

RKR Franck-Condon Factors and r -centroids of the $d^3\Pi_g-a^3\Pi_u$, $e^3\Pi_g-a^3\Pi_u$, $C^1\Pi_g-A^1\Pi_u$, and $D^1\Sigma_u^+-X^1\Sigma_g^+$

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RKR Franck–Condon Factors and r -centroids of the $d^3\Pi_g-a^3\Pi_u$, $e^3\Pi_g-a^3\Pi_u$, $C^1\Pi_g-A^1\Pi_u$, and $D^1\Sigma_u^+-X^1\Sigma_g^+$ Band Systems of C_2 Radical

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Rydberg-Klein-Rees (RKR) Franck–Condon factors and r -centroids were computed for the $d^3\Pi_g-a^3\Pi_u$ Swan system, the $e^3\Pi_g-a^3\Pi_u$ Fox-Herzberg system, the $C^1\Pi_g-A^1\Pi_u$ Deslandres-d'Azambuja system, and the $D^1\Sigma_u^+-X^1\Sigma_g^+$ Mulliken system of C_2 radical for the $v'=0-8$; $v''=0-8$ matrix using reported molecular constants.

Key words: C_2 radical, RKR potential, Franck-Condon factor, r -centroid

1. Introduction

The C_2 radical is found in hydrocarbon flames, electrical discharges through carbon containing materials, carbon arc emission, heads of comets, and the atmospheres of certain types of stars. Many emission and absorption band systems between various electronic states of C_2 radical have been observed in a wide spectral range.¹⁻¹²⁾ Molecular constants of C_2 radical obtained from high-resolution vibrational and rotational analyses have been compiled by Huber and Herzberg.¹³⁾ In order to determine rovibrational population of C_2 radical from emission spectra, Franck-Condon factors (FCFs) are necessary. Nicholls calculated FCFs of several transitions of C_2 radical using Morse potentials.¹⁴⁾ When Rydberg-Klein-Rees (RKR) potentials are used,¹⁵⁻¹⁷⁾ more reliable FCFs can be obtained.¹⁸⁾

In this study, FCFs and r -centroids of the $d-a$, $e-a$, $C-A$, and $D-X$ band systems of C_2 radical are calculated using RKR potentials. Results obtained are compared with previously reported data.^{14,19,20)} FCFs obtained in this work is used for the determination of

rovibrational distributions of the d , e , C , and D states of C_2 radical formed by the energy-transfer reactions of metastable $Ne(^3P_{0,2})$ atoms with C_2H_2 and C_2D_2 .^{21,22)}

2. FCF and r -centroids

2.1. Franck–Condon factors (FCF)

The expression for band intensities in emission is given as

$$I_{v'jv''} \propto N_{v'j} Re^2(\bar{r}_{v'v''}) q_{v'v''} v_{v'jv''}^3 S_{jv''} / g_{j'} \quad (1)$$

where $N_{v'j}$ is the rotational population in a given vibrational level, $Re(\bar{r}_{v'v''})$ the electronic transition moment, $q_{v'v''}$ the FCF, $v_{v'jv''}$ the transition frequency, $S_{jv''}$ the rotational line strength, and $g_{j'} = 2j' + 1$.²³⁾ FCFs are expressed as,

$$q_{v'v''} = [\int \Psi_{v'}(r) \Psi_{v''}(r) dr]^2 \quad (2)$$

where $\Psi_{v'}(r)$ and $\Psi_{v''}(r)$ are the wave functions of v' and v'' levels.

2.2. r -centroids

r -centroids ($\bar{r}_{v'v''}$) is the r -coordinate of the centroid of the area represented by the overlap integral and defined as:

$$\bar{r}_{v'v''} = \frac{\int \Psi_{v'}(r) r \Psi_{v''}(r) dr}{\int \Psi_{v'}(r) \Psi_{v''}(r) dr} \quad (3)$$

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3. Results and discussion

3.1 Energy-level diagram and emission systems

Figure 1 shows energy-level diagram of C_2 radical in the $a^3\Pi_u$, $d^3\Pi_g$, and $e^3\Pi_g$ triplet states and in the $X^1\Sigma_g^+$, $A^1\Pi_u$, $C^1\Pi_g$, and $D^1\Sigma_u^+$ singlet states. Their molecular constants are given in Table 1. The $a^3\Pi_u$ state is located just above the ground $X^1\Sigma_g^+$ state. Among these states, the $d^3\Pi_g$ - $a^3\Pi_u$ Swan system, the $e^3\Pi_g$ - $a^3\Pi_u$ Fox-Herzberg system, the $C^1\Pi_g$ - $A^1\Pi_u$ Deslandres-d'Azambuja system, and the $D^1\Sigma_u^+$ - $X^1\Sigma_g^+$ Mulliken system are known to occur. As shown in the names of above emission systems, two

Nobel prize winners, Herzberg and Mulliken, contributed to the first observation of two emission systems and the determination of molecular states of C_2 radical. This indicates that C_2 radicals are an important diatomic radical for the understanding of molecular structure and reactions of carbon-containing molecules in flame, discharge, and comet.

Among molecular constants given in Table 1, equilibrium internuclear distance (r_e) and vibrational frequency (ω_e) are two key parameters, which affect FCFs. The r_e values of the d, C, and D states are close to the ground X state, whereas they increase by factors of 5.6, 6.1, and 23.5% for the a, A and e states,

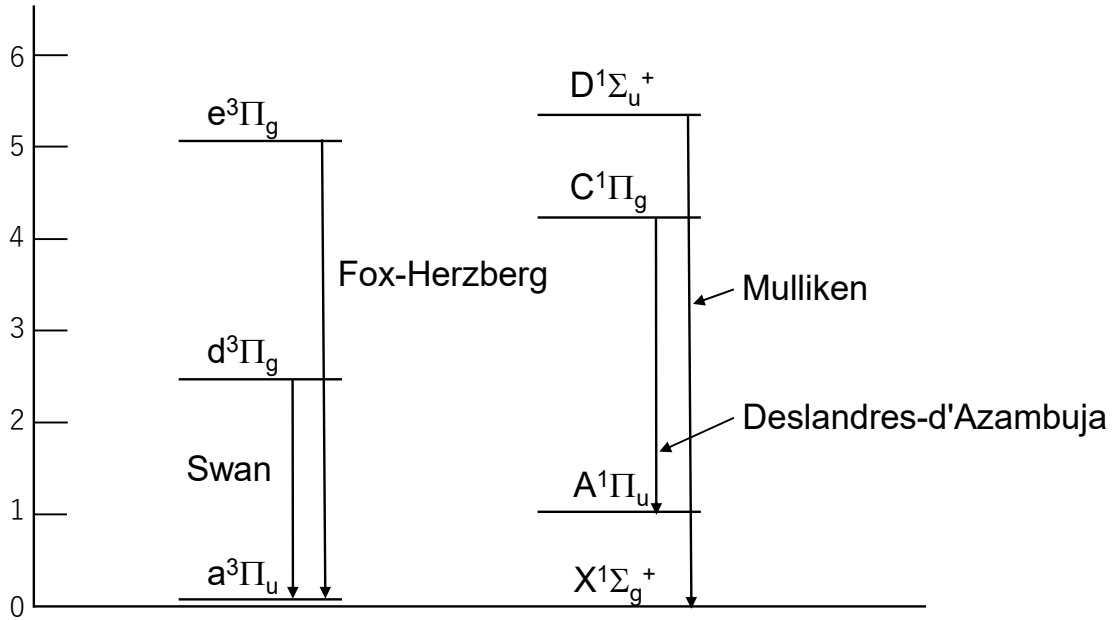


Fig. 1. Energy-level diagram and emission systems of C_2 radicals, for which RKR FCFs and r -centroids are calculated.

Table 1. Molecular constants of C_2 molecules (Ref. 13) used for the calculations of RKR FCFs and r -centroids.

State	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	D_e ($10^{-6} cm^{-1}$)	r_e (\AA)
$D^1\Sigma_u^+$	43239.44	1829.57	13.94	1.8332	0.0196	7.32	1.2380
$e^3\Pi_g$	40796.65	1106.56	39.260	1.1922	0.0242	6.3	1.5351
$C^1\Pi_g$	34261.3	1809.1	15.81	1.7834	0.0180	6.8	1.2552
$d^3\Pi_g$	20022.50	1788.22	16.440	1.7527	0.01608	6.74	1.2661
$A^1\Pi_u$	8391.00	1608.35	12.078	1.61634	0.01686	6.44	1.31843
$a^3\Pi_u$	716.24	1641.35	11.67	1.63246	0.01661	6.44	1.31190
$X^1\Sigma_g^+$	0	1854.71	13.340	1.81984	0.01765	6.92	1.24253

respectively, due to increasing the antibonding character of the molecular orbital of an excited electron. The ω_e value decreases by 1.4, 2.5, 3.6, 11.5, 13.3, and 40.3% for the D, C, d, a, A, and e states in comparison with that of the ground X state, respectively. Similar equilibrium geometries for the D and X states lead to small Δr_e and $\Delta \omega_e$, thus narrow FC envelopes are expected for the D–X transition. On the other hand, relatively large Δr_e and $\Delta \omega_e$ values between the d and a states, between the e and a states, and between the C and A states will give broad FC envelopes.

3.2 RKR FCFs and r -centroids

Tables 2–5 show RKR FCFs and r -centroids of the d–a, e–a, C–A, and D–X transitions of C_2 radical, respectively. RKR FCFs of these transitions are plotted for v' and v'' in Figs. 2–5. RKR FCFs for the d–a, e–a, and C–A transitions obtained in this study are similar to those of Morse FCFs reported by Nicholls.¹⁴⁾ FCFs and r -centroids for the d–a and e–a transitions are similar to those of RKR FCFs and r -centroids reported by Jain.¹⁹⁾ FCFs and r -centroids for the D–X transition are in reasonable agreement with the reported data of Sorkhabi et al. calculated using RKR potentials.²⁰⁾ Based on our present calculations, the following tendencies are found.

- (a) $\Delta v' = 1, 0,$ and -1 sequences are dominant for the d–a Swan system for which Δr_e (3.6%) and $\Delta \omega_e$ (–8.2%) values are relatively large (Table 2 and Fig. 2).
- (b) $v' = 0$ and 1 progressions are dominant for the e–a Fox-Herzberg system for which very large differences exist in Δr_e (–15%) and $\Delta \omega_e$ (48%) values (Table 3 and Fig. 3).
- (c) $\Delta v' = 3, 2, 1, 0,$ and $-1, -2,$ and -3 sequences are dominant for the C–A Deslandres-d’Azambuja system for which Δr_e (5.0%) and $\Delta \omega_e$ (–11%) values are relatively large (Table 4 and Fig. 4).
- (d) Only $\Delta v' = 0$ sequence is dominant for the D–X Mulliken system for which Δr_e (0.37%) and $\Delta \omega_e$ (1.4%) values are very small (Table 5 and Fig. 5).

4. Summary and Conclusion

RKR FCFs and r -centroids were computed for the d–a, e–a, C–A, and D–X band systems for the $v' = 0-8$; $v'' = 0-8$ matrix using reported precise molecular constants. Results obtained were in reasonable agreement with

reported data. Reliable data obtained in this study can be used to determine rovibrational distributions of d, e, C, and D states of C_2 radical produced in various conditions (flame, plasma discharge, and comet).

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Table. 2. RKR FCFs and r -centroids of the $d^3\Pi_g-a^3\Pi_u$ Swan system of C_2 .

	v''								
	0	1	2	3	4	5	6	7	8
0	0.7263 (0) ^{a)}	0.2183 (0)	0.4558 (-1)	0.8151 (-2)	0.1379 (-2)	0.2315 (-3)	0.3893 (-4)	0.6371 (-5)	
	1.2938	1.2244	1.1681	1.1176	1.0738	1.0363	1.0026	0.9665	
1	0.2453 (0)	0.3411 (0)	0.2829 (0)	0.9905 (-1)	0.2494 (-1)	0.5412 (-2)	0.1096 (-2)	0.2132 (-3)	0.3928 (-4)
	1.3691	1.3070	1.2317	1.1757	1.1250	1.0802	1.0410	1.0053	0.9676
2	0.2746 (-1)	0.3708 (0)	0.1367 (0)	0.2639 (0)	0.1390 (0)	0.4614 (-1)	0.1231 (-1)	0.2922 (-2)	0.6440 (-3)
	1.4633	1.3791	1.3274	1.2383	1.1827	1.1318	1.0864	1.0456	1.0080
3	0.9617 (-3)	0.6720 (-1)	0.4223 (0)	0.4347 (-1)	0.2120 (0)	0.1588 (0)	0.6648 (-1)	0.2115 (-1)	0.5755 (-2)
	1.6138	1.4761	1.3905	1.3679	1.2440	1.1891	1.1379	1.0920	1.0500
v' 4		0.2626 (-2)	0.1083 (0)	0.4369 (0)	0.9172 (-2)	0.1565 (0)	0.1614 (0)	0.8219 (-1)	0.3040 (-1)
		1.6518	1.4905	1.4035	1.4833	1.2479	1.1949	1.1431	1.0970
5	0.1945 (-5)	0.5503 (-5)	0.4020 (-2)	0.1440 (0)	0.4397 (0)	0.6604 (-3)	0.1101 (0)	0.1530 (0)	0.9176 (-1)
	1.4481	0.3286	1.7061	1.5070	1.4183	2.1414	1.2482	1.2002	1.1471
6		0.1172 (-4)	0.8489 (-4)	0.4117 (-2)	0.1699 (0)	0.4465 (0)	0.5515 (-4)	0.7562 (-1)	0.1397 (0)
		1.5231	1.0775	1.7956	1.5259	1.4349	-2.4208	1.2416	1.2054
7			0.3403 (-4)	0.4296 (-3)	0.2559 (-2)	0.1825 (0)	0.4649 (0)	0.7606 (-4)	0.5161 (-1)
			1.6056	1.2949	1.9899	1.5482	1.4530	-2.9078	1.2223
8				0.5729 (-4)	0.1306 (-2)	0.4364 (-3)	0.1788 (0)	0.4952 (0)	0.2000 (-3)
				1.7194	1.4119	2.9154	1.5749	1.4715	4.7600

^{a)} (n) is power of 10 multiplying the entry. Top entry each block FCFs. Bottom entry each block r -centroids in Å.

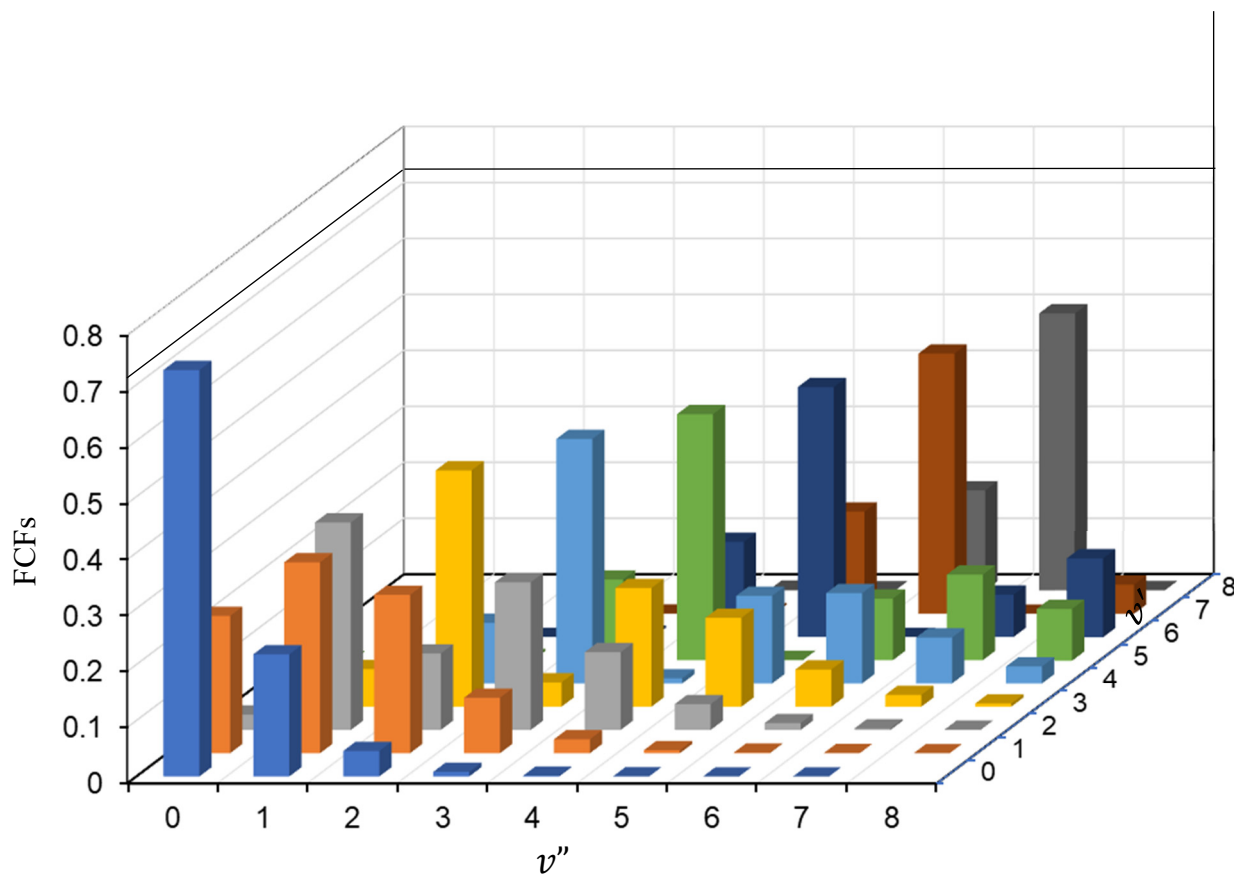
**Fig. 2.** RKR FCFs of the $d^3\Pi_g-a^3\Pi_u$ Swan system of C_2 .

Table. 3. RKR FCFs and r -centroids of the $e^3\Pi_g-a^3\Pi_u$ Fox-Herzberg system of C_2 .

		v''								
		0	1	2	3	4	5	6	7	8
0		0.2155 (-2) ^{a)}	0.1701 (-1)	0.6080 (-1)	0.1322 (0)	0.1970 (0)	0.2144 (0)	0.1764 (0)	0.1123 (0)	0.5612 (-1)
	r -centroids	1.4222	1.4434	1.4664	1.4908	1.5164	1.5433	1.5717	1.6020	1.6340
1		0.8810 (-2)	0.5064 (-1)	0.1167 (0)	0.1332 (0)	0.6606 (-1)	0.2308 (-2)	0.3337 (-1)	0.1241 (0)	0.1740 (0)
	r -centroids	1.4085	1.4282	1.4498	1.4727	1.4957	1.5022	1.5578	1.5832	1.6129
2		0.1984 (-1)	0.8232 (-1)	0.1135 (0)	0.4623 (-1)	0.7553 (-3)	0.6046 (-1)	0.9539 (-1)	0.3354 (-1)	0.2912 (-2)
	r -centroids	1.3962	1.4142	1.4342	1.4549	1.5148	1.5104	1.5335	1.5567	1.6118
3		0.3274 (-1)	0.9664 (-1)	0.6902 (-1)	0.7883 (-3)	0.4584 (-1)	0.7112 (-1)	0.8861 (-2)	0.2584 (-1)	0.8969 (-1)
	r -centroids	1.3850	1.4012	1.4189	1.4136	1.4692	1.4908	1.5064	1.5516	1.5729
4		0.4465 (-1)	0.9153 (-1)	0.2459 (-1)	0.1526 (-1)	0.6763 (-1)	0.1433 (-1)	0.2023 (-1)	0.6927 (-1)	0.1635 (-1)
	r -centroids	1.3747	1.3889	1.4018	1.4361	1.4519	1.4703	1.5080	1.5280	1.5444
5		0.5362 (-1)	0.7372 (-1)	0.2339 (-2)	0.4505 (-1)	0.4030 (-1)	0.3417 (-2)	0.5803 (-1)	0.1840 (-1)	0.1706 (-1)
	r -centroids	1.3652	1.3769	1.3662	1.4192	1.4346	1.4738	1.4867	1.5061	1.5488
6		0.5881 (-1)	0.5152 (-1)	0.2022 (-2)	0.5717 (-1)	0.8230 (-2)	0.3370 (-1)	0.3845 (-1)	0.3661 (-2)	0.5671 (-1)
	r -centroids	1.3563	1.3650	1.4247	1.4046	1.4104	1.4490	1.4678	1.5074	1.5235
7		0.6014 (-1)	0.3109 (-1)	0.1316 (-1)	0.4760 (-1)	0.5790 (-3)	0.5193 (-1)	0.5103 (-2)	0.3833 (-1)	0.2782 (-1)
	r -centroids	1.3480	1.3528	1.3912	1.3901	1.4831	1.4319	1.4406	1.4803	1.5027
8		0.5801 (-1)	0.1572 (-1)	0.2508 (-1)	0.2814 (-1)	0.1295 (-1)	0.4057 (-1)	0.3751 (-2)	0.4952 (-1)	0.7054 (-4)
	r -centroids	1.3403	1.3395	1.3762	1.3743	1.4157	1.4145	1.4617	1.4609	1.4100

^{a)} (n) is power of 10 multiplying the entry. Top entry each block FCFs. Bottom entry each block r -centroids in Å.

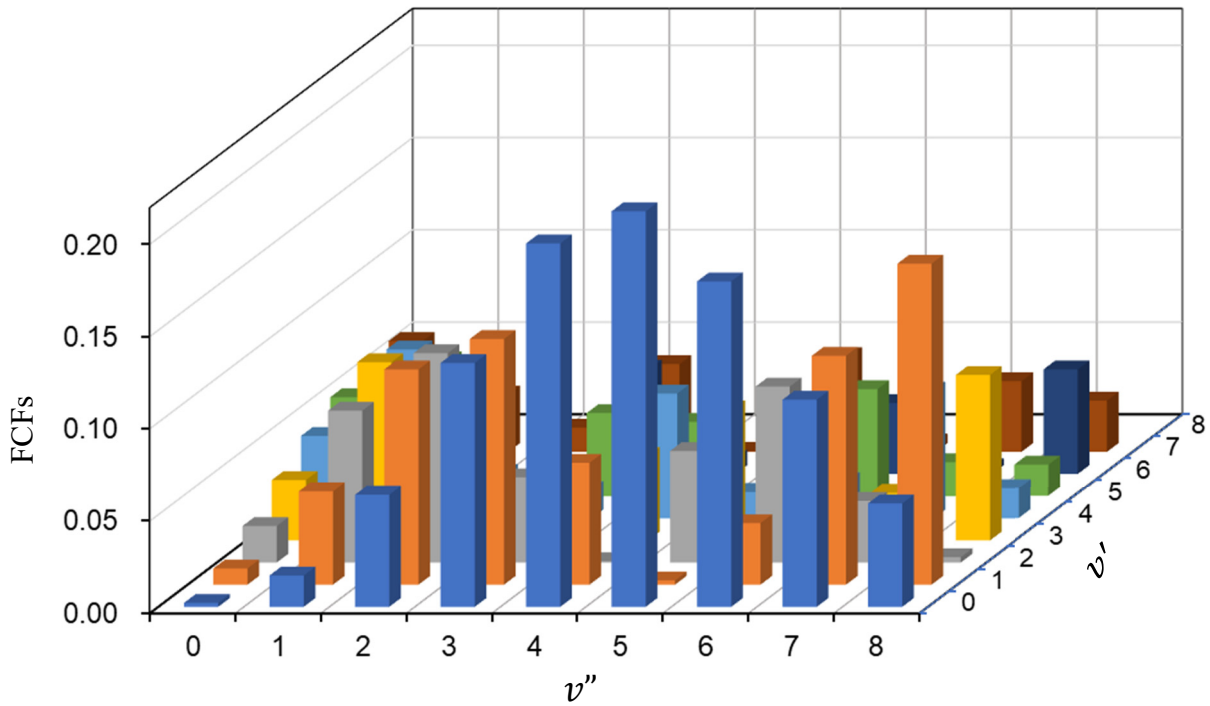


Fig. 3. RKR FCFs of the $e^3\Pi_g-a^3\Pi_u$ Fox-Herzberg system of C_2 .

Table 4. RKR FCFs and r -centroids of the $C^1\Pi_g-A^1\Pi_u$ Deslandres-d'Azambuja system of C_2 .

		v''								
		0	1	2	3	4	5	6	7	8
0		0.5447 (0) ^{a)}	0.3048 (0)	0.1082 (0)	0.3145 (-1)	0.8224 (-2)	0.2031 (-2)	0.4871 (-3)	0.1156 (-3)	0.2754 (-4)
	r	1.2913	1.2418	1.1990	1.1608	1.1263	1.0947	1.0657	1.0392	1.0150
1		0.3558 (0)	0.8518 (-1)	0.2622 (0)	0.1794 (0)	0.7812 (-1)	0.2738 (-1)	0.8508 (-2)	0.2467 (-2)	0.6884 (-3)
	r	1.3468	1.3091	1.2508	1.2066	1.1680	1.1334	1.1018	1.0728	1.0463
2		0.8856 (-1)	0.3841 (0)	0.2837 (-3)	0.1398 (0)	0.1859 (0)	0.1172 (0)	0.5343 (-1)	0.2042 (-1)	0.7032 (-2)
	r	1.4110	1.3565	1.0082	1.2617	1.2146	1.1754	1.1405	1.1088	1.0799
3		0.1038 (-1)	0.1901 (0)	0.2869 (0)	0.4693 (-1)	0.4497 (-1)	0.1470 (0)	0.1348 (0)	0.7894 (-1)	0.3660 (-1)
	r	1.4894	1.4198	1.3677	1.2854	1.2784	1.2233	1.1829	1.1476	1.1159
4		0.5592 (-3)	0.3339 (-1)	0.2691 (0)	0.1688 (0)	0.1101 (0)	0.3425 (-2)	0.9156 (-1)	0.1287 (0)	0.9684 (-1)
	r	1.5964	1.4984	1.4288	1.3816	1.3018	1.3429	1.2334	1.1907	1.1549
5		0.1053 (-4)	0.2355 (-2)	0.6711 (-1)	0.3138 (0)	0.7569 (-1)	0.1465 (0)	0.5189 (-2)	0.4227 (-1)	0.1045 (0)
	r	1.7866	1.6073	1.5075	1.4384	1.4023	1.3128	1.2071	1.2472	1.1991
6			0.5204 (-4)	0.5956 (-2)	0.1079 (0)	0.3250 (0)	0.2075 (-1)	0.1493 (0)	0.3015 (-1)	0.1101 (-1)
	r		1.8070	1.6183	1.5168	1.4485	1.4459	1.3228	1.2522	1.2745
7				0.1490 (-3)	0.1171 (-1)	0.1518 (0)	0.3099 (0)	0.6989 (-3)	0.1272 (0)	0.6015 (-1)
	r			1.8288	1.6296	1.5262	1.4595	1.7948	1.3328	1.2681
8					0.3206 (-3)	0.1971 (-1)	0.1955 (0)	0.2785 (0)	0.5210 (-2)	0.9264 (-1)
	r				1.8534	1.6413	1.5361	1.4719	1.2262	1.3431

^{a)} (n) is power of 10 multiplying the entry. Top entry each block FCFs. Bottom entry each block r -centroids in Å.

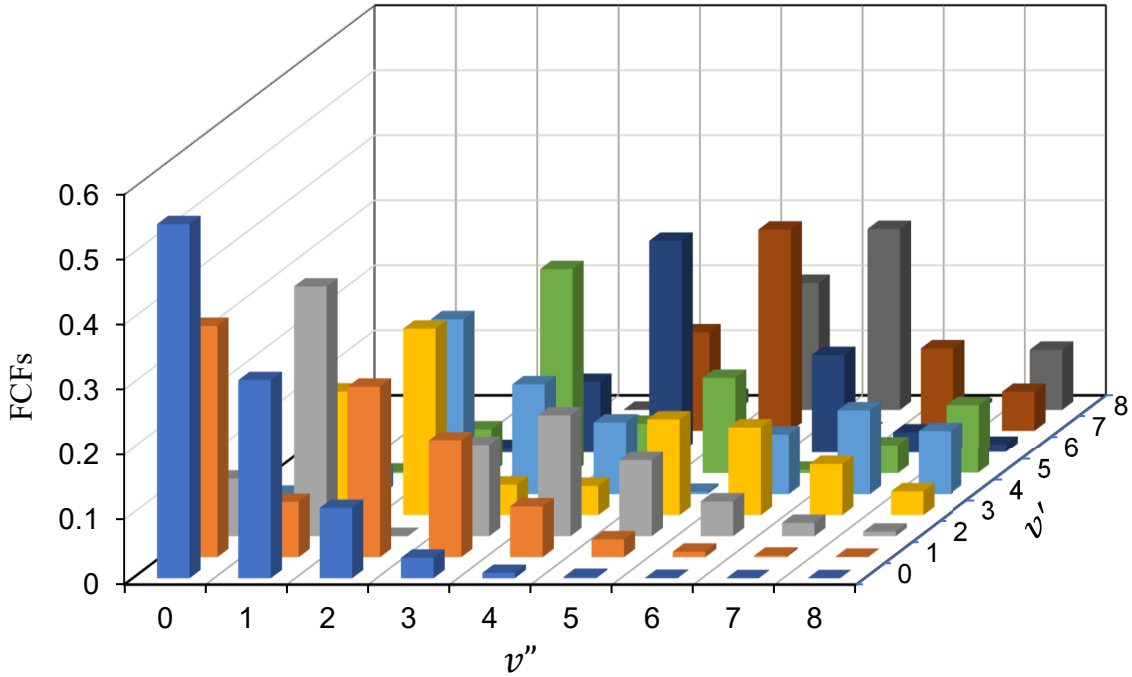
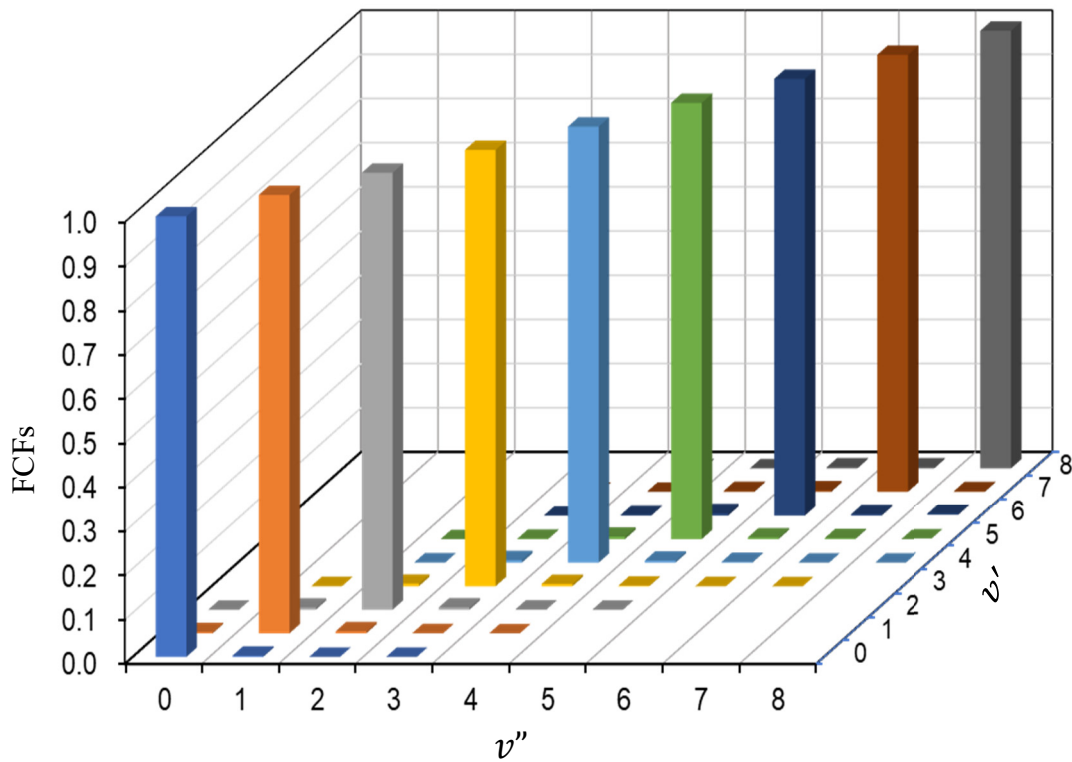
**Fig. 4.** RKR FCFs of the $C^1\Pi_g-A^1\Pi_u$ Deslandres-d'Azambuja system of C_2 .

Table 5. RKR FCFs and r -centroids of the $D^1\Sigma_u^+-X^1\Sigma_g^+$ Mulliken system of C_2 .

		v''								
		0	1	2	3	4	5	6	7	8
0		0.9971 (0)	0.2749 (-2)	0.1720 (-3)	0.4115 (-5)					
		1.2453	0.4992	0.8594	0.6162					
1		0.2833 (-2)	0.9923 (0)	0.4394 (-2)	0.4640 (-3)	0.1420 (-4)				
		1.9816	1.2555	0.4130	0.8684	0.6079				
2		0.9267 (-4)	0.4673 (-2)	0.9892 (0)	0.5141 (-2)	0.8365 (-3)	0.3056 (-4)			
		1.2096	2.0631	1.2659	0.3027	0.8790	0.5986			
3			0.2820 (-3)	0.5639 (-2)	0.9876 (0)	0.5182 (-2)	0.1260 (-2)	0.5254 (-4)	0.1309 (-5)	
			1.2483	2.1631	1.2765	0.1577	0.8915	0.5882	0.1098	
v' 4				0.5675 (-3)	0.5858 (-2)	0.9871 (0)	0.4699 (-2)	0.1714 (-2)	0.7898 (-4)	0.2178 (-5)
				1.2873	2.2894	1.2873	-0.0399	0.9062	0.5769	0.0823
5				0.1363 (-5)	0.9439 (-3)	0.5473 (-2)	0.9874 (0)	0.3862 (-2)	0.2185 (-2)	0.1087 (-3)
				-0.2664	1.3267	2.4551	1.2982	-0.3223	0.9233	0.5649
6					0.4387 (-5)	0.1401 (-2)	0.4637 (-2)	0.9883 (0)	0.2837 (-2)	0.2664 (-2)
					0.1265	1.3671	2.6838	1.3093	-0.7546	0.9428
7					0.1316 (-5)	0.1124 (-4)	0.1922 (-2)	0.3517 (-2)	0.9894 (0)	0.1783 (-2)
					1.6861	0.3899	1.4089	3.0222	1.3206	-1.4916
8						0.2111 (-5)	0.2472 (-4)	0.2487 (-2)	0.2298 (-2)	0.9905 (0)
						1.7625	0.5830	1.4526	3.5791	1.3322

^{a)} (n) is power of 10 multiplying the entry. Top entry each block FCFs. Bottom entry each block r -centroids in Å.

**Fig. 5.** RKR FCFs of the $D^1\Sigma_u^+-X^1\Sigma_g^+$ Mulliken system of C_2 .