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Franck–Condon factors for diatomic molecules with anharmonic corrections

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Abstract

Some of the band systems of several astrophysically important molecules are calculated and compared with the results obtained by calculations based on realistic Klein–Dunham and Rydberg–Klein–Rees potential functions. The Morse potential is approximated by means of a fourth-order anharmonic oscillator model. In the second-quantized formalism, the anharmonic Hamiltonian is diagonalized by using the Bogoliubov–Tyablikov transformation. The diagonalization process gives a shift in the frequency associated with each normal mode of harmonic vibration of the molecules presented here. The Franck–Condon factors are estimated using this new frequency within the framework of a harmonic oscillator. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Diatomic molecules; Franck–Condon factors; Morse potential

1. Introduction

The relative intensity of vibrational bands in electronic spectra or photoelectron spectra depends primarily on the square of the vibrational overlap integrals of electronic states which participate in the transitions. These transitions are usually known as the Franck–Condon factors (FCFs) and they are important quantities widely used in many branches of physical and chemical sciences. Among the various potential functions proposed to calculate such factors,

Morse [1] in 1929 proposed his potential function to describe diatomic molecules. The Morse function enjoys a great popularity, thanks to its simple form and the relation between the parameters of analytical functions and the observable spectroscopic constants. On the other hand, the vibrational overlap integrals used to evaluate the FCFs contain the vibrational wave function of both the lower electronic state (basic) and the upper electronic state (excited) and they were calculated for the first time in 1939 by Hutchisson [2] using two harmonic oscillator wave functions. It is important to comment that, when simple molecular systems are studied, those harmonic integrals can be solved directly; however, to make the experimental work more efficient, it is convenient to obtain general formulae to calculate them. An attempt made by Manneback [3] in 1951 and

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after him by Wagner [4] and Ansbacher [5] in 1959, used integral–differential methods to obtain such formulae. A year later Koide [6], who used second-quantization formalism, derived various formulae of which, Ansbacher's is undoubtedly the most elegant and useful. Besides, Katriel and Adam [7,8] reported closed formulae of particular cases. In 1983, Palma and Morales [9] obtained Ansbacher's relations by using complex variable and second quantization techniques, for the harmonic potential.

For the evaluation of the Morse FCFs there are many approaches, such as those reported by Ramjee et al. [10], Ta-You Wu [11] and Chang and Karplus [12]. In the present work, we calculate the FCFs for the Morse potential, based on the second quantization formalism proposed a few years ago by Palma et al. and Recamier [13,14]. Such formalism allows us to algebraically obtain the frequencies associated with each one of the vibrational molecular states. In addition, the method allows us to find an expression for the frequency, in terms of well-known spectroscopic constants, which in addition, includes anharmonic corrections. The FCFs were estimated by using recurrence relations with the corrected harmonic frequency [13].

In summary, this method, besides retaining the harmonic simplicity, takes into account the anharmonic effects through spectroscopic constants. In addition to this method, results of some interstellar molecules are presented, for which, there are no experimental data.

2. Theory

The use of Morse potential to treat anharmonic effects in molecules is well known. In the particular case of the calculation of FCFs, some authors have derived analytical expressions [15,16] which have become very cumbersome when they are applied to real systems. To overcome this problem we have devised a calculation method, which retains the simplicity inherent in the harmonic approximation and, at the same time, some of the anharmonic effects could be included.

Let us consider the Morse potential function

$$V(x) = D_e[\exp(-2ax) - 2\exp(-ax)] \quad (1)$$

where a is the range parameter and D_e is the dissociation energy. By making a power expansion of this function up to the fourth order, the Hamiltonian of the system can be written as:

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{1}{2}\omega_e^2\hat{x}^2 + A\hat{x}^3 + B\hat{x}^4. \quad (2)$$

In order to proceed, it is convenient to introduce the ladder operators \hat{a} and \hat{a}^+ :

$$\hat{a} = \sqrt{\frac{\mu\omega_e}{2\hbar}}\hat{x} + i\frac{1}{\sqrt{2\hbar\mu\omega_e}}\hat{p} \quad (3)$$

$$\hat{a}^+ = \sqrt{\frac{\mu\omega_e}{2\hbar}}\hat{x} - i\frac{1}{\sqrt{2\hbar\mu\omega_e}}\hat{p}.$$

By retaining only linear and quadratic terms, the normal form of the anharmonic Hamiltonian (2) can be expressed as

$$\hat{H} = \hbar\omega_e[\hat{a}^+\hat{a} + 1/2] + 3\lambda[\hat{a}^+ + \hat{a}] + 6\gamma[\hat{a}^2 + 2\hat{a}^+\hat{a} + (\hat{a}^+)^2 + 1/2], \quad (4)$$

where \hat{a} and \hat{a}^+ are the ladder operators for the harmonic oscillator, and λ , γ , are constants that depend on Morse parameters:

$$\lambda = -\left(\frac{\hbar}{2\mu\omega_e}\right)^{3/2} D_e a^3 \quad (5)$$

$$\gamma = \frac{7}{12}\left(\frac{\hbar}{2\mu\omega_e}\right)^2 D_e a^4. \quad (6)$$

Eq. (4) is a quadratic functional of boson operators \hat{a} , \hat{a}^+ and it can be diagonalized by using the Bogoliubov–Tyablikov transformation [17], for which, we calculate the commutator:

$$[\hat{H}, \hat{a}^+] = (\hbar\omega_e + 12\gamma)\hat{a}^+ + 12\gamma\hat{a} + 3\lambda \quad (7)$$

and by using the same notation as in Ref. [17] to identify the coefficients A and B from Eq. (4), we obtain the 'matrix' \mathbf{M} in a straightforward way

$$\mathbf{M} = (A - B)^{1/2}(A + B)(A - B)^{1/2} = \hbar\omega_e(\hbar\omega_e + 24\gamma) \quad (8)$$

where $A = \hbar\omega_e + 12\gamma$ and $B = 12\gamma$.

The energy (or equivalent to the frequency) is thus

Table 1

Spectroscopic constants of C₂ (Ref. [18]), CN (Ref. [20]), CO (Ref. [20]) and SiO (Ref. [20])

Molecule	State	r_e (Å)	ω_e (cm ⁻¹)	$\omega_e x_e$ (cm ⁻¹)	ω'_e (cm ⁻¹) ^a
C ₂	$\mu = 6.0000$				
	$a^3\Pi_u$	1.3119	1641.35	11.67	1661.65
	$d^3\Pi_g$	1.2661	1788.22	16.44	1816.76
CN	$\mu = 6.4622$				
	$X^2\Sigma^+$	1.1719	2068.70	13.14	2091.58
	$A^2\Pi_i$	1.2328	1814.43	12.88	1836.84
	$B^2\Sigma^+$	1.1508	2164.13	20.25	2199.28
CO	$\mu = 6.8562$				
	$X^1\Sigma^+$	1.1283	2170.21	13.46	2193.64
	$A^1\Pi$	1.2352	1515.61	17.25	1545.50
	$a^3\Pi_r$	1.2094	1739.25	14.47	1764.39
SiO	$\mu = 10.1767$				
	$X^1\Sigma^+$	1.5102	1242.03	6.047	1252.57
	$A^1\Pi$	1.6212	851.51	6.143	862.19

^a New harmonic frequency calculated from the spectroscopy constants.

given by:

$$E = \mathbf{M}^{1/2} = \hbar\omega_e \left[1 + \frac{24\gamma}{\hbar\omega_e} \right]^{1/2}. \quad (9)$$

Therefore, the new frequency which contains anharmonic corrections through the spectroscopic

Table 2

Franck–Condon factors for the $d^3\Pi_g(\nu) \leftarrow a^3\Pi_u(\nu')$ transition of C₂ (swan) calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	7.240–1	–	–	–
	7.323–1	1.661–1	6.476–2	2.282–2
	7.230–1	2.234–1	4.519–2	7.299–3
1	2.460–1	3.300–1	–	–
	2.618–1	3.814–1	1.566–1	1.057–1
	2.442–1	3.303–1	2.961–1	1.012–1
2	–	3.700–1	1.170–1	–
	3.130–3	4.342–1	1.993–1	9.845–2
	3.108–2	3.603–1	1.182–1	2.834–1
3	–	–	4.120–1	2.230–2
	2.740–3	7.552–3	5.424–1	1.079–1
	1.690–3	7.962–2	3.903–1	2.347–2

constant γ , is:

$$\omega' = \omega_e \left[1 + \frac{24\gamma'}{\hbar\omega_e} \right]^{1/2}. \quad (10)$$

Using Eq. (6), γ is calculated in terms of the reduced mass μ of the system, the oscillation frequency ω_e and the following expressions for D_e and a in terms of the anharmonic constant $\omega_e x_e$ [18]:

$$D_e = \frac{\omega_e^2}{4\omega_e x_e} \quad (11)$$

$$a = 2.4354 \times 10^7 (\mu\omega_e x_e)^{1/2}. \quad (12)$$

Thus, the value of γ substituted on Eq. (10) leads to calculate ω' directly, which contains anharmonic corrections.

3. Results and discussion

The formalism presented in this work for the FCFs gives us a simple and direct way to study the diatomic molecular systems whose potential contains both harmonic and anharmonic effects. Given that molecules vibrate in an anharmonic way, it is necessary to approximate a potential function, which describes

Table 3

Franck–Condon factors for the $A^2\Pi_i(\nu) \leftarrow X^2\Sigma^+(\nu')$ transition of CN (red) calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	4.990–1 5.001–1 4.975–1	3.710–1 3.742–1 3.688–1	1.110–1 1.037–1 1.138–1	1.740–2 1.571–2 1.837–2
1	3.200–1 3.167–1 3.238–1	4.560–2 4.726–2 4.574–2	3.500–1 3.599–1 3.419–1	2.230–1 2.210–1 2.244–1
2	1.260–1 1.259–1 1.274–1	2.400–1 2.358–1 2.458–1	1.220–2 1.081–2 1.097–2	2.100–1 2.249–1 2.031–1
3	3.990–2 4.085–2 3.859–2	1.950–1 1.909–1 2.006–1	9.890–2 9.683–2 1.051–1	9.050–2 8.622–2 8.373–2

the real movement of molecules in the best way. We used the Morse potential to do that in this work.

The molecular data of the band systems considered in this paper are shown in Table 1 together with the spectroscopic constants ω_e , $\omega_e x_e$, and ω'_e , in cm^{-1} .

The FCFs obtained for the band systems of astrophysical interest are displayed in Tables 2–7. The molecular systems studied here are

Table 4

Franck–Condon factors for the $B^2\Sigma^+(\nu) \leftarrow X^1\Sigma^+(\nu')$ transition of CN (violet) calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	9.200–1 9.067–1 9.118–1	7.400–2 4.835–2 8.183–2	5.000–3 3.348–2 6.010–3	0.000000 7.048–3 3.700–4
1	7.900–2 7.820–2 8.604–2	7.760–1 7.719–1 7.512–1	1.290–1 4.442–1 1.449–1	1.400–2 7.311–2 1.647–2
2	1.000–3 1.324–2 2.190–3	1.470–1 1.309–1 1.605–1	6.600–1 6.666–1 6.120–1	1.630–1 2.310–2 1.916–1
3	0.000000 1.067–3 5.210–6	2.000–3 4.259–2 6.450–3	2.010–1 1.519–1 2.243–1	5.750–1 5.762–1 4.426–1

Table 5

Franck–Condon factors for the $A^1\Pi(\nu) \leftarrow X^1\Sigma^+(\nu')$ transition of CO (4th positive calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	1.150–1 1.145–1 1.196–1	2.630–1 2.243–1 2.959–1	2.850–1 2.469–1 3.165–1	1.950–1 1.939–1 1.882–1
1	2.210–1 2.346–1 2.085–1	1.530–1 1.472.1 1.425–1	3.000–3 1.099–2 2.272–4	– 2.934–2 1.498–1
2	2.350–1 2.605–1 2.196–1	1.200–2 7.222–3 1.020–2	9.460–2 7.026–2 1.004–1	– 1.141–1 8.402–2
3	1.830–1 1.947–1 1.777–1	2.000–2 4.159–2 1.851–2	1.180–1 1.082–1 1.055–1	– 6.004–3 1.332–3

C_2 : $d^3\Pi_g - a^3\Pi_u$, CN: $A^2\Pi_i - X^2\Sigma^+$ and $B^2\Sigma^+ - X^2\Sigma^+$, CO: $A^1\Pi - X^1\Sigma^+$ and $a^3\Pi_r - X^1\Sigma^+$ and SiO: $A^1\Pi - X^1\Sigma^+$. For each table, rows are labeled by ν and columns by ν' .

The FCFs for each band system have been computed by using recurrence relations. The calculations obtained in this work are the lower inputs in each table and they are compared with two different values.

Table 6

Franck–Condon factors for the $a^3\Pi_r(\nu) \leftarrow X^1\Sigma^+(\nu')$ transition of CO (cameron) calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	2.660–1 2.647–1 2.684–1	3.800–1 3.652–1 3.845–1	2.400–1 2.385–1 2.420–1	8.800–2 9.722–2 8.233–2
1	3.180–1 3.281–1 3.133–1	2.880–1 3.000–2 2.539–2	1.050–1 8.763–2 1.196–1	2.680–1 2.434–1 2.884–1
2	2.180–1 2.245–1 2.184–1	5.400–2 5.604–2 5.010–2	1.600–1 1.542–1 1.482–1	– 1.443–3 1.076–3
3	1.140–1 1.125–1 1.164–1	1.610–1 1.738–1 1.551–1	– 3.850–3 7.930–3	1.300–1 1.219–1 1.264–1

Table 7

Franck–Condon factors for the $A^1\Pi(\nu) \leftarrow X^1\Sigma^+(\nu')$ transition of SiO calculated by: (i) Klein–Dunham and RKR analysis (Ref. [19], uppermost entries), (ii) the Morse of Sharp (Ref. [20], middle entries) and present work (lowermost entries)

$\nu\lambda\nu'$	0	1	2	3
0	1.410–1	2.780–1	2.740–1	1.780–1
	1.427–1	2.763–1	2.710–1	1.773–1
	1.472–1	3.311–1	3.136–1	1.585–1
1	2.570–1	1.300–1	–	–
	2.644–1	1.268–1	7.168–5	9.496–2
	2.279–1	1.147–1	1.060–2	2.098–1
2	2.510–1	–	1.230–1	–
	2.578–1	5.800–5	1.249–1	9.133–2
	2.209–1	1.710–3	1.228–1	5.154–2
3	1.750–1	–	1.000–1	–
	1.758–1	7.353–2	9.381–2	6.917–3
	1.678–1	3.458–2	9.027–2	1.262–2

Firstly, to the values obtained by McCallum et al. [19] based on a realistic Klein–Dunham and Rydberg–Klein–Rees (RKR) potential functions. Secondly, to the values obtained by Sharp [20], who used a recursive analytic method based on the Morse potential function, except for the CN violet system, where Doktorov’s method was used [21].

Table 2 shows the values for the FCFs calculated for the C_2 (Swan) molecule. We found that the FCFs agreed with those given by McCallum et al. [19]. In the best case, for example 0–0, 1–0, 1–1 and 2–2 bands match up to the two first digits. In the worst case, for example 3–2 band, the difference is just 0.02. Comparing the results obtained by Sharp and the results of this work it can be seen that, there is an improvement, when anharmonic effects are considered.

According to Table 1, the ω_e values are considerably different for the two electronic states ($A^2\Pi_1-X^2\Sigma^+$) in the CN(Red) system. However, in the same table, the values of $\omega_e x_e$ for the two states, are very similar; consequently, we would expect good agreement for the FCFs with the values provided by

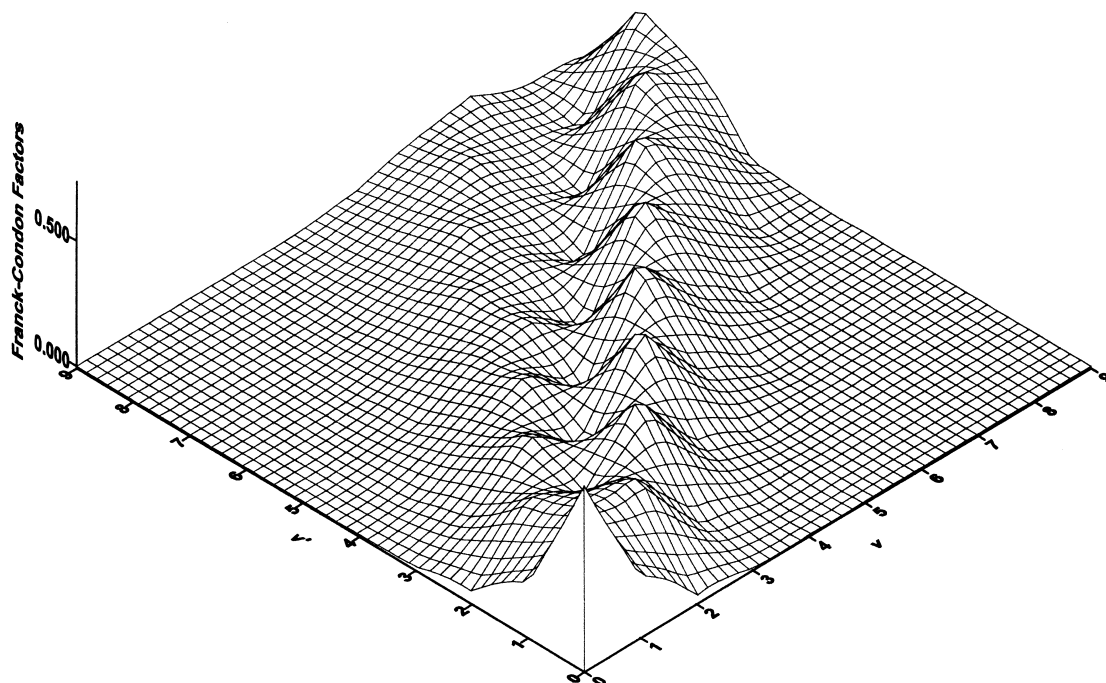


Fig. 1. The Franck–Condon factors in 3D for the $d^3\Pi_g(\nu) \leftarrow a^3\Pi_u(\nu')$ transition of C_2 (swan).

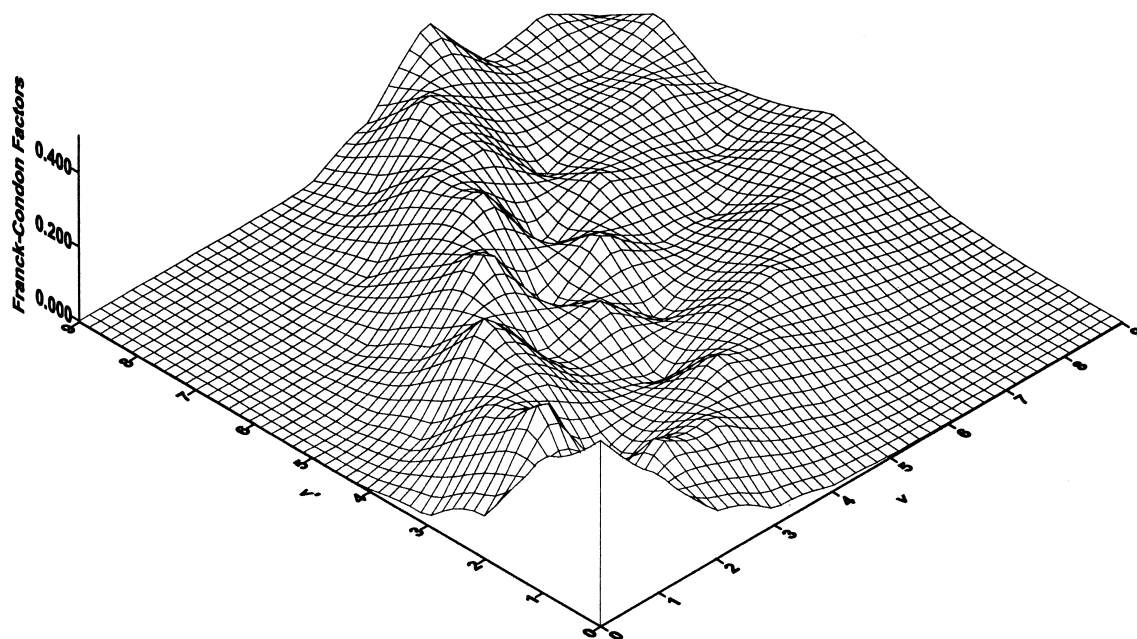


Fig. 2. The Franck–Condon factors in 3D for the $A^2\Pi_i(\nu) \leftarrow X^2\Sigma^+(\nu')$ transition of CN (red).

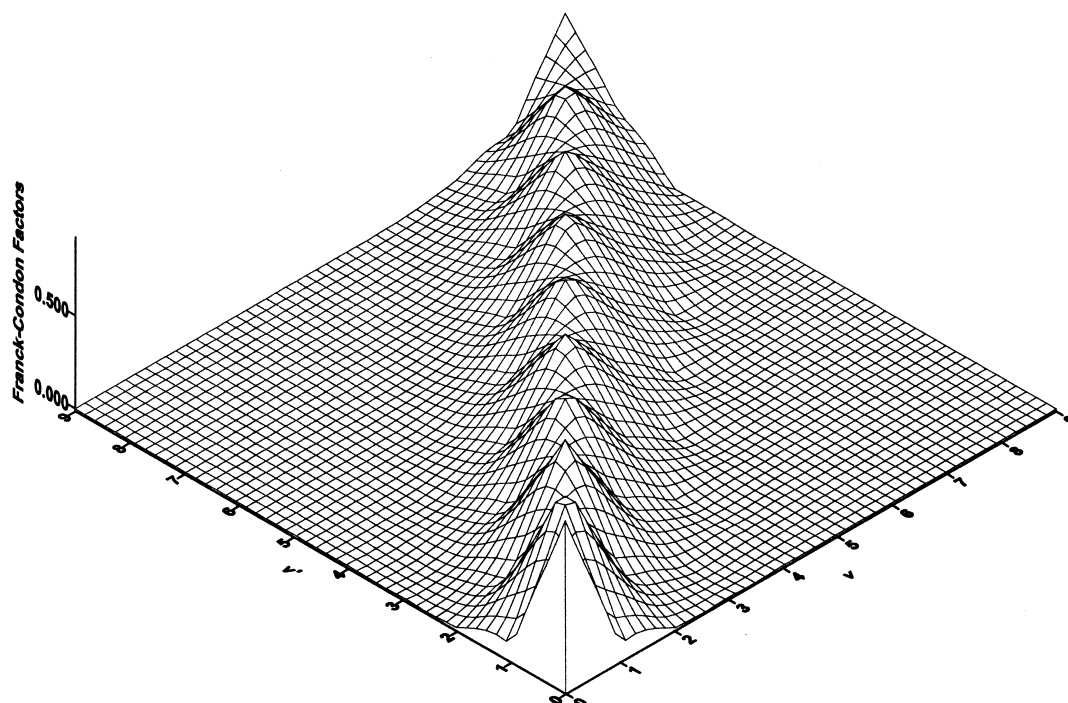


Fig. 3. The Franck–Condon factors in 3D for the $B^2\Sigma^+(\nu) \leftarrow X^1\Sigma^+(\nu')$ transition of CN (violet).

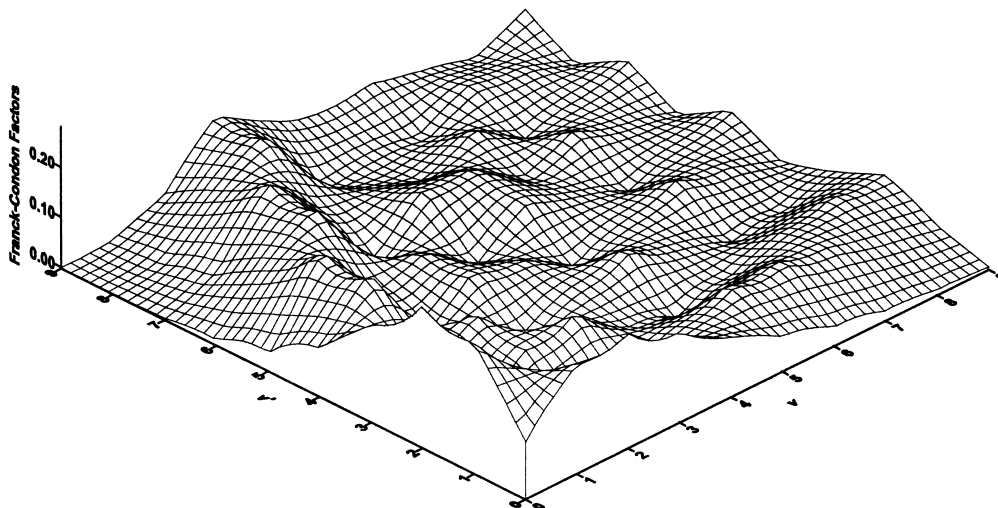


Fig. 4. The Franck–Condon factors in 3D for the $A^1\Pi(v) \leftarrow X^1\Sigma^+(v')$ transition of CO (4th positive).

McCallum et al. shown in Table 3. It is important to observe that, despite some small differences in the values, for the majority of the bands calculated by our method, generally, the values obtained are good because they differ in two digits only. In addition, there are small differences with the values obtained by Palma et al. [13] due to the difference in the constants used for the two electronic states, from those given in Table 1.

In some of the bands of Table 4, for the CN violet

system, our results are in agreement with those calculated by McCallum et al.

Due to high cosmic abundance of carbon and oxygen, CO is one of the more important molecules in astrophysics; consequently, many of the spectroscopic constants of CO are well known, particularly for the ground state. We calculated the FCFs for the CO system and if the FCFs of the main diagonal and the upper triangular matrix are observed in Table 5, it can be seen that the values calculated by Sharp are better

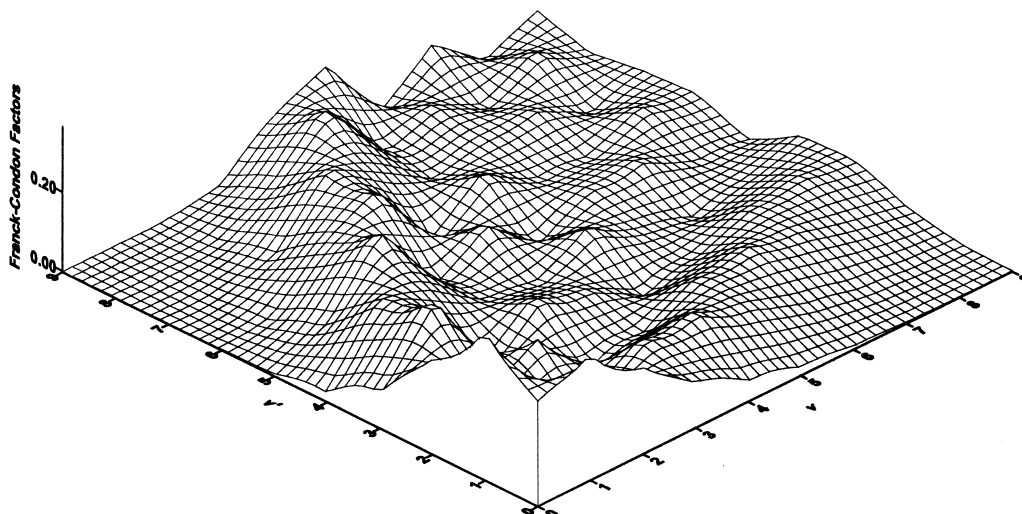


Fig. 5. The Franck–Condon factors in 3D for the $a^3\Pi_r(v) \leftarrow X^1\Sigma^+(v')$ transition of CO (cameron).

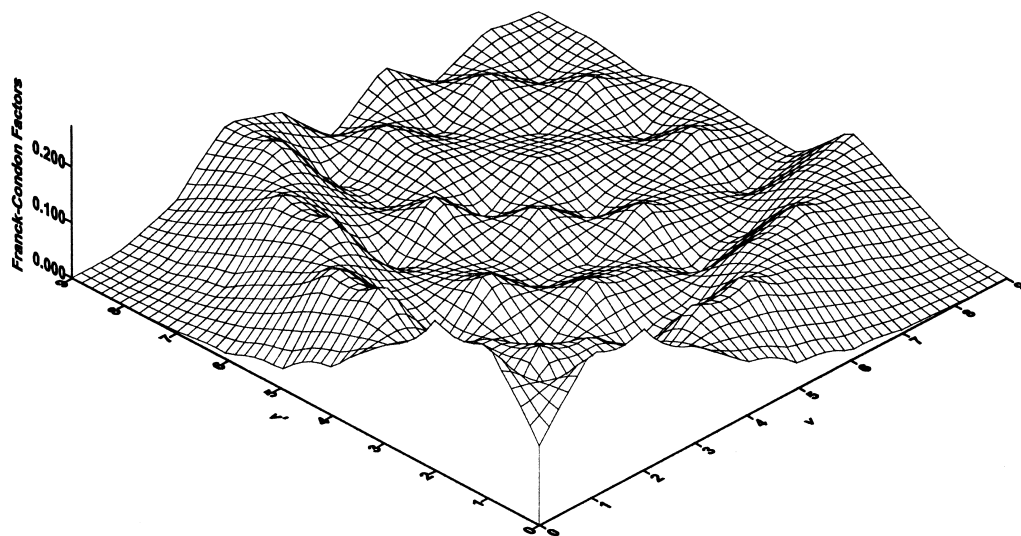


Fig. 6. The Franck–Condon factors in 3D for the $A^1\Pi(v) \leftarrow X^1\Sigma^+(v')$ transition of SiO.

than those calculated by us; however, for the FCFs in the lower triangular matrix, our results are better than those obtained by Sharp.

Despite the Cameron system being very weak, it is still an important system. As can be seen in Table 1, the values of ω_e and r_e are different for those two electronic states ($A^1\Pi-X^1\Sigma^+$). In Table 6 the results of McCallum, Sharp and ours are compared and we can see that there is a better agreement with the values of RKR than those reported in the CO (4th positive) system.

The final system that we discuss here, is the SiO system, because it is an interesting system to study. The values of ω_e and r_e are considerably different for the two electronic states. A selection of some of the bands given by McCallum and Sharp are reproduced in Table 7 and they have been compared with our results. From Table 7, we can observe that, our results are quite different from those obtained by Sharp et al., for the majority of the transitions calculated here.

Although the results for the majority of the bands in the systems calculated here are very similar, among these, when we use the three methods for the calculation of FCFs; in general, we have achieved a moderate approximation to the RKR values due to the inclusion of anharmonic effects, except for the SiO system, obviously.

It can be seen from the graphics that there is a

region that can be identified as a transition probability region, which depends on the spectroscopic constants. In Figs. 1–3 the region is reduced around the main diagonal of the FC matrix; and for the rest of the systems (Figs. 4–6), the region is bounded by a parabola which defines the probabilities of major transition. In the first case, the fact that the probabilities are concentrated in the main diagonal, is due to the difference between the distances of equilibrium of each one of the electronic states being close to zero; therefore, the FCFs are proportional to the probability density of two wave vibrational functions of only one electronic state. However, in the second case, the transition probability between the two electronic states is maintained.

4. Conclusion

The method proposed here gives some improvement on the calculation of FCFs. This improvement comes out because we are considering the harmonic part up to the quartic term. Not all the terms can be incorporated into the scheme of the second quantization; for example, the cubic term does not appear in the final formula of the Hamilton operator. Some attempts have been done [22] to solve this problem but the complexity increases when more number of

terms are taken in account. The problem of extracting the harmonic part of the anharmonic terms is still an open question. Work along this line is in progress.

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