid of the observed bands vary systematically from band to band of a system. In the case of very small overlap integrals, r-centroids have irregular behavior, and such values are not used in our consideration. The sequence difference $\Delta\bar{r} = r_{v'+1,v''+1} - r_{v',v''}$ for the observed bands are found generally to be constant for the strong sequences. In G-X, L-X, $[20.6]^3\Gamma_5$ -X and $[34.7]^3\Gamma_5$ -X systems the sequence difference is found to be constant amounting to about 0.01(Å). But in the case of K-X system, the sequence difference is not a constant and is varying from 0.004-0.01 (Å). For all these band systems, it is found that the r-centroids increase systematically with increasing wavelength of the corresponding v', v'' bands, which is expected for transitions between states with $r'_e > r''_e$ and the bands are red degraded. For example the wavelength and wavenumbers versus r-centroids of few bands of $\Delta v = 3$ sequence of the G-X system are displayed in Table 9 and wavelength versus r-centroids are plotted in Fig.3 which show a systematic relationship. Nicholls et al. [11] have shown that $r_{0,0}$ is usually greater than $(r'_e + r''_e)/2$ for systems whose potentials are not very anharmonic. In the present case, $r_{0,0}$ is found to be slightly greater than $(r'_e + r''_e)/2$ by 0.004, 0.005, 0.005, 0.004 and 0.005 respectively, suggesting that the potentials are almost harmonic. The vibrational sum rule is satisfied for lower and upper states progressions up to (2, v''), (v' , 0) progressions for G-X, $[20.6]^3\Gamma_5$ -X and up to (2, v''), (v' , 1) progressions for K-X, L-X and to (2, v''), (v' , 2) progressions for $[34.7]^3\Gamma_5$ -X, indicating that further experimental work will not be helpful to observe more bands in these progressions. To assess the reliability of r-centroids values we have calculated the factor $Y_{v',v''}^{(n)}$ for $n = 3$. In terms of this factor 1% agreement means that this quantity, which should be exactly 1, is smaller than 1.01 or $|1 - Y_{v',v''}^{(n)}| < 0.01$. According to McCallum [30] the obtained values may be considered reliable for which $|1 - Y_{v',v''}^{(3)}| < 0.02$.

Figures and Tables

Table 1: Spectroscopic constants of the different states of $^{59}\text{Co}^{19}\text{F}$

Constant ^a	$X^3\Phi_4$	$G^3\Phi_4$	$K^3\Phi_4$	$L^3\Phi_4$	$[20.6]^3\Gamma_5$	$[34.7]^3\Gamma_5$
T_e	0	10385.4033	18912.2894	19252.1574	20679.3781	34694.0474
T_0	-338.8650 ^b	10046.5383 ^c	18573.4244 ^d	18913.2924 ^e	20340.5131 ^f	34355.1824 ^g
ω_e	677.59	580.3556	673.72	646.37	630.54	685.65
$\omega_e x_e$	2.16	2.72447	4.28	2.76	3.40	3.61
$\omega_e y_e$	-0.161	0.007257	-	-	-	-
B_e	0.389824	0.3530152	0.3781	0.3785	0.3702	0.3829
α_e	0.003317	0.0026928	0.0029	0.0028	0.0023	0.0029
α_e Calc. ^h	0.001822	0.002291	0.003010	0.002261	0.002648	0.002656
$r_e(\text{Å})$	1.734924	1.823137	1.761624	1.760690	1.780322	1.750546
Ref	[12]	[9]	[10-11]	[10-11]	[10]	[8]

^a All values are in data units of cm^{-1} , unless otherwise noted.

^b Adjusted T_e of the X state to give $T_0 = 0 \text{ cm}^{-1}$.

^{c, d, e, f, g} Adjusted T_e of the state to give the corresponding ν_{00} value of [9],[10],[11]and [8].

^h α_e calculated using the Pekeris relation.

Table 2: Transition Probability parameters For $G^3\Phi_4 - X^3\Phi_4$ band system of $^{59}\text{Co}^{19}\text{F}$

$v' \backslash v''$	0	1	2	3	4	5	6	$\Sigma_{v''} q_{v'v''}$
0	10336.670	9663.919	8996.942	8336.699	7684.157	7040.282	6406.041	
	0.967	1.035	1.112	1.200	1.301	1.420	1.561	
	0.357	0.400	0.188	0.048	0.007	0.001	0.000	1.000
	1.783	1.829	1.879	1.935	1.998	2.072	2.174	
	0.002	0.000	0.002	0.004	0.006	0.010	0.016	
1	10911.600	10238.850	9571.871	8911.629	8259.087	7615.212	6980.970	
	0.917	0.977	1.045	1.122	1.211	1.313	1.433	
	0.339	0.000	0.225	0.285	0.122	0.026	0.003	1.000
	1.743	1.640	1.840	1.889	1.944	2.008	2.084	
	0.000	0.213	0.003	0.000	0.003	0.006	0.009	
2	11481.140	10808.400	10141.420	9481.176	8828.634	8184.759	7550.517	
	0.871	0.925	0.986	1.055	1.133	1.222	1.324	
	0.186	0.135	0.096	0.055	0.272	0.193	0.056	0.992
	1.707	1.753	1.789	1.856	1.898	1.953	2.018	
	0.002	0.004	0.005	0.011	0.002	0.002	0.005	
3	12045.350	11372.600	10705.620	10045.380	9392.840	8748.965	8114.723	
	0.830	0.879	0.934	0.996	1.065	1.143	1.232	
	0.078	0.202	0.011	0.162	0.000	0.199	0.241	0.892
	1.673	1.715	1.777	1.800	2.111	1.910	1.963	
	0.003	0.001	0.021	0.001	0.097	0.004	0.001	
4	12604.260	11931.510	11264.540	10604.290	9951.750	9307.875	8673.634	
	0.793	0.838	0.888	0.943	1.005	1.074	1.153	
	0.028	0.143	0.119	0.012	0.140	0.024	0.115	0.582
	1.641	1.680	1.724	1.742	1.810	1.832	1.924	
	0.005	0.002	0.004	0.023	0.002	0.020	0.008	
5	13157.920	12485.170	11818.190	11157.950	10505.410	9861.532	9227.291	
	0.760	0.801	0.846	0.896	0.952	1.014	1.084	
	0.009	0.073	0.152	0.038	0.062	0.080	0.071	0.485
	1.611	1.648	1.688	1.737	1.762	1.822	1.850	
	0.006	0.004	0.000	0.011	0.008	0.007	0.009	
6	13706.360	13033.620	12366.640	11706.400	11053.850	10409.980	9775.738	
	0.730	0.767	0.809	0.854	0.905	0.961	1.023	
	0.003	0.030	0.109	0.116	0.002	0.100	0.028	0.387
	1.583	1.618	1.656	1.697	1.788	1.773	1.838	
	0.008	0.005	0.002	0.003	0.054	0.003	0.016	
$\Sigma_{v'} q_{v'v''}$	0.999	0.983	0.900	0.715	0.605	0.622	0.514	

For each $v' \rightarrow v''$ The listed quantities are $\nu_{v'v''}$ (cm^{-1}), $\lambda_{v'v''}$ (μm), $q_{v'v''}$, $\bar{r}_{v'v''}$ ($\text{\AA}$), $|1 - Y_{v'v''}^{(3)}|$

Table 3: Transition Probability Parameters for $K^3\Phi_4 - X^3\Phi_4$ band system

$v' \backslash v''$	0	1	2	3	$\Sigma_{v''} q_{v'v''}$
0	18909.843	18237.096	17570.119		
	0.529	0.548	0.569		
	0.905	0.093	0.001		1.000
	1.753	1.887	2.183		
	0.002	0.012	0.064		
1	19575.003	18902.256	18235.279		
	0.511	0.529	0.548		
	0.085	0.740	0.170		0.996
	1.621	1.764	1.897		
	0.020	0.005	0.011		
2	20231.605	19558.858	18891.880	18231.637	
	0.494	0.511	0.529	0.549	
	0.008	0.143	0.608	0.234	0.993
	1.549	1.624	1.777	1.907	
	0.022	0.020	0.009	0.009	
3	20879.644	20206.897	19539.919	18879.677	
	0.479	0.495	0.512	0.530	
	0.001	0.021	0.180	0.502	0.703
	1.491	1.549	1.628	1.790	
	0.026	0.023	0.019	0.014	
$\Sigma_{v'} q_{v'v''}$	1.000	0.997	0.960	0.735	

Table 4: Transition Probability Parameters for $L^3\Phi_4 - X^3\Phi_4$ band system

$v' \backslash v''$	0	1	2	3	$\Sigma_{v''} q_{v'v''}$
0	19236.420	18563.670			
	0.520	0.539			
	0.914	0.084			0.998
	1.753	1.897			
	0.002	0.014			
1	19877.270	19204.520	18537.540	17877.300	
	0.503	0.521	0.539	0.559	
	0.081	0.762	0.152	0.006	1.000
	1.615	1.763	1.908	2.105	
	0.022	0.006	0.013	0.034	
2	20512.600	19839.850	19172.870	18512.630	
	0.488	0.504	0.522	0.540	
	0.006	0.139	0.639	0.207	0.990
	1.507	1.621	1.774	1.920	
	0.042	0.021	0.010	0.012	
3		20469.660	19802.680	19142.440	
		0.489	0.505	0.522	
		0.014	0.180	0.540	0.734
		1.511	1.626	1.785	
		0.042	0.020	0.014	
$\Sigma_{v''} q_{v'v''}$	1.000	0.999	0.971	0.752	

Table 5: Transition Probability Parameters For $[20.6]^3\Gamma_5 - X^3\Phi_4$ band system

$v' \backslash v''$	0	1	2	3	$\Sigma_{v''} q_{v'v''}$
0	20655.560	19982.820	19315.840		
	0.484	0.500	0.518		
	0.761	0.217	0.022		0.999
	1.762	1.847	1.947		
	0.002	0.004	0.011		
1	21279.300	20606.560	19939.580		
	0.470	0.485	0.502		
	0.201	0.414	0.330	0.053	0.998
	1.683	1.773	1.858	1.957	
	0.005	0.007	0.003	0.010	
2	21896.240	21223.500	20556.520	19896.280	
	0.457	0.471	0.487	0.503	
	0.034	0.279	0.214	0.381	0.908
	1.616	1.689	1.786	1.869	
	0.012	0.004	0.013	0.001	
3	22506.380	21833.640	21166.660	20506.420	
	0.444	0.458	0.472	0.488	
	0.004	0.075	0.295	0.103	0.477
	1.548	1.620	1.695	1.802	
	0.020	0.010	0.002	0.023	
$\Sigma_{v''} q_{v'v''}$	0.999599	0.98523	0.8603	0.5366	

Table 6: Transition Probability parameters for $[34.7]^3\Gamma_5 - X^3\Phi_4$ band system

$v' \setminus v''$	0	1	2	3	$\Sigma_{v''} q_{v'v''}$
0	34697.740	34024.990			
	0.288	0.294			
	0.967	0.033			1.000
	1.748	1.976			
	0.002	0.035			
1	35376.170	34703.420	34036.440		
	0.283	0.288	0.294		
	0.031	0.908	0.062		1.000
	1.518	1.758	1.989		
	0.076	0.005	0.034		
2	36047.380	35374.630	34707.650	34047.410	
	0.277	0.283	0.288	0.294	
	0.002	0.054	0.858	0.086	1.000
	1.472	1.513	1.769	2.003	
	0.032	0.084	0.009	0.034	
3	36711.370	36038.620	35371.640	34711.400	
	0.272	0.278	0.283	0.288	
	0.000	0.005	0.071	0.817	0.893
	1.403	1.469	1.508	1.781	
	0.049	0.033	0.093	0.012	
$\Sigma_{v''} q_{v'v''}$	1.000	1.000	0.991	0.903	

Table 7: FCFs for $G^3\Phi_4 - X^3\Phi_4$ band system

$v' \setminus v''$	0	1	2	3	4	5	6	$\Sigma_{v''} q_{v'v''}$
0	0.357	0.400	0.187	0.048	0.007	0.001	0.000	
	0.357	0.400	0.187	0.048	0.007	0.001	0.000	
	0.357	0.400	0.188	0.048	0.007	0.001	0.000	1.000
	0.357	0.400	0.187	0.048	0.007	0.001	0.000	
	0.346	0.382	0.195	0.061	0.013	0.002	0.000	
1	0.339	0.000	0.225	0.285	0.122	0.026	0.003	
	0.339	0.000	0.225	0.285	0.122	0.026	0.003	
	0.339	0.000	0.225	0.285	0.122	0.026	0.003	1.000
	0.339	0.000	0.225	0.285	0.122	0.026	0.003	
	0.345	0.002	0.180	0.267	0.147	0.047	0.010	
2	0.186	0.135	0.096	0.055	0.271	0.193	0.056	
	0.186	0.135	0.096	0.055	0.271	0.193	0.056	
	0.186	0.135	0.096	0.055	0.272	0.193	0.056	0.992
	0.186	0.135	0.096	0.055	0.272	0.193	0.056	
	0.192	0.130	0.115	0.021	0.205	0.207	0.096	
3	0.078	0.202	0.011	0.162	0.000	0.198	0.241	
	0.078	0.202	0.011	0.162	0.000	0.198	0.241	
	0.078	0.202	0.011	0.162	0.000	0.199	0.241	0.892
	0.078	0.202	0.011	0.162	0.000	0.199	0.241	
	0.079	0.211	0.005	0.166	0.011	0.097	0.213	
4	0.028	0.143	0.119	0.012	0.140	0.024	0.115	
	0.028	0.143	0.119	0.012	0.140	0.024	0.115	
	0.028	0.143	0.119	0.012	0.140	0.024	0.115	0.582
	0.028	0.143	0.119	0.012	0.140	0.024	0.116	
	0.027	0.152	0.116	0.027	0.110	0.074	0.019	
5	0.009	0.073	0.152	0.038	0.062	0.080	0.071	
	0.009	0.073	0.152	0.038	0.062	0.080	0.071	
	0.009	0.073	0.152	0.038	0.062	0.080	0.071	0.485
	0.009	0.073	0.152	0.038	0.061	0.080	0.071	

	0.008	0.076	0.163	0.026	0.091	0.034	0.122	
6	0.003	0.030	0.109	0.116	0.002	0.100	0.028	
	0.003	0.030	0.109	0.116	0.002	0.100	0.028	
	0.003	0.030	0.109	0.116	0.002	0.100	0.028	0.387
	0.003	0.030	0.109	0.116	0.002	0.100	0.028	
	0.002	0.031	0.120	0.115	0.000	0.117	0.000	
$\Sigma_{v'} q_{v'v''}$	0.999	0.983	0.900	0.715	0.605	0.622	0.514	

The result order is respectively for Le Roy, Tele, Espy, Jarman and Felenbok

Table 8: r -Centroids for $G^3\Phi_4 - X^3\Phi_4$ band system

$v' \setminus v''$	0	1	2	3	4	5	6
0	1.783	1.829	1.879	1.935	1.998	2.072	2.174
	1.783	1.829	1.879	1.935	1.998	2.072	2.174
	1.783	1.829	1.879	1.935	1.998	2.072	2.174
	1.783	1.829	1.879	1.935	1.998	2.072	2.174
	1.781	1.826	1.873	1.920	1.969	2.017	2.066
1	1.743	1.640	1.840	1.889	1.944	2.008	2.084
	1.743	1.640	1.840	1.889	1.944	2.008	2.084
	1.743	1.640	1.840	1.889	1.944	2.008	2.084
	1.743	1.639	1.840	1.888	1.944	2.008	2.084
	1.743	1.767	1.834	1.880	1.927	1.975	2.023
2	1.707	1.753	1.789	1.856	1.898	1.954	2.018
	1.707	1.753	1.789	1.856	1.898	1.953	2.018
	1.707	1.753	1.789	1.856	1.898	1.953	2.018
	1.707	1.753	1.789	1.856	1.898	1.953	2.018
	1.705	1.751	1.792	1.845	1.887	1.933	1.981
3	1.673	1.715	1.777	1.800	2.110	1.910	1.963
	1.673	1.715	1.777	1.800	2.111	1.910	1.963
	1.673	1.715	1.777	1.800	2.111	1.910	1.963
	1.673	1.715	1.777	1.800	2.109	1.910	1.963
	1.670	1.714	1.772	1.801	1.839	1.894	1.940
4	1.641	1.680	1.724	1.742	1.810	1.832	1.924
	1.641	1.680	1.724	1.742	1.810	1.832	1.924
	1.641	1.680	1.724	1.742	1.810	1.832	1.924
	1.641	1.680	1.724	1.742	1.810	1.832	1.924
	1.636	1.678	1.723	1.757	1.809	1.851	1.904
5	1.611	1.648	1.688	1.737	1.762	1.822	1.850
	1.611	1.648	1.688	1.737	1.762	1.822	1.850
	1.611	1.648	1.688	1.737	1.762	1.822	1.850
	1.611	1.648	1.688	1.737	1.762	1.822	1.850
	1.604	1.644	1.686	1.735	1.768	1.819	1.859
6	1.583	1.618	1.656	1.697	1.788	1.773	1.838
	1.583	1.618	1.656	1.697	1.788	1.773	1.838
	1.583	1.618	1.656	1.697	1.788	1.773	1.838
	1.583	1.618	1.655	1.697	1.787	1.773	1.838
	1.574	1.612	1.652	1.695	1.669	1.777	1.892

The result order is respectively for Le Roy, Tele, Espy, Jarman and Felenbok

Table 9: Wave numbers, Wavelengths and r -centroids
of few bands of $\Delta v=3$ sequence of $G^3\Phi_4-X^3\Phi_4$

(v', v'')	$\bar{r}_{v'v''}$ (Å)	$\nu_{v'v''}$ (cm^{-1})	$\lambda_{v'v''}$ (Å)
(3,0)	1.6727	12045.35	8302.0
(4,1)	1.6802	11931.51	8381.2
(5,2)	1.6882	11818.19	8461.5
(6,3)	1.6967	11706.40	8542.3
(7,4)	1.7065	11597.14	8622.8
(8,5)	1.7203	11491.42	8702.1

Fig. 1: PECs for the $X^3\Phi_4$, $G^3\Phi_4$, $K^3\Phi_4$, $L^3\Phi_4$, $[20.6]^3\Gamma_5$ & $[34.7]^3\Gamma_5$
States of $^{59}\text{Co}^{19}\text{F}$

Fig. 2: 3-D Pars of FCF's for the G-X transition

Fig. 3: Variation of r -centroids with λ for $\Delta v=3$ sequence of G-X

5. CONCLUSION

FCFs and r -centroids for the G-X, K-X, L-X, $[20.6]^3\Gamma_5$ -X and $[34.7]^3\Gamma_5$ -X systems of cobalt monofluoride have been calculated for the first time using the Morse and RKR potentials. The generated values using Morse potential show's deviation with those generated by RKR potentials even for low v -level transitions, however, both sets of the results follow the same pattern. This deviation does not depend on Morse program that we used but on nature of Morse model. We also checked the Morse result using the standard program LEVEL8 which gives fairly the same result presented here. The calculated values of FCFs may help in the search and experimental identification of new bands in these systems. On the other hand, the r -centroid values will be helpful in studies of variations in electronic transition moment with internuclear distance as well as in the search for other molecular properties as a function of r .

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