

Franck-Condon factors for some abundant umbral molecules

G. C. Joshi, U. C. Joshi, L. M. Punetha and M. C. Pande

Uttar Pradesh State Observatory, Manora Peak, Naini Tal 263 129

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Abstract. Some of the molecular transitions in UV in sunspots are pointed out and Franck-Condon factors for some of these have been calculated.

Key words : Franck-Condon factors—sunspot umbrae.

1. Introduction

Sunspots present favourable conditions for the formation of molecules. Prominent electronic transitions of some of the abundant molecules fall in the ultraviolet region also. However, the sunspot ultraviolet spectrum is still largely unexplored except for the successful detection of CO(A — X) and H₂ Lyman bands (Bartoe *et al.* 1978; Jordan *et al.* 1978).

As a part of the program of predicting the umbral absorption spectrum in the ultraviolet, theoretical investigations regarding the visibility and the role, as sources of quasi-continuous opacity, of SiO, SH, O₂ and NO have been carried out (Joshi *et al.* 1978, 1979a, 1979b; Joshi & Pande 1979). Although the list of abundant molecules (Gaur *et al.* 1973; Gaur 1977) in the umbral spectrum in the yet unexplored ultraviolet electronic transitions is still long (tables 1 and 2), the predictions for

Table 1. Transitions between 350.0 nm to 207.4 nm originating from ground electronic states of molecules which have already been established to be present in sunspots through transitions other than mentioned here

Molecule	Transition	$\omega_{00}(\text{cm}^{-1})$
Ca ⁴⁰ H ¹	D ² Σ ⁺ — X ² Σ ⁺	40187.2
	K ² Σ ⁺ — X ² Σ ⁺	32691.1
	L ² Π — X ² Σ ⁺	32739.3
	G ² Σ ⁺ — X ² Σ ⁺	34819.5
	J ² Π — X ² Σ ⁺	35068.5
	F ² Σ ⁺ — X ² Σ ⁺	36797.1
C ¹² H ¹	C ² Σ ⁺ — X ² Π _r	31778.1
	E ² Σ ⁺ — X ² Σ ⁺	35550.6
Mg ²⁴ H ¹	C ² Π _r — X ² Σ ⁺	41235.9
	E ¹ Σ ⁺ — X ¹ Σ ⁺	37683.5
Mg ²⁴ O ¹⁶	F ¹ Π — X ¹ Σ ⁺	37879.1
	G ¹ Π — X ¹ Σ ⁺	39868.6
	C ² Σ ⁺ — X ² Π _r	30820.4
Si ²⁸ H ¹	B ² Σ ⁺ — X ² Π _r	30830.2

Table 2. Transitions between 350.0 nm to 207.4 nm originating from ground electronic states of molecules which are abundant in umbral atmosphere but have electronic transitions (from ground state) falling in the ultraviolet only

Molecule	Transition	$\omega_{00}(\text{cm}^{-1})$
Al ²⁷ Cl ³⁵	A ¹ Π — X ¹ Σ ⁺	38237.7
Al ²⁷ F ¹⁹	A ¹ Π — X ¹ Σ ⁺	43949.7
*Al ²⁷ H ¹	C ¹ Σ ⁺ — X ¹ Σ ⁺	44597.9
*Al ²⁷ O ¹⁶	C ² Π — X ² Σ ⁺	33092.0
		33018.0
C ¹² S ³²	A ¹ Π — X ¹ Σ ⁺	38797.6
Mg ²⁴ F ¹⁹	A ² Π _r — X ² Σ ⁺	27863.7
	B ² Σ ⁺ — X ² Σ ⁺	37187.5
	C ² Σ ⁺ — X ² Σ ⁺	42589.6
N ¹⁴ O ¹⁶	A ² Σ ⁺ — X ² Π _r	44080.5
	B ² Π _r — X ² Π _r	45392.1
O ₂ ¹⁶	B ³ Σ _u ⁻ — X ³ Σ _g ⁻	49358.2
P ³¹ N ¹⁴	A ¹ Π — X ¹ Σ ⁺	39688.5
P ₂ ³¹	A ¹ Π _g — X ¹ Σ _g ⁺	34434.3
	C ¹ Σ _u ⁺ — X ¹ Σ _g ⁺	46788.0
S ₂ ³²	B ³ Σ _u ⁻ — X ³ Σ _g ⁻	31689.0
S ³² H ¹	A ² Σ ⁺ — X ² Π ₁	30662.4
Si ₂ ²⁸	N ³ Σ _u ⁻ — X ³ Σ _g ⁻	46762.2
	L ³ Π — X ³ Σ _g ⁻	28602.2
	K ³ Σ _u ⁻ — X ³ Σ _g ⁻	30768.8
Si ²⁸ Cl ³⁵	B ² Σ ⁺ — X ² Π _r	33987.1
	C ² Π — X ² Π _r	34193.6
		41039.9
		41235.0
Si ²⁸ F ¹⁹	B ² Σ ⁺ — X ² Π _r	34638.5
	C ² Δ — X ² Π _r	39454.1
	C ² Π — X ² Π _r	42052.1
	D ² Π — X ² Π _r	46700.2
	D ² Σ ⁺ — X ² Π _r	47491.4
Si ²⁸ O ¹⁶	A ¹ Π — X ¹ Σ ⁺	42640.7
Si ²⁸ S ³²	D ¹ Π — X ¹ Σ ⁺	34908.5
Si ³² O ¹⁶	A ³ Π — X ³ Σ _g ⁻	38255.0
		38095.0
	B ³ Σ ⁻ — X ³ Σ _g ⁻	37940.0
		41370.0

*This molecule has electronic transition (from ground state) in the visible region also.

these transitions could not be made because of the non-availability of electronic oscillator strengths, Franck-Condon factors (hereafter abbreviated as F-C-F) and other related quantities.

Though the techniques for calculating F-C-Fs for molecular electronic transitions are well known, these factors are still not available for most of the transitions listed in tables 1 and 2. Since the F-C-Fs are important for determining intensities of the corresponding molecular bands, a program for calculating F-C-Fs has been undertaken.

We here report the F-C-Fs calculated for some of the transitions listed in tables 1 and 2, namely the D — X (SiF), F — X (CaH), A — X (AlF), C — X (P₂),

C — X (SiCl) and N — X, K — X (Si₂) transitions. In obtaining these F-C-Fs we have used the molecular constants given by Barrow (1973, 1975, 1979), Huber & Herzberg (1979) and Suchard (1975).

2. Calculations

The Franck-Condon factor ($q_{v'v''}$) in any given case is defined as :

$$q_{v'v''} = \langle v' | v'' \rangle^2$$

where $\langle v' | v'' \rangle$ is the overlap integral and v' and v'' represent the upper and lower vibrational states of the molecule. We have calculated these factors using the r_e -shift method given by Jarman & Fraser (1953), who give a closed-form solution of these factors for Morse potential. The values of F-C-Fs for the above mentioned transitions, are tabulated in tables 3a to 3g. The figures given after the mantissa and the sign are the corresponding exponents.

Table 3(a). Franck-Condon factors of the D ²Σ⁺ — X ²Π_r transition of SiF

$v' \setminus v''$	0	1	2	3	4	5
0	5.320-1	2.650-1	7.486-2	1.581-2	2.775-3	4.271-4
1	2.809-1	1.217-1	2.664-1	1.367-1	4.165-2	9.496-3
2	6.745-2	3.205-1	3.632-3	1.928-1	1.872-1	8.498-2
3	9.619-3	1.476-1	2.484-1	2.140-2	9.492-2	1.845-1
4	8.993-4	3.172-2	2.090-1	1.470-1	7.893-2	2.720-2
5	5.762-5	4.005-3	6.445-2	2.378-1	6.123-2	1.295-1

Table 3(b). Franck-Condon factors of the F ²Σ⁺ — X ²Σ⁺ transition of CaH

$v' \setminus v''$	0	1	2	3	4	5
0	8.320-1	1.345-1	1.702-2	2.070-3	2.566-4	3.309-5
1	1.458-1	5.655-1	1.987-1	3.711-2	5.777-3	8.509-4
2	7.939-3	2.615-1	3.539-1	2.608-1	7.885-2	1.820-2
3	1.371-4	2.386-2	3.460-1	1.960-1	2.645-1	1.111-1
4	4.998-7	5.910-4	4.756-2	3.997-1	8.836-2	2.394-1
5	3.237-15	2.844-6	1.590-3	7.850-2	4.235-1	2.579-2

Table 3(c). Franck-Condon factors of the A ¹Π — X ¹Σ⁺ transition of AlF

$v' \setminus v''$	0	1	2	3	4	5
0	9.925-1	4.427-3	1.008-4	3.446-6	1.529-7	8.268-9
1	4.517-3	9.836-1	8.549-3	2.861-4	1.277-5	6.932-7
2	1.486-5	8.947-3	9.750-1	1.251-2	5.679-4	3.237-5
3	7.538-8	4.505-5	1.329-2	9.665-1	1.619-2	9.166-4
4	3.037-10	3.148-7	9.104-5	1.754-2	9.583-1	1.963-2
5	7.526-15	1.711-9	8.211-7	1.533-4	2.171-2	9.503-1

Table 3(d). Franck-Condon factors of the $C\ ^1\Sigma_u^+ - X\ ^1\Sigma_g^+$ transition of P_2

$\begin{array}{c} \diagdown \\ u \\ \diagup \\ u'' \end{array}$	0	1	2	3	4	5
0	1.867-4	1.430-3	5.403-3	1.341-2	2.454-2	3.533-2
1	1.163-3	3.709-3	1.817-2	6.018-2	3.327-2	2.407-2
2	3.768-3	1.578-2	2.791-2	2.471-2	8.506-3	1.419-5
3	8.453-3	2.449-2	2.499-2	7.159-3	6.923-4	1.281-2
4	1.477-2	2.763-2	1.227-2	1.026-4	1.208-2	1.478-2
5	2.141-2	2.333-2	1.694-3	7.662-3	2.031-2	1.563-4

Table 3(e). Franck-Condon factors of the $C\ ^2\Pi - X\ ^2\Pi_r$ transition of $SiCl$

$\begin{array}{c} \diagdown \\ u \\ \diagup \\ u'' \end{array}$	0	1	2	3	4	5
0	9.824-2	1.907-1	1.973-1	1.447-1	8.447-2	4.181-2
1	2.144-1	1.141-1	2.945-3	3.355-2	9.168-2	1.021-1
2	2.233-1	1.760-4	9.300-2	8.369-2	7.058-3	1.749-2
3	1.476-1	7.559-2	7.820-2	3.550-3	7.690-2	6.077-2
4	6.948-2	1.576-1	1.511-5	9.121-2	2.542-2	1.594-2
5	2.477-2	1.367-1	6.755-2	4.294-2	3.528-2	8.207-3

Table 3(f). Franck-Condon factors of the $N\ ^3\Sigma_u^- - X\ ^3\Sigma_g^-$ transition of Si_2

$\begin{array}{c} \diagdown \\ u \\ \diagup \\ u'' \end{array}$	0	1	2	3	4	5
0	3.414-1	3.659-1	1.546-1	3.312-2	3.847-3	2.402-4
1	2.945-1	4.152-4	2.292-1	2.463-1	8.671-2	1.402-2
2	1.567-1	1.249-1	7.313-2	7.476-2	2.714-1	1.586-1
3	6.714-2	1.703-1	1.158-2	1.409-1	3.755-3	2.183-1
4	2.558-2	1.214-1	9.721-2	9.387-3	1.304-1	1.290-2
5	9.115-3	6.526-2	1.236-1	2.719-2	5.861-2	7.065-4

Table 3(g). Franck-Condon factors of the $K\ ^3\Sigma_u^- - X\ ^3\Sigma_g^-$ transition of Si_2

$\begin{array}{c} \diagdown \\ u \\ \diagup \\ u'' \end{array}$	0	1	2	3	4	5
0	2.836-1	3.371-1	1.532-1	3.377-2	3.765-3	2.007-4
1	2.594-1	5.757-4	1.898-1	2.359-1	8.748-2	1.375-2
2	1.494-1	8.677-2	8.244-2	4.965-2	2.849-1	1.568-1
3	7.029-2	1.412-1	2.122-3	1.301-1	2.345-4	1.909-1
4	2.972-2	1.129-1	6.273-2	2.035-2	1.028-1	2.155-2
5	1.184-2	6.825-2	9.857-2	8.918-3	6.976-2	2.074-2

3. Discussion

For low values of the vibrational quantum number, the calculations based on more realistic potentials, such as Klein-Dunham or the R K R potentials, agree well with

those based on Morse potential. We calculated the R K R potentials vis-a-vis the Morse potentials for above mentioned transitions and found that both potentials match for low values of vibration quantum numbers ($v'' \leq 5$). Typical values for Morse and R K R potentials for the A $^1\Pi$ state of the molecule AlF are given in table 4. This can also be seen from the fact that the F-C-Fs as calculated by Murty (1979) for MgO ($B - A$) agree to the third place of decimal with those calculated by McCallum *et al.* (1970) for the same transition. Further, under sunspot conditions the higher vibrational levels will not be populated significantly, and therefore we restricted our calculations up to vibrational quantum number $v'' = 5$ only.

Table 4. Morse and RKR potentials for the A $^1\Pi$ state of AlF

r (Å)	Morse (cm $^{-1}$)	RKR (cm $^{-1}$)
1.481	4234.5	4240.5
1.494	3491.4	3496.4
1.510	2734.5	2740.4
1.528	1968.1	1972.4
1.553	1190.1	1192.4
1.591	400.0	400.5
1.714	400.8	400.5
1.767	1193.9	1192.4
1.807	1974.9	1972.4
1.842	2743.5	2740.4
1.873	3499.5	3496.4
1.902	4242.6	4240.5

Regarding the dependence of F-C-Fs on rotational states we found that for all the transitions except CaH (F - X), the vibration-rotation interaction factor γ is < 0.001 . For CaH (F - X) γ is 0.004 to 0.006. The interaction is not important for molecules with $\gamma \leq 0.001$.

In preparing tables 1 and 2 we considered the following points :

(i) abundances of the constituent elements of the molecule, (ii) dissociation energy range corresponding to sunspot conditions, and (iii) species included in the reduced equation.

In Zwaan's (1965, 1974) sunspot model, the integrated number I per cm 2 in a column above optical depth $\tau_{0.5\mu m} \approx 3$ were considered. All the molecules having $\log I$ values above 16 were considered from the list given by Gaur *et al.* (1973), Gaur (1977) and Joshi (1980). Only the electronic transitions which fall redwards of 207.4 nm (absorption lines) were considered. Shortward of 207.4 nm, the metal opacity due to AlI increases drastically and the continuous absorption masks the line absorption.

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