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Calculating Franck Condon Factor (FCF) for $X^1\Sigma^+$-$A^1\Pi$ Transition of SiO Molecule in Supernova Ejecta by Using Hua Potential

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Abstract: The present work concerns by study of spectroscopic properties for Silicon monoxide SiO which is founded in supernova ejecta type II. Franck Condon Factor of SiO molecule had been calculated theoretically for ground state $X^1\Sigma^+$ and excited state $A^1\Pi$ by special integrals by depending on spectroscopic constants for this molecule. Our results are compared with experimental results and appear good convergence. The potential of this molecule is studied in this work by using Hua potential function, the results appear that potential curve of SiO molecule for ground state $X^1\Sigma^+$ and excited state $A^1\Pi$ converge with experimental results, and getting on minimum value of potential in ($r = r_e$), also results of Franck Condon Factors converge with experimental results.

Key word: Hua function, ($X^1\Sigma^+$ - $A^1\Pi$) band system of SiO molecule, Franck Condon Factors.

Nomenclature

T_e: Electronic energy above ground state (cm^{-1})
ω_e: The fundamental vibration frequency (cm^{-1})
$\omega_e x_e$: The anharmonicity constant (cm^{-1})
α_e : The vibration, rotation interaction constant (cm^{-1})
B_e: The rotational constant at equilibrium bond length (cm^{-1})
r_e: Equilibrium bond length of the molecule (Å)
μ_e: The reduced mass of the molecule (gm)
K_e: Force constant (dynes/cm)

1. Introduction

Spectroscopic studies of diatomic molecules are useful in the fields such as astrophysics, astronomy and combustion physics. Most of the molecules we know are in the atmosphere of the cool stars where they exist in sufficient numbers to make their band spectrum to observe. Spectroscopy happens to be the most versatile remote sensing tool of astronomers. Spectroscopic investigations have revealed the existence of SiO in various astrophysical sources such as supernova ejecta [1].

The silicon monoxide (SiO) molecule was detected for the first time in the interstellar medium by Wilson et al. [2] through the J = 3 → 2 radio line emission from the galactic source Sagittarius B2, shortly after the first detection of the interstellar CO molecule. In supernovae like in other environments, the nucleation will take place via the formation of a molecular phase in the ejecta. And Detection of CO, SiO in SN type II. Since then, SiO has been detected in a variety of astrophysical objects such as supernova ejecta and the modeling of observed molecular spectra showed that the SiO molecule, in contrast to CO, is mostly present in regions associated with warm, dense, and shocked gas [1, 3].

In several prior works, Mcgergor, et al. [4], calculated Franck Condon Factor and r-centroids for some bands of the SiO $A^1\Pi$-$X^1\Sigma^+$ band system by classical integral equations and Reddy et al. [5]

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calculated the potential energy curves for the electronic ground states of astrophysically important YO, CrO, BN, ScO, SiO and AlO molecules using the five-parameter Hulburt-Hirschfelder function. The r-Centroids and Franck-Condon factors for the bands of $B^2\sum^+$ -$^2\sum^+$ of YO, $B^5\prod$ - $X^5\prod$ of CrO, $A^3\prod$ - $X^3\prod$ of BN, $B^2\sum^+$ - $X^2\sum^+$ of ScO, $E^1\sum^+$ - $X^1\sum^+$ of SiO and $D^2\sum^+$ - $X^2\sum^+$ and $B^2\sum^+$ - $X^2\sum^+$ of AlO molecules have been determined. The Franck-Condon factors are evaluated by the approximate analytical method of Jarmain and Fraser. The absence of the bands in these systems is explained.

Melendez et al. [6] calculated some of the band systems of several astrophysically important molecules (C2, CO, CS, SiO) and compared with the results obtained by calculations based on realisitic Klein-Duunham and Rydberg-Klein-Rees potential functions. The morse potential is approximated by means of a four- order anharmonic oscillator model. In the second quantized formalism, the anharmonic Hamiltonian is diagonalized by using the Bogoiubov-Tyabliko transformation. The diagonalization process gives a shift in the frequency associated with each normal mode of harmonic vibration of the molecules presented her. The Franck Condon Factors are estimated using this new frequency within the framework of a harmonic oscillator .

Majedifar and Islampour [7] are dealing with the calculation of Franck-Condon factors by using Hua potential on (Li_2, CN, N_2, CO) molecules. The advantages of this function have been observed, and the numerical methods are used to obtain Franck-Condon factors for the band systems.

2. Theoretical Section: Hua Potential function and Franck Condon Factor

Classically, the Franck-Condon principle is the approximation that an electronic transition is most likely to occur without changes in the positions of the nuclei in the molecular entity and its environment. The resulting state is called a Franck–Condon state, and the transition involved, a vertical transition. The quantum mechanical formulation of this principle is that the intensity of a vibronic transition is proportional to the square of the overlap integral between the vibrational wavefunctions of the two states that are involved in the transition [4].

For many problems in molecular spectroscopy, such as study of lectronic absorption and emission of a molecular system, preliminary it is necessary to have Franck-Condon factors for transition between vibrational states of upper and lower electronic states of the molecule. In fact, the Franck-Condon factors represent one of the most useful and comprehensive concepts for the study of radiative and non-radiative processes in molecular systems. Intensity of a vibronic transition is controlled by Franck-Condon factor that is defined as the square of the vibrational overlap (or Franck-Condon) integral [8, 9]:

$$q_{v'v''} = \left| \int \Psi_{v'} . \Psi_{v''} . dr \right|^2 \tag{1}$$

where, $\Psi_{v'}$ and $\Psi_{v''}$ are the vibrational wave functions corresponding to the vibrational levels of the upper and lower electronic states v', v'', respectively. Sincethe molecules vibrate in an anharmonic way, it is necessary to use a potential function, which describes the real movement of the molecules in the best way. We have employed the Hua potential to obtain the vibrational wave functions and have calculated the Franck-Condon factors.

Calculating Franck-Condon factors is related with time-independent Schrödinger equation:

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + U(r) \right] \Psi_v = E_v \Psi_v \tag{2}$$

The most accurate values of Franck-Condon factors are obtained using the true Rydberg-Klein-Rees (RKR) potential curves. To construct the RKR potential curves we need a set of sufficient spectroscopic data. However, all of the spectroscopic data for all molecules in all their electronic states is not available. In the absence of exact expressions for the vibrational wave function ψ_v one may use the eigenfunctions derived from some approximate potential functions.

Consequently, the methods for the calculation of Franck-Condon factors depend on the choice of approximate eigenfunction Ψ_v obtained by the solving Schrödinger equation with approximate potential functions. The various potential functions have been proposed to calculate these factors, such as Morse, which is the most popular empirical potential function because of its simple form. We use the eigen functions of Schrödinger equation for Hua potential function. Hua potential function has the form [8]:

$$U_{Hua}(r) = D_e\left[\frac{1-e^{-b(r-r_e)}}{1-ce^{-b(r-r_e)}}\right]^2 \tag{3}$$

where, $b = a(1 - c)$ where a, r_e and D_e have the same physical significant as in the Morse potential function and c is an additional constant. This potential function indicate an alternative way to evaluate anharmonic overlap integrals starting from the wave functions of Hua potential function.

Consider the wave functions of Hua potential [8]:

$$\Psi_v = N_v\left[\frac{b}{v!}\times\frac{\Gamma[2\rho_\circ(v)+v+1]}{\Gamma[2\rho_\circ(v)+v]}\times\frac{\Gamma[2\rho_c+v+1+2\rho_\circ(v)]}{\Gamma[2\rho_c+v+1]\Gamma[2\rho_\circ(v)]}\times\frac{2\rho_c+2v+1+2\rho_\circ(v)}{2\rho_c+2v+1}\right]^2 x^{\rho_\circ(v)}(1-x)^{\rho_c+\frac{1}{2}} \times F[-v,1+v+2\rho_\circ(v)+2\rho_c,1+2\rho_c,1+2\rho_\circ(v);x] \tag{4}$$

where, $F[\ldots]$ is the Jacobi Polynomial, $\Gamma[\ldots]$ is the Gamma function,

$N_v = 1$ for $c > 0$, and for $c < 0$ N_v equal:

$$N_v = \left[\frac{\sin\sin(2\rho_\circ(v)-2\rho)\pi}{\sin\sin(-2\rho\pi)}\right]^{1/2} \tag{5}$$

$$\rho_\circ(v) = \frac{\left[t^2(Q-1)-\rho_c\bar{v}-\frac{\bar{v}^2}{2}-\frac{1}{8}\right]}{(\rho_c+\bar{v})} \tag{6}$$

$$t = \frac{2D_e}{\hbar\bar{\omega}_e(1-c)} \tag{7}$$

$$x = ce^{-b(r-r_e)} \tag{8}$$

$$\bar{\omega}_e = a\left(\frac{2D_e}{\mu}\right)^{1/2} \tag{9}$$

$$\bar{v} = v + \frac{1}{2} \tag{10}$$

$$\rho_c = \pm\left[\frac{1}{4}+t^2(Q-1)^2\right]^{1/2} \tag{11}$$

$$Q = \frac{1}{c} \tag{12}$$

here, $\bar{\omega}_e$ is the vibrational frequency in cm-1and ± in Eq. (11) refers to the sign of c. We denote various quantities in Eq. (4) for two states v', v'' by a single and a double prime, respectively, and choose x' as the variable in the integral Eq. (1), and in continue omit the prime from for simplicity, then we have :

$$dr = -\frac{dx'}{b'x'} = -\frac{dx''}{b''x''}, x'' = hx'^{\gamma} \tag{13}$$

$$h = \frac{c''e^{b''(r_e'-r_e'')}}{c'^{\gamma}}, \gamma = \frac{b''}{b'} \tag{14}$$

Using this variable, the integral in Eq. (1) can be written as [7]:

$$I(v',v'') = -\frac{N_{v'}.N_{v''}}{b'}\int_0^1 \frac{(hx^{\gamma})^{\rho_\circ(v')}}{x} \times\left[1-(hx^{\gamma})\right]^{\rho'+1/2} x^{\rho_\circ(v'')}(1-x)^{\rho''+1/2} \times F\left[-v',1+v'+2\rho_\circ(v')+2\rho',1+2\rho_\circ(v');hx^{\gamma}\right] \times F\left[-v'',1+v''+2\rho_\circ(v'')+2\rho'',1+2\rho_\circ(v'');x\right]dx \tag{15}$$

for (c> 0).

And:

$$I(v',v'') = -\frac{N_{v'}.N_{v''}}{b'}\int_0^\infty \frac{(hx^{\gamma})^{\rho_\circ(v')}}{x} \times\left[1-(hx^{\gamma})\right]^{-\rho'+1/2} x^{\rho_\circ(v'')}(1-x)^{-\rho''+1/2} \times F\left[-v',1+v'+2\rho_\circ(v')-2\rho',1+2\rho_\circ(v');hx^{\gamma}\right] \times F\left[-v'',1+v''+2\rho_\circ(v'')-2\rho'',1+2\rho_\circ(v'');x\right]dx \tag{16}$$

3. Results and Discussion

Spectroscopic properties of SiO molecule which is found in supernova ejecta are studied such as potential curves for “Hua function” for ground $X^1\Sigma^+$ state and exited state $A^1\Pi$ (Eq. (3)) (Tale 1).

3.1 Results of Hua Potential Function

To calculate Hua potential for SiO molecule Eq. (3) is used for the ground state $X^1\Sigma^+$ and the excited state $A^1\Pi$ by depending on dissociation energy, bond length, spectroscopic constants and c parameter [8], which equal to (-0.055) for ground state $X^1\Sigma^+$ and (0.066) for excited state $A^1\Pi$ and here are the results of Hua potential for SiO molecule for the ground state $X^1\Sigma^+$and the excited state $A^1\Pi$ in Table 2 and Fig. 1.

The calculations appear the maximum value of Hua potential is (40,330 cm^{-1}) in ground state of SiO molecule at (r = 1.2 Å) which is the minimum value of bond length. At bond length (r = 1.5 Å), which is the equilibrium bond length of the molecule for ground state $X^1\Sigma^+$, the potential equal zero , then the potential increase by increasing bond length until reach at the point which happen in it the dissociation because that the diatomic molecules dissociate when the value of (r) increase to determinate limit. That behavior of potential is similar to behavior the excited state of this molecule except the potential don't equal zero at the equilibrium bond length but equal to (38,652 cm^{-1}) which is also minimum value of the potential.

The $X^1\sum^+$ potential-curves from Hua calculations are compared with the experimental RKR curve of Timothey and Hinry [10] as in Table 3 and Fig. 2. Both of the theoretical curves are in quantitative agreement with experiment. The Hua potential curve for the $A^1\Pi$ state is compared with the corresponding experimental RKR curve in Table 4 and Fig. 3. As can be seen, the computed and experimental shape are in general agreement [10]. Therefore behavior results of Hua potential is similar to behavior results of experimental values.

3.2 Results of Franck Condon Factor (FCF)

To calculate Franck-Condon factor, Eqs. (15) and (16) are used, and here are the results in Table 5. The obtained Franck-Condon factors are agreed with those of Mcgergor, Nichols and Jarmain [4], and Melendez et al. [6]. The vibrational sum rule is satisfied for this system, the Δv = 0 sequence is the most intense of all sequences in $X^1\Sigma^+$-$A^1\Pi$ system of SiO.

Due to high cosmic abundance of Silicon and Oxygen, SiO is one of the more important molecules in astrophysics; consequently, many of the spectroscopic constants of SiO are well known, particularly for the ground state. It is seen from the Table 5 that the (0, 1), (0, 2), (1, 0) and (2, 0) bands are strongest and that the FC system of the successive bands in the Δv =0 sequence fall off rapidly in the

Table 1 The spectroscopic constants for SiO molecule measured (cm^{-1}) [10, 11].

Spectroscopic constant	$X^1\Sigma^+$	$A^1\Pi$
T_e	0	42,835.4
ω_e	1,241.5	852.8
$\omega_e x_e$	5.966	6.430
B_e	0.7267	0.630
r_e (Å)	1.5097	1.620
α_e	0.0050	0.0066
$\mu_{e\,(gm)}$	10.1767	10.1767
Ke (dynes/cm)	6.2×10^5	2.7×10^5

Table 2 Hua potential function for ground state $X^1\Sigma^+$ and exited state $A^1\Pi$.

	$X^1\Sigma^+$	$A^1\Pi$
r (A°)	$U_{Hua}(r)$ cm^{-1}	$U_{Hua}(r)$ cm^{-1}
1.2	40.330	112.924
1.3	14.518	64.528
1.5	0	38.652
1.9	7.255	39.523
2	12.099	41.943
2.4	29.844	43.556
2.8	37.542	44.363
3	40.330	44.422
3.2	41.943	44.412

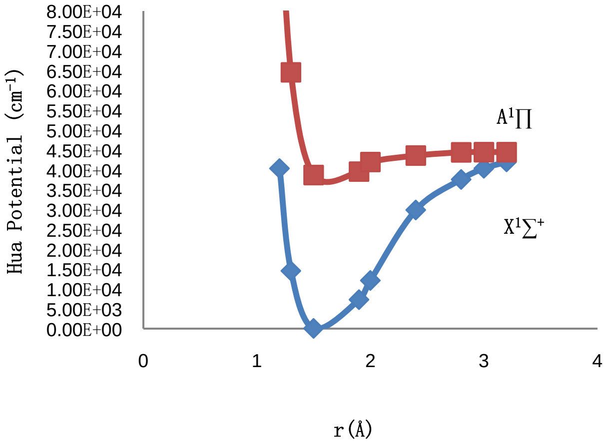

Fig. 1 Calculated Hua potential curves for $X^1\sum^+$ and $A^1\prod$ states.

Table 3 Comparing Hua function and experimental for ground state $X^1\Sigma^+$.

r (Å)	Hua Potential	Experimental Potential [10]
1.2	54.481	50.396
1.3	22.793	16.938
1.5	0	0
1.9	14.764	12.099
2	18.834	14.518
2.4	32.514	30.037
2.8	39.751	37.652
3	41.231	39.341
3.2	41.352	40.221

Table 4 Comparation Hua function and experimental for excited state $A^1\Pi$.

r (Å)	Hua Potential	Experimental potential [7]
1.2	72.950	80.254
1.3	41.485	53.235
1.5	29.976	36.254
1.9	28.800	34.297
2	31.428	36.225
2.4	37.428	40.330
2.8	39.845	41.943
3	42.114	43.521
3.2	43.556	43.888

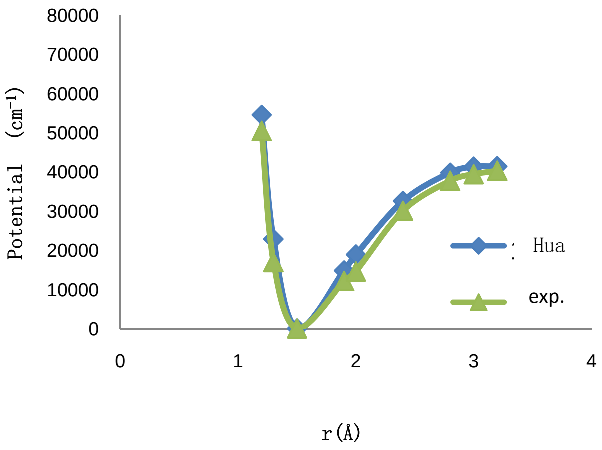

Fig. 2 Theoretical potential calculated by Hua potential compare with experimental curves for ground state $X^1\Sigma^+$.

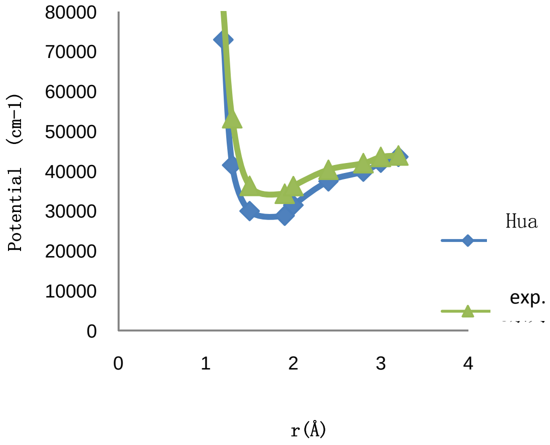

Fig. 3 Theoretical potential calculated by Hua potential compare with experimental curves for excited state $A^1\Pi$.

Table 5 Franck-Condon factors of SiO molecule $X^1\Sigma^+$-$A^1\Pi$ transition.

V`` V`	0	1	2	3	4	5
0	0.1205	0.2684	0.2116	0.1992	0.0988	0.0372
1	0.2215	0.1621	0.0072	0.0851	0.1722	0.1528
2	0.2421	0.0213	0.0767	0.1125	0.0071	0.0692
3	0.1975	0.0182	0.1262	0.0643	0.0782	0.0833
4	0.1105	0.0916	0.0421	0.0072	0.0541	0.0344
5	0.0811	0.1312	0.0603	0.0805	0.0511	0.0722

Table 6 Franck-Condon factors of SiO molecule $X^1\Sigma^+$-$A^1\Pi$ transition [4].

V`` V`	0	1	2	3	4	5
0	0.14	0.27	0.27	0.17	0.08	0.03
1	0.26	0.12	0.001	0.09	0.19	0.16
2	0.25	0.01	0.12	0.08	0.001	0.07
3	0.17	0.07	0.09	0.012	0.11	0.05
4	0.09	0.15	0.001	0.10	-	-
5	0.04	0.16	0.03	0.06	-	-

A-X system of SiO as v' and v" increase. The magnitude of the FC factors from Table 5 indicates that the sum rule is satisfied for v' and v" progressions. The FC factors for the (1, 2), (2, 4) and (4, 2) bands are found to be small in the case of $X^1\Sigma^+$- $A^1\Pi$ system of SiO molecule in comparison with others, indicting its absence. The magnitude of the FC factors for (0, 3) and (3, 0) bands indicates that these bands are of equal intensity. The Frank-Condon factors for the Mcgergor, et al. Table 6 [4] are near than our results with simple errors ratio. In case (1, 2), (2, 4) and (4, 2), FC factors are small and they may not be probably be noticed experimentally. (0, 1) band is the strongest one among all the bands observed in the A-X system of SiO molecule.

4. Conclusions

One of important molecules in interstellar medium, a variety of astrophysical objects and supernova ejecta is Silicon monoxide (SiO) molecule, specially in type II. The potentials of SiO molecule by using Hua function for ground $X^1\Sigma^+$ state and exited state $A^1\Pi$ are in good agreement with experimental results and the important notice that bond length (r) with spectroscopic constants have an effect upon values of the potential. The Franck-Condon factors have good values by using integral method depending on Hue potential function and vibration quantum number for ground $X^1\Sigma^+$ state and exited state $A^1\Pi$. Our results are agreed with Franck-Condon principle and the experimental results, too.

References

[1] A. Sarangi, I. Cherchnef, Dust and Molecule Synthesis in Type IIP Supernova: Reconciling IR & Sub-mm Observations, Klingelbergstrasse 82, Basel, Switzerland, 2012.

[2] R.W. Wilson, A.A. Penzias, K.B. Jefferts, M. Kutner, P. Thaddeus, Ap. J. L 97(1971) 167.

[3] C. Isabelle, L. Simon, Primordial Massive Supernovae as the first molecular factories in the early universe, The Astrophysical Journal L123 (2008) 683.

[4] A.T. Mcgergor, R.W. Nichols, W.R. Jarmain, Franck Condon Factor and r-centroids for some bands of the SiO $A^1\Pi$-$X^1\Sigma^+$ band system, Canadian Journal of Physics 39 (8) (1961) 1215-1216.

[5] R.R. Reddy, Y. Nazeer, K. Rama, P. Abdulazeem, S. Anjaneyulu, RKRV potential energy curves, dissociation energies, r-centroids and Franck-Condon Factors of YO, CrO, BN, ScO, SiO and AlO molecules, Astrophysics and Space Science 262 (1999) 223-240.

[6] F.J. Melendez, L. Sandoval, A. Palma, Franck Condon Factor for diatomic molecules with anharmonic corrections, Journal of Molecular Structure (Theochem) 580 (2002) 91-99.

[7] H. Majedifar, R. Islampour, Calculation of Franck-Condon factors for a number of band systems of diatomic molecules using Hua Potential, Iran. J. Chem. Chem. Eng. 31 (2) (2012)25-35.

[8] W. Hua, Four-parameter exactly solvable potential for diatomic molecules, Phys. Rev. A 42 (1990) 2524.

[9] R. Islampour, R.G. Alden, G.Y.C. Wu, S.H. Lin, Effect of temperature, energy gap and distortion of potential surfaces on photo induced intermolecular electron transfer, J. Phys. Chem. 97 (1993) 6793.

[10] G. Timothy, F. Henery, Potential curves for the valence-excited states of Silicon Monoxide: A theoretical study, The Journal of Chemical Physics 56 (2) (1972) 958.

[11] K.P. Huber, G. Herzberg, NIST Standard Reference Database, Material Measurement Laboratory, Data Gateway, Chemistry Web Book, 2011.