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Franck–Condon Factors and R–Centroids of Some Molecular Transitions of Sio and Baf Molecules

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Abstract

Franck–Condon factors and r-centroids were computed for some molecular transitions of SiO and BaF molecules using molecular constants and Hua potential depending on theoretical calculations, also plotting the potential energy curves of ground state for these molecules and we got to high value of potential in minimum value of bond length. So minimum value of potential that in bond length equal to bond length at equilibrium distance and after that when bond length reach to highest values, that lead to dissociation in these bonds and as result of that the molecule be stable.

Keywords— SiO and BaF Molecules, Hua potential, Franck-Condon factor, r– centroid.

INTRODUCTION .I

Several decades ago, the Spectroscopic investigations of the emission, absorption, and scattering of electromagnetic radiation that is associated with transitions between atomic or molecular energy levels provide extensive information about atomic and molecular structure. Moreover, Diatomic molecules and their positive ions have gained increasing interest over the past years in both experimental and theoretical studies because of their importance in astrophysical processes and in many chemical reactions. Theoretical investigations are an essential tool for researchers in the field of physics and other subjects that are connected to it [1]. Molecular vibrational spectroscopy is a technique that measures the frequency of vibrations in molecules and it is a more complicated field than atomic spectroscopy since its covers the electronic transitions. Vibrational and rotational degrees of freedom are involved in the study of molecules too. In the field of scientific study, theoretical representations focus primarily on the information pertaining to molecules, atoms, and solid-state materials in terms of both data and graphical visualizations. Different techniques with varying advantages have been offered for producing the wave functions of various band systems of diatomic molecules, and the Spectroscopic investigations of these molecules have applications in variety of branches of science, including astronomy, astrophysics, and combustion physics [2][3]. Franck–Condon factors (FCFs) are essential quantities for each molecular band system, Because they are used in the computation of the relative band intensity, which is a crucial source of information for quantitative spectroscopy, high temperature chemistry, and astrochemistry. They are also important for the determination of the molecular structure, the population of the levels in the upper electronic state involved in transition, radiative lifetimes, vibrational temperature, and the kinetics of energy transfer, and plenty of other applications. On the other hand, having knowledge of r-centroids has been proven to be highly valuable in the discussion of the change of the electronic transition moment with the internuclear spacing as well as in other molecular features. The variation of r-centroids with band wavelengths is a useful connection between experimental observations, which are frequently described as a function of wavelength, and theoretical results, which are commonly formulated in terms of internuclear separation[3] [4]. In this study, the linear diatomic molecules SiO and BaF have their FCFs and r-centroids determined for $E^1\sum^+ \rightarrow X\sum^+$ and $A^2\prod_r \rightarrow X^2\sum^+$ electronic transitions using the empirical Hua potential function.The solutions to these equations have been determined and computed by creating specified complicated functions with the using of MATLAB. The P.E curves of these molecules with different (r) values were studied, with the highest and lowest energy determined as a function of (r) at the ground and excited state, and then it has been drawn using the Excel program. Silicon monoxide (SiO) is of considerable interest to astrophysical experts. It has been detected in the massive stellar as well as in a broad range of astrophysical objects, which are closely linked to heated, dense, and shocked gas. SiO has been of importance in the field of entrance physics investigations. Since 1958, when Kivel and Camms conducted research on the $A^1\Pi$-$x^1\Sigma^+$ band system to assist in better understanding the spectrum of shock-heated air polluted by quartz [5]. While BaF is a non-linear molecule in the gaseous form, and it is often observed in nature as uncommon mineral. Because of its massive band gap, it finds wider usage in UV and IR spectroscopy, as well as in a variety of optical technologies [6][7].

THEORETICAL SECTION .II

Since the 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.The potential energy of a molecule arises due to the electronic, vibrational and rotational levels of the atoms. The electronic and vibrational energy levels of a diatomic molecule in a given electronic state are often described by potential energy along Y-axis and inter-nuclear distance along X-axis in a diagram called potential energy curve [4]. In the field of physical chemistry, determining whether or not there is a linkage between the potential energy curves and the internuclear space of diatomic molecules is of the utmost importance. The examination of concepts like photo-dissociation, molecular scattering, electric charge, and chemical kinetics rely on the background knowledge of these functions. Spectroscopy has been shown to play a very important position in a broad range of research fields of study. The associated surface close equilibrium potential energy curves, at which a number of molecules dwell, may be analyzed with spectroscopy to get information that is direct and unambiguous. It is therefore necessary to have a solid grasp of the subject of molecular spectroscopy, and it is primarily reliant on the degree of estimation accuracy of the state of the molecule that is being questioned in relation to both its ground and excited state[8]. The ground state of the electron has no radiation conceivable, while the excited state with energy range has vibrational and rotational modes. The construction of accurate potential energy curve is importance for the understanding the molecular spectrum. P.E minima detemine the possible structures and are thus related to band strength and valence. It is necessary for the potential energy to become closer and closer to reaching a limiting value, which corresponds to the dissociation energy of the molecule. The curvatures of the potential energy surface, the second derivatives of the potential energy with respect to (r) are force constants for the various modes of vibration and detemine the vibrational and rotational energy levels of the molecule. Therefore, it is of great importance to have a suitable representation of the potential energy as a function of the relative positions of the nuclei[3] [9].

SPECTROSCOPIC CONSTANTS .III

In theory, there are varieties of essential and well-known spectroscopic parameters that have a direct impact on the construction of the P.E curve, these spectral constants that includes in our study are detailed in table I below

SPECTROSCOPIC COSTANTS OF SIO AND BAF [5], [7], [10], [11]. .TABLE I

Molecule	**Reduced mass, μ**	**State**	**equilibrium bond length, r_e**	**Electronic energy, T_e**	**vibration frequency, ω_e**	**anharmonicity constant, $\omega_e\chi_e$**	**rotational constant at (r_e), B_e**	**ro-vibration interaction constant, α_e**
SiO	10.1767	$X\sum$ -	1.5097	0	1239.5	5.92	0.724	0.0049
		$E^{1}\sum^{+}$	1.7394	52859	673.5	4.15	0.546	0.0053
BaF	16.698	$X^{2}\sum^{+}$	2.126	0	468.9	1.79	0.215	0.0012
		$A^{2}\prod_{r}$	2.183	11646.9	436.7	1.82	0.211	0.0012

Where:
μ: Reduced mass of the molecule (gm).
r_e: Equilibrium inter nuclear distance (A°).
T_e: Electronic energy above the ground state (cm^{-1}).
ω_e: the Vibrational spacing (cm^{-1}).
$\omega_e\chi_e$: Anharmonic correction to the vibrational spacing (cm^{-1}).
B_e: Rigid rotator rotatioal Spacing at r_e (cm^{-1}).
α_e: NonRigid rotator correction to B_e (cm^{-1}).

METHOD OF COMPUTATION .IV

Franck–Condon Factors (FCFs) .A

In its traditional form, the Franck-Condon principle is an approximation that states it is most likely for a vertical electronic transition to occur without changes in the locations of the nuclei. The state that is produced as a result is known as a Franck–Condon state. According to the quantum mechanical formulation of this principle, the intensity of a vibronic transition)the absorption or emission of a photo(is proportional to the square of the overlap integral between the vibrational wave functions of the two states that involved in the transition. Which are calculated by comparing these WFs. FCFs are an important entity in the diatomic molecular spectra, it is defined as the ratios between the intensities of a continuum band below and above a peak intensity at an internal wave number. in a more elucidating notion, it's an overlap of the WF's of two vibrational states taking part in a transition, These factors give an idea about the intensity of a band appearing in the band systems of a molecule [12]. The hereunder is a formula for the band intensities seen within emission:

$$I_{v'j'v''j''} \propto \frac{N_{v'j'} R^{2}_{e(\bar{r}_{v'v''})} q_{v'v''} v^{3}_{v'j'v''j''} S_{j'j''}}{g_{j'}} \quad (1)$$

Where $N_{v'j'}$is the rotational population in a given vibrational level, $R^2_{e(\bar{r}_{v'v''})}$ the electronic transition moment, $q_{v'v''}$ Is the FCFs, $v^3_{v'j'v''j''}$ the transition frequency, $S_{j'j''}$ the rotational line strength, and$(g_{j'} = 2j' + 1)$ [8]. The FCFs evaluation are described as:

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

Where $\Psi_{v'}(r)$ and $\Psi_{v'}{}'(r)$ are the vibrational wave functions of vibrational levels of the upper and lower electronic states v' and v" levels respectively[13].

r-centroids .B

The r–centroid (sometimes called r-Centrix) is the r-coordinate of the centroid of the region that is indicated by the overlap integral. it is an interpolation point for radiation angles in which each photon has equal probability to be absorbed or emitted. And Its definition is as follows[11]:

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

The empirical hua potential function .C

Over a course of several decades, a variety of theoretical determinations has been put forward for the primary objective of performing a computation of the spectroscopic factors. After the discovery of quantum mechanics, these several methods include the empirical Hua potential function. The time-independent Schrodinger equation (TISE) is involved in the process of calculating FCFs:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + U_{hua}(r)\right]\Psi_v = E_v\Psi_v \tag{4}$$

The method that have the most precise values and results in the determination of FCFs is by Utilizing Rydberg-Klein-Rees (RKR) potential curves. It is require a complete and adequate collection of spectroscopic informations to create these curves. Twenty-one empirical potential functions for the ground states of fourteen first- and second-row diatomic molecules were analysed, compared, and fitted to experimental RKR data. The functions with a greater number of parameters are generated more accurate fits. The four-parameter Hua potential function has been analysed and founded to be the most accurate potential function. Moreover, it has the added benefit of creating TISE. For this reason, we choose this function for the purpose of our task. However, according to the fact that the spectroscopic evidences for all molecules in all of their electronic states is not always readily accessible, It is possible to insert the Eigen functions that obtained from the approximate potential functions in the case of the lack of accurate equations for Ψ_v. As a consequence of this, the procedures for calculating FCFs depend on the approximate Eigen function Ψ_v that is selected during the solution of TISE using approximate potential functions. In our investigation, we make use of the Eigen functions of TISE for the Hua potential function in order to compute these factors and we provide a softer strategy to calculating anharmonic overlap integrals, beginning with the wave functions of the Hua potential function. The form of Hua's potential function is as follows:

$$U_{hua}(r) = D_{\mathrm{e}}\left[\frac{1-e^{-b(r-r_e)}}{1-c_r e^{-b(r-r_e)}}\right]^2 \tag{5}$$

$$b = a(1-c_r) \tag{6}$$

Here (a) is a factor that is derived from the data acquired by molecular spectroscopy, r_e is the equilibrium bond length, D_e is the dissociation energy and (c_r) is an extra constant that is utilized to reduce the relative deviations. The anharmonic overlap integrals in the equations (2) and (3) are obtained using this expression starting from the wave functions of Hua potential function [14]:

$$\Psi_{\mathrm{v}} = N_{\mathrm{v}}\left[\frac{b}{v!}\times\frac{\Gamma[2\rho_{\circ}(v)+v+1]}{\Gamma[2\rho_{\circ}(v)+v]}\times\frac{\Gamma[2\rho_{C}+v+1+2\rho_{\circ}(v)]}{\Gamma[2\rho_{C}+v+1]\Gamma[2\rho_{\circ}(v)]}\times\frac{2\rho_{C}+2v+1+2\rho_{\circ}(v)}{2\rho_{C}+2v+1}\right]^{2} x^{\rho_{\circ}(v)}(1-x)^{\rho_{C}+\frac{1}{2}}F[{}^{-}v,1+v+2\rho_{\circ}(v)+2\rho_{C},1+2\rho_{\circ}(v);x] \tag{7}$$

Where the closed arches for F […] is the Jacobi Polynomial and Γ […] is the Gamma function. We indicate different values in Equation (7) for two states v', v" by a single prime and a double prime, respectively, And $N_v = 1$ for c > 0, and for c < 0 N_v equal to:

$$N_{\mathrm{v}} = \left[\frac{sinsin\ sinsin\ (2\rho_{\circ}(v)-2\rho)\pi}{sinsin\ sinsin\ ({}^{-}2\rho\pi)}\right]^{\frac{1}{2}} \tag{8}$$

$$\rho_{\circ}(v) = \frac{\left[t^{2}(Q-1)-\rho_{C}(v^{-})-\frac{(v^{-})^{2}}{2}-\frac{1}{8}\right]}{(\rho_{C}+v^{-})} \tag{9}$$

$$t = \frac{2D_{e}}{\hbar\omega_{e}(1-c_{r})} \tag{10}$$

$$x = c_{r}e^{-b(r-r_{e})} \tag{11}$$

$$\omega_{e} = a\left(\frac{2D_{e}}{\mu}\right)^{\frac{1}{2}} \tag{12}$$

$$v^{-} = v+\frac{1}{2} \tag{13}$$

$$\rho_{c} = \pm\left[\frac{1}{4}+t^{2}(Q-1)^{2}\right]^{\frac{1}{2}} \tag{14}$$

Here the ± in Eq. (14) refers to the sign of (c_r).

$$Q = \frac{1}{c_{r}} \tag{15}$$

If we pick x' as a variable in the Integral Equation (2) and if we continue by omitting the prime from x' for the sake of simplicity, then we obtain:

$$dr = -\frac{dx'}{b'x'} = \frac{dx''}{b''x''} \tag{16}$$

$$x'' = ox'^{\gamma} \tag{17}$$

$$o = \frac{c''e^{b''(r'_{e}-r''_{e})}}{c'^{\gamma}} \tag{18}$$

$$\gamma = \frac{b''}{b'} \tag{19}$$

The integral defined by equation (2) may be reformulated using these above factors for the purpose of Clarifying the Intensity (FCFs) of the given transition (v"-v') as follows:

$$I_{(v',v'')} = \frac{N_{v'}N_{v''}}{b'}\int_{0}^{1}\frac{(ox^{\gamma})^{\rho\square(v')}}{x}[1-(ox^{\gamma})]^{\rho'+\frac{1}{2}}x^{\rho\square(v'')}(1-x)^{\rho''+\frac{1}{2}}F[{}^{-}v',1+v'+2\rho_{\circ}(v')+2\rho',1+2\rho_{\circ}(v');ox^{\gamma}]\times$$

$$F[{}^{-}v'', 1 + v'' + 2\rho_{\circ}(v'') + 2\rho'', 1 + 2\rho_{\circ}(v''); x]dx \;\ldots\; (\text{For } c_r>0) \tag{20}$$

$$I_{(v',v'')} = \frac{N_{v'}N_{v''}}{b'} \int_0^{\infty} \frac{(ox^{\gamma})^{\rho\square(v')}}{x} [1 - (ox^{\gamma})]^{-\rho' + \frac{1}{2}} x^{\rho\square(v')} (1 - x)^{\rho'' + \frac{1}{2}} F[{}^{-}v', 1 + v' + 2\rho_{\circ}(v') - 2\rho', 1 + 2\rho_{\circ}(v'); ox^{\gamma}]$$
$$F[{}^{-}v'', 1 + v'' + 2\rho_{\circ}(v'') - 2\rho'', 1 + 2\rho_{\circ}(v''); x]dx \;\ldots\; (\text{For } c_r<0) \tag{21}$$

The calculation of Equations (15) and (16) is a challenging endeavour. Despite the fact that the direct integration is easy to do and may be accomplished in a straightforward manner [13].

CALCULATIONS AND RESULTS .V

In this paper, we are going to deal with the actual calculations and evaluated FCFs for $E^1\sum^+ \rightarrow X\sum^+$ and $A^2\prod_r \rightarrow X^2\sum^+$ electronic transitions for Sio and BaF molecules respectively by utilizing the functions and equations that have already been discussed. The solutions of equation (5) and other equations have been determined and computed by creating specified complicated functions with the using of MATLAB. As well as basing our conclusions of this program on the spectral constants of our molecules in table I as an input dataset which correspond to the states involved in the transitions.

Franck–Condon Factors results .A

Using the definition of FCFs in equations (2), Moreover the WFs of Hua potential function in equation (5-21), the FCFs(or the Intensity of the transitions) for the first five consecutive vibration states (v) of these molecules Beginning from the GS (v'' = 0) and moving up to the excited state (v' = 5). As shown in the table II for Sio molecule and table III for BaF molecule.

Franck–Condon Factors for $E^1\sum^+ \rightarrow X\sum^+$ transition of SiO molecule. .TABLE II

(v'-v'') electronic transition	***0***	***1***	***2***	***3***	***4***	***5***
0	0.001	0.004	0.017	0.043	0.089	0.103
1	0.002	0.021	0.063	0.109	-	-
2	0.008	0.053	0.109	-	-	-
3	0.091	-	0.101	-	-	-
4	0.051	0.109	-	-	-	-
5	-	-	-	-	-	-

Table II illustrates that the FCFs values of the observed SiO molecule transitions have on the whole rather low, because the transitions between these vibration levels are quite slight, particularly in the bands (0,0), (0,1), (0,2), (1,0), (1,1), and (2,0). In contrast, the bands (0,5), (1,3), (2,2), (3,2) and (4,1) seem to have a greater intensity in the spectrum.

Franck–Condon Factors for $A^2\prod_R \rightarrow X^2\sum^+$ transitions BaF molecule. .TABLE III

(v'-v'') electronic transition	***0***	***1***	***2***	***3***	***4***	***5***
0	0.693	0.263	0.039	-	-	-
1	-	0.278	0.369	0.099	0.014	0.758
2	0.052	0.308	0.077	-	-	-
3	-	0.114	0.291	-	0.497	-
4	-	0.056	-	-	-	-
5	-	-	-	-	-	-

There are faint bands such in (0,2), (1,4) and(2,0) bands in the BaF molecule transitions shown in table III. However, there is a clear differentiation between these bands and the others, Because of the higher intensities of the transitions that take place in some bands like (0,0), (1,2), (1,5), (2,1) and (3,4).the band intensities here have a relative bigger values than those of the SiO molecule. It is important to point out that the absence of data in the cells of tables II and III indicates that there have been no observed transitions between the two limiting vibrational levels.

r-centroids results .B

The results of the computation of the r-centroid values for $E^1\sum^+ \rightarrow X\sum^+$ transition of a SiO molecule and $A^2\prod_r \rightarrow X^2\sum^+$ transition of a BaF molecule are presented in tables IV and V, respectively.

R-CENTROIDS FOR THE $E^1\sum^+ \rightarrow X\sum^+$ TRANSITION OF SIO MOLECULE. .TABLE IV

(v'-v'') electronic transition	***0***	***1***	***2***	***3***	***4***	***5***
0	1.606	1.626	1.646	1.666	1.685	1.705
1	1.595	1.615	1.635	1.655	1.675	1.694
2	1.584	1.604	1.624	1.644	1.664	1.683
3	1.573	1.594	1.614	1.633	1.653	1.673
4	1.563	1.583	1.603	1.623	1.643	1.662
5	1.552	1.573	1.593	1.613	1.632	1.652

R-CENTROIDS FOR THE $A^2\prod_R \rightarrow X^2\sum^+$ TRANSITION OF BAF MOLECULE. .TABLE V

(v'-v'') electronic transition	***0***	***1***	***2***	***3***	***4***	***5***
0	2.156	2.241	2.337	2.451	2.583	2.748
1	2.086	2.162	2.247	2.343	2.455	2.589
2	2.024	2.092	2.167	2.252	2.349	2.461
3	1.967	2.029	2.097	2.173	2.258	2.355
4	1.916	1.973	2.035	2.103	2.179	2.264
5	1.869	1.921	1.978	2.041	2.109	2.184

When we take a gander at tables IV and V, we can see obviously that the r-centroid values of the vertical electronic transitions from the same ground vibration state (v'') to either of the excited states (v') that are attained by the electron arriving from the ground state gradually increase with the increase in the value of (v'') ($\underline{r}_{0,0} < \underline{r}_{0,1} < \underline{r}_{0,2} \dots \underline{r}_{v'v''}$). It should be also observed that the r-centroid values for the transitions take place in the BaF molecule are relatively larger than those in the SiO molecule. This is attributed to that the intensity of the BaF transitions is higher, as was discussed before.

Hua potential function results .C

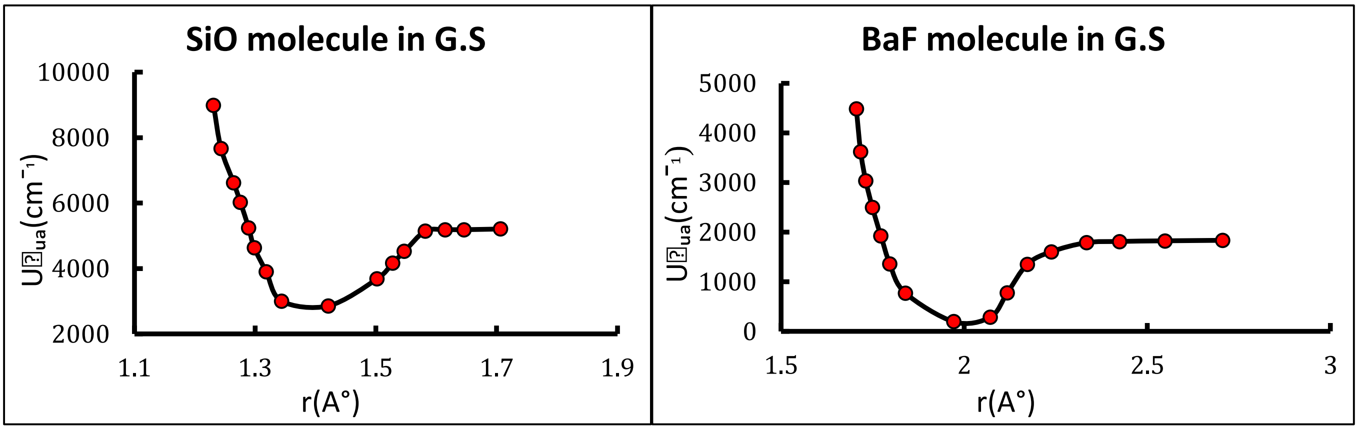
The Hua potential function values for different r values of SiO and BaF at the G.S are listed in Table VI. Equ. (5) And Hua's wave function equations were included in the measurement of the result.

SIO AND BAF IN G.S. .TABLE VI

SiO		**BaF**	
bond length, r(A°)	***Hua potential function, $U_{(Hua)}(cm^{-1})$***	***bond length, r(A°)***	***Hua potential function, $U_{(Hua)\,)}(cm^{-1})$***
1.2311	8986.7	1.7056	4482.2
1.2435	7670.2	1.7173	3624.7

SiO		BaF	
1.2644	6620.6	1.7314	3035.4
1.2755	6031.2	1.7496	2497.8
1.2892	5246.3	1.7724	1927.6
1.2985	4641.7	1.7972	1353.2
1.3183	3906.5	1.8394	775.4
1.3438	3009.8	1.9723	192.8
1.4212	2863.5	2.0714	287.8
1.5017	3686.2	2.1178	775.7
1.5276	4165.6	2.1726	1353.6
1.5471	4528.4	2.2384	1606.8
1.5816	5147.7	2.3341	1787.9
1.6145	5188.8	2.4242	1812.8
1.6462	5191.3	2.5481	1825.3
1.7065	5211.2	2.7056	1835.2

Following table IV is a graph in Fig. 1 depicting the P.E curve for both Sio and BaF molecule in G.S, with the X-axis representing r values and the Y-axis representing $U_{(Hua)}$ values.



Potential energy curve fo SiO and BaF in the ground state .Fig. 1

The energy curves of the molecules that were used in our research can be seen in the figure (1) up there. These molecules had certain values of (r) that assigned to them, and their potential energy curves were computed with the help of the Hua potential function in equation (5) and thier eigenfunctions in equation (7). In this regard, it has been shown that the potential energy curves of these molecules resemble that of the diatomic molecule that ocsillating in anharmonic manner more closely, both in terms of their structure and their attributes. where it has the greatest amount of energy at (SiO:r=1.2311A$^{\circ}$, U_{Hua}=8986.7 cm^{-1}, BaF: r=1.7056A$^{\circ}$, U_{Hua}=4482.2cm^{-1}) A later energy regression happens as (r) grows until we reach the minimum energy of the curve (SiO:r=1.4212A$^{\circ}$, U_{Hua}=2863.5cm^{-1}, BaF: r=1.9723A$^{\circ}$, U_{Hua}=192.8cm^{-1}). In this case, the BaF curve has a lower minimum energy than the SiO curve. These molecules will reach the point where their bonds are dissociated at (SiO:r=1.7065A$^{\circ}$, U_{Hua}=5211.2cm^{-1}, BaF:r=2.7056A$^{\circ}$, U_{Hua}=1835.2cm^{-1}) and when (r) is increased further, it will emit a thermal energy as a result of their dissociation.

CONSULUSION .VI

Silicon monoxide (SiO) and barium fluoride (BaF) are two chemical compounds that are considered to be among the most significant in the interstellar and astrophysical medium. This work is primarily focused on finding a correct solution to the Schrodinger equation for the Hua potential function and making use of eigenfunctions of this potential. The spectral and molecular information of these molecules are calculated previously by many researches using some empirical potential functions like Morse potential function, Deng Fan potential function, Varshni potential function, and a few other functions . These functions were proposed approximately 100 years ago or a little less. In this particular research, the potential energy curve was computed and drawn, as well as the FCFs and r-centroids being computed for the $E^{1}\sum^{+}\rightarrow X\sum^{+}$ transition of SiO molecules and $A^{2}\prod_{r}\rightarrow X^{2}\sum^{+}$ transition of BaF molecules. When using the Hua potential function and its associated eigenfunctions, it is anticipated that the obtained findings will be more accurate and will come closer to the Rydberg-Klein-Rees (RKR) potential curve. Because we use an integral technique that is dependent on the Hua potential function and the vibration quantum number for our constrained transitions, the FCFs that we have here have excellent values, and this method is in agreement with the Franck-Condon principle. The fact that the bond length (r) and spectroscopic constants have an influence upon of the potential values is the most significant point to take away from this work.

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