Calculation of New Five ParametersPotentialand Dissociation Energy for (X$^1\Sigma^+$- A$^1\Pi$) Band System of Diatomic Molecule

Adil N. Ayyash[1], Zeyad A. Salih[2]

[1]Physics Department, College of Science, University of Anbar, Iraq

[2]Physics Department, College of Science, AL-Mustansyria University, Iraq

Abstract: *The present work concerns by study of potential curve and dissociation energy for Diatomic moleculeSiO which is founded in supernova ejecta type II. Dissociation energy had been calculated theoretically for ground state X$^1\Sigma^+$ and excited state A$^1\Pi$ of SiO molecule by Gaydenrelation and by depending on spectroscopic constants for this molecule. Our results are compared with experimental results and appear good convergence, also showed an important effect for bond length (r) for occur the dissociation. The potential of this molecule is studied in this work by using new five parameters 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.*

Keyword: New five parameters function , dissociation energy.

1. Introduction

The silicon monoxide SiO molecule is of considerable astrophysical interest. It is detected in the interstellar medium and in a variety of astrophysical objects which are mostly associated with warm, dense, andshocked gas. Because of the interaction between high velocities jets emerging from a young star and the surrounding molecular environment a large fraction of the SiO relative to hydrogen molecule are found in the high velocity gas components of molecular outflows. Spectroscopic studies of diatomic molecules are useful in the fields such as astrophysics, astronomy and combustion physics[1].

Because of SiO occurs in a wide range of gaseous environments at temperatures up to about 10000 K, it is a molecule of considerable interest in both astrophysics and entry physics. The astrophysical interest in SiO results from its occurrence in stellar atmospheres and in the interstellar medium near M-type stars. Specifically, calculations by Dolan1 show SiO to be an important constituent in the atmospheres of normal (oxygen rich) dwarf, giant, and supergiant stars, as well as in giants and supergiants having equal abundances of carbon and oxygen. The abundance of SiO is, apparently, a fairly sensitive function of the effective temperature and surface gravity of stars. Measurement of the strength of the vibration-rotation bands in the X$^1\sum^+$ ground-state manifold of SiO may, therefore, useful for spectral classification of late-type stars. [2]

SiO has been of interest in entry physics studies since 1958 when Kivel and Camms studied the A$^1\prod$-x$^1\sum^+$ band system to aid in understanding the spectrum of shock-heated air contaminated by quartz. The SiO molecule is of current interest at NASA because of the proposal to use the so-called "volume reflecting heat shield, " which consists of SiO2, for Jupiter entry. Such heat shields are designed to reflect much of the radiation that impinges on the surface of the probe and thus are efficient for entry conditions where intense shock layer emission is present[3].

2. Theoretical Section

Dissociation Energy

The empirical equation for the diatomic molecule, which in many cases is quite accurate, was proposed by Morse and D_e is again the dissociation energy from the potential minimum. Note that for r-r$_e$ = ∞,V$_m$=D$_e$. This dissociation energy differs from the measured dissociation energy of a molecule; however the quantity De is the energy that would be necessary to dissociate the molecule if it could be at the minimum of the potential energy curve. Because of the zero point energy, this is impossible, and therefore [4]:

$$D_e = D_0 + 1/2 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (1)$$

D_0 is the measured dissociation energy and 1/2 v$_0$ is the zero point energy measured in cm-1 unit and the values of D$_e$ and D$_0$ have the same units. The relation for dissociation energy is called Gaydon relation [5]:

$$D_e = \frac{\omega_e{}^2}{(5\omega_e\chi_e - 2B)} \dots\dots\dots\dots\dots\dots\dots (2)$$

New Five Parameters Function

A new function, which had been expressed for potential curves as a molecule is formed and electrons of each atom are shared by the molecule as a whole. The electron energy as a function of inter nuclear distance is distorted in such a way so as to provide a potential well for finite vibrational levels. Clearly to calculate this potential function quantum mechanically is a formidable task. There are then mainly two ways of determining the potential function of a stable diatomic molecule. One of these is the so-called Rydberg-Klein-Rees (RKR) procedure which is based on the WKB approximation and essentially amounts to the construction of potential function from the known energy spectrum. Since energy spectrum cannot be written in a closed mathematical form and is represented by the Dunham expansion as a power series, a large amount of spectroscopic data is

required. This potential is thus suitable for those molecular states for which sufficient data are available.

Another approach is to use the empirical potential function where all stable potential curves can be fitted to certain algebraic expressions, the best example is the Morse function and the five-parameter potential function is [6]:

$$V(\chi_o) = e^{-t_o\chi_o}\frac{K_o}{\chi_o} - a - b_o\chi_o - c_o\chi_o^2 \quad \ldots\ldots\ldots\ldots\ldots..(3)$$

Where χ_o =r/re , r being the internuclear distance and re the equilibrium bond length , K_o, a, b_o, c_o and t_o are the parameters to determined from molecular spectroscopic data .

The potential energy curve calculations on several stable diatomic molecular states can be solved by equations (3). These states front the work are chosen for ground state since it provides extensive RKR data covering a wide range of r [7].

New five parameters function" is a function for diatomic molecules had been used to calculate the potential curves of molecules,a number of three to five parameter functions are used in potential curve calculations of stable diatomic molecules, and New five parameters functionwritten as [6]:

$$U_r = D_e[(1 - e^{-x_o}) + c_o x_o^3 e^{-2x_o}(1 + b_o x_o)]\ldots\ldots........(4)$$
$$x_o = \frac{\omega_e(r - r_e)}{2(D_e B_e)^{\frac{1}{2}}r_e}\ldots\ldots\ldots\ldots\ldots\ldots..(5)$$
$$c_o = 1 + a_1\left(\frac{D_e}{a_0}\right)^{\frac{1}{2}}\ldots\ldots\ldots\ldots\ldots\ldots.\ldots(6)$$
$$b_o = 2 - \left[\frac{\frac{7}{12} - \left(\frac{D_e a_2}{a_0}\right)}{c}\right]\ldots\ldots\ldots\ldots\ldots(7)$$
$$a_{0=}\frac{\omega_e^2}{4B_e} \quad \text{and} \quad a_1 = -1 - \left(\frac{\alpha_e \omega_e}{6B_e^2}\right)\ldots..(8)$$

3. Results and Discussion

Spectroscopic properties of SiO molecule which is found in supernova ejecta are studied such as potential curves for new five parameters function for ground $X^1\Sigma^+$ state and excited state $A^1\Pi$ (eq. 4) compared with experimental curvesfor ground $X^1\Sigma^+$ state and exited state $A^1\Pi$, then dissociation energy is obtained using (eq. 2) compared with experimental energy.

Table 1: The spectroscopic constants for SiO moleculemeasured (cm^{-1})[8,9].

Spectroscopic	$X^1\Sigma^+$	$A^1\Pi$
T_e	0	42835.4
ω_e	1241.5	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
K_e (dynes/cm)	6.2×10^5	2.7×10^5

Where:
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 (A$^\circ$)
μ_e: the reduced mass of the molecule (gm)
K_e: force constant (dynes/cm)

4. Result of Dissociation Energy

In order to obtain dissociation energy, the relation is used (eq. (2)), and here are the results in table (2). The D_e values are found to be (54316.66cm-1)and (23543.79cm-1) for $X^1\Sigma^+$ and $A^1\Pi$ respectively, that dissociation due to approaching the bond length (r) from infinity values, where this is one of three conditions of potential curve. These results are in good agreement with the values (66947.8 cm-1) and (22165.1 cm-1) for $X^1\Sigma^+$ and $A^1\Pi$ respectively that have been calculated by Timothey and Hinry [8], and the values (65334.6 cm-1) for $X^1\Sigma^+$ of Gaydon [10] and (28231 cm-1) for $A^1\Pi$ of Verma and Mulliken [11].

Table 2: Dissociation energy obtained (cm^{-1})

State	D_e (cm^{-1})	Experimental
$X^1\Sigma^+$	54316.66	66947.8 [8] 65334.6 [10]
$A^1\Pi$	23543.79	22165.1 [8] 28231 [11]

5. Results Of New Five Parameters Potential Curve:

To calculate new five parameters potential for SiO molecule (eq. (4)) is used for the ground state $X^1\Sigma^+$ and the excited state $A^1\Pi$, and here are the results in table (3) and figure (1). The calculations show that the maximum value of new five parameters potential is at (r = 1.2 A°) that means the minimum value of bond length gives us maximum potential in ground state of SiO molecule. At bond length (r = 1.5 A°), which is the equilibrium bond length of the molecule for ground state $X^1\Sigma^+$, the potential equal zero , then the potential increases by increasing bond length until reach at the point which happen in it the dissociation because of that the diatomic molecules dissociate when the value of (r) increases to determinate limit. That behavior of potential is similar to the behavior the excited state $A^1\Pi$ of this molecule except the potential don't equal zero at the equilibrium bond length but equal to (35521 cm-1) which is also minimum value of the potential.

The $X^1\Sigma^+$ potential-curve from the New five parameters calculations are compared with the experimental RKR curve of Timothey and Hinry [8] as in table (4) and Fig. (2).The theoretical curve is in quantitative agreement with experiment. The New five parameters potential curve for the $A^1\Pi$ state are compared with the corresponding experimental RKR curve in table (5) and Fig. (3). As can be seen, the computed and experimental shape are in general agreement .Therefore behavior results of New five parameters potential is in good agreement with experimental values.

Paper ID: SUB151396   1212

Table 3: New five parameters potential function for ground state X1Σ+ and exited state A1Π

r (A°)	$X^1\Sigma^+$ $U_{Varsh}(x)$ cm^{-1}	$A^1\Pi$ $U_{Varsh}(x)$ cm^{-1}
1.2	56963	84800
1.3	33658	44755
1.5	0	35521
1.9	24153	33742
2	26514	34996
2.4	34513	38581
2.8	39232	41886
3	41231	42544
3.2	42521	42222

Fig(1):Calculated new five potential curves for $X^1\Sigma^+$ and $A^1\Pi$ states.

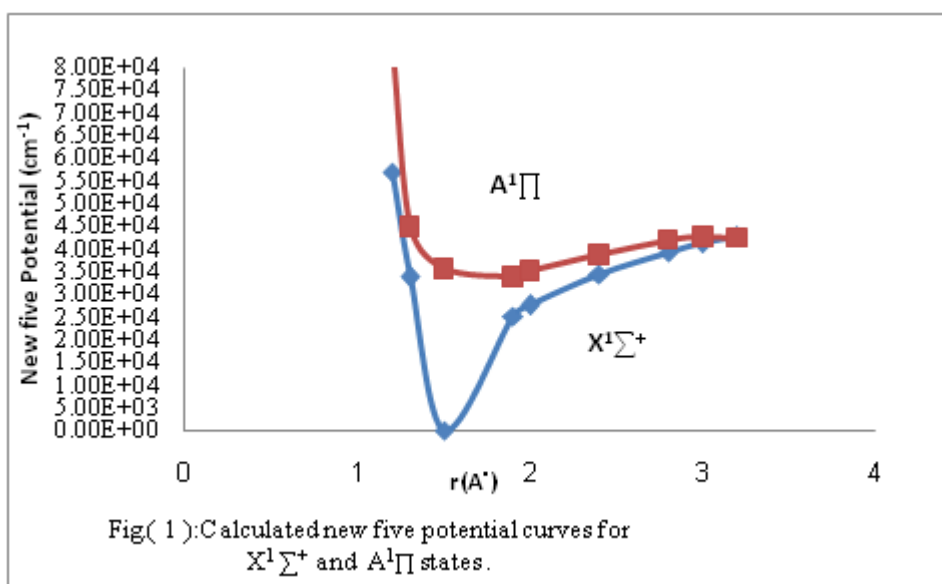**Table 4:** Comparing New five parameters potential and experimental for ground state X1Σ+

r (A°)	New five parameters potential	Experimental potential [8]
1.2	56963	50396
1.3	33658	16938.6
1.5	0	0
1.9	27035	12099
2	29544	14518.2
2.4	34513	30037
2.8	39232	37652.4
3	41231	39341
3.2	42521	40221.1

Fig. (2):Theoretical potential calculated by New five parameter potential compared with experimental curve for ground state $X^1\Sigma^+$

Fig. (3):Theoretical potential calculated by New five parameter potential compared with experimental curve for excited state $A^1\Pi$
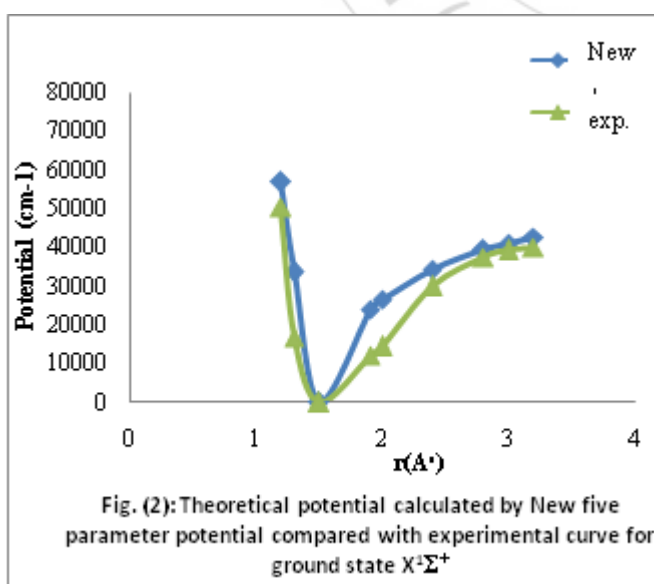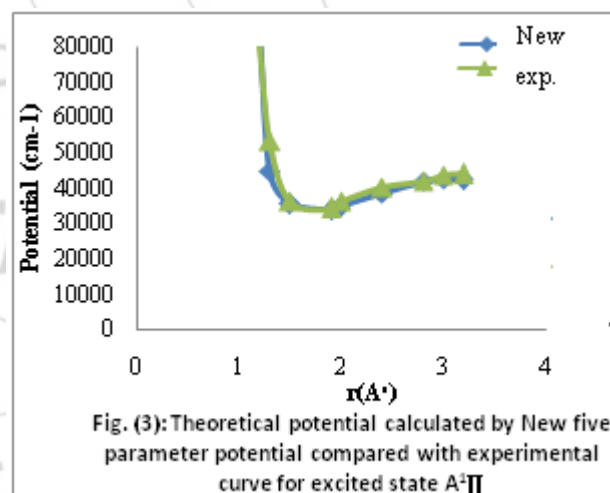
Table 5: Comparation New five parameters and experimental for excited state $A^1\Pi$

r (A°)	New five parameters potential	Experimental potential [8]
1.2	84800	80254
1.3	44755	53235.5
1.5	35521	36254.4
1.9	33742	34297.1
2	34996	36225.1
2.4	38581	40330
2.8	41886	41943.1
3	42544	43521
3.2	42222	43888

6. 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.

Dissociation energies of SiO molecule have calculated for ground $X^1\Sigma^+$ state and exited state $A^1\Pi$ and showed that bond length (r) has an effect upon the values of the dissociation energies, where the dissociation happen when (r) approach from infinity values. that meaning near from experimental values. The potentials of SiO molecule by using New five Parameters 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.

References

[1] Wilson, R. W., Penzias, A. A., Jefferts, K. B., Kutner, M., and Thaddeus, P., ApJ, 167, L97(1971).

[2] Cudaback D. D., Gaustad J. E., and Knacke R. F., Astrophys.Lett.166, L49 (1971).

[3] Howe J. T., Green M. J., and Weston K. C., AIAA J. 11, 989 (1973).

[4] Schadee A., J. Quan. Spectrosc.Radiat.Transf., (1978).

[5] Teik-Cheng L.,"Obtaining The Varshni Potential Function Using The 2-Body Kaxiras–Pandey Parameters", J. Serb. Chem. Soc.V. 74, No.12, P.1423–1428, (2009).

[6] Rafi M., Al-Tuwirqi R., Farhan H. and Khan I. A., "A new four-parameter empirical potential energy function for diatomic molecules" J. Pramana of physics V. 68, No. 6 p. 959–965, (2007).

[7] Atkins P. W., Physical Chemistry, 6th edition, Oxford university press, Oxford, (2001).

[8] Timothy G. and Henery F., potential curves for the valence – excited states of Silicon Monoxide: A theoretical study, The journal of chemical physics, V.56 No. 2 (1972).

[9] Huber K.P. and Herzberg G.,NIST Standard Reference Database , Material measurement laboratory, Data Gateway, Chemistry WebBook. Data collected 1977 , published (2011).

[10] Gaydon A. G., Dissociation energies and spectra of diatomic molecules, Chapman and Hall, London, (1968).

[11] Verma R. D. and Mulliken R. D., Can. J. Phys. 39, 908, (1961).

Author Profile

Dr. Adil N. Ayyash, Date ofBirth 30/8/1978 in Baghdad, Specialization(Molecular Physics), Work Adress: (Physics Department, College of Science, University of Anbar). Scientific Certification: Ph.D in Molecular physics (2014) College of Science, AL-MustansriyahUniversity, Baghdad, Iraq.

Dr. Zeyad A. Saleh, Date ofBirth 30/12/1958 in Baghdad, Specialization(Molecular Physics), Work Adress: (Physics Department, College of Science,AL-Mustansriyah University). Scientific Certification: Ph.D in Molecular physics (2005) College of Science, University of Baghdad, Baghdad, Iraq.