

CALCULATION OF VARSHNI POTENTIAL, HUA POTENTIAL AND DISSOCIATION ENERGY FOR ($X^1\Sigma^+$ - $A^1\Pi$) BAND SYSTEM OF SiO MOLECULE IN SUPERNOVA EJECTA

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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. Dissociation energy had been calculated theoretically for ground state $X^1\Sigma^+$ and excited state $A^1\Pi$ of SiO molecule by Herzberg relation 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 more of potential function as (Varshni potential function) and (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 ($r=r_e$), but the dissociation happen when (r) approach from (∞).

KEYWORDS: Varshni and Hua Function, Dissociation Energy, ($X^1\Sigma^+$ - $A^1\Pi$) Band System of SiO Molecule

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 $J = 3 \rightarrow 2$ 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].

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 $r-r_e = \infty$, $V_m = -D_e$. This dissociation energy differs from the measured dissociation energy of a molecule; however the quantity D_e 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]:

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

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.

Another relation for dissociation energy is called Gaydon relation [5]:

$$D_e = \frac{\omega_e^2}{(5\omega_e x_e - 2B)} \quad (2)$$

Another relation for dissociation energy is called Herzberg relation [4]:

$$D_e = \frac{\omega_e^2}{4\omega_e x_e} \quad (3)$$

Varshni Function and Hua Potential Function

One of functions of potential is Varshni function which is different from Morse function by term (r/r_e) so the function had written as [5]:

$$U(x) = D_e \left(1 - \frac{r}{r_e} e^{-\beta x}\right)^2 \quad (4)$$

$$x = r - r_e$$

$$\beta = \left[\frac{8\pi^2 \mu (\omega_e x_e) c}{h} \right]^{1/2} \quad (5)$$

On the other hand, another function of potential called Hua potential function has the form [6]:

$$U_{\text{Hua}}(r) = D_e \left[\frac{1 - e^{-b(r-r_e)}}{1 - c e^{-b(r-r_e)}} \right]^2 \quad (6)$$

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 [6]. This potential function indicate an alternative way to evaluate anharmonic overlap integrals starting from the wave functions of Hua potential function.

RESULTS AND DISCUSSIONS

Spectroscopic properties of SiO molecule which is found in supernova ejecta are studied such as potential curves for two functions began with potential Varshni function for ground $X^1\Sigma^+$ state and excited state $A^1\Pi$ (eq. 4) compared with other function "Hua function" for ground $X^1\Sigma^+$ state and excited state $A^1\Pi$ (eq. 6) then dissociation energy is obtained using (eq. 3) compared with experimental energy.

Table 1: The Spectroscopic Constants for SiO Molecule Measured (cm^{-1}) [7,8]

Spectroscopic Constant	$X^1\Sigma^+$	$A^1\Pi$
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
μ_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 (Å)
- μ_e : the reduced mass of the molecule (gm)
- K_e : force constant (dynes/cm)

RESULTS OF DISSOCIATION ENERGY

In order to obtain dissociation energy, the relations are used (eq. 3), and here are the results in table (2). The D_e values are found to be (64587.7 cm^{-1}) and (28276.3 cm^{-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 of Timothy and Hinry [7], and the values (65334.6 cm^{-1}) for $X^1\Sigma^+$ of Gaydon [9] and (28231 cm^{-1}) for $A^1\Pi$ of Verma and Mulliken [10].

Table 2: Dissociation Energy Obtained (cm^{-1})

State	D_e (cm^{-1})	Experimental
$X^1\Sigma^+$	64587.7 cm^{-1}	66947.8 [7] 65334.6 [9]
$A^1\Pi$	28276.3 cm^{-1}	22165.1 [7] 28276.3 cm^{-1}

RESULTS OF POTENTIAL CURVE

Results of Varshni Potential Function

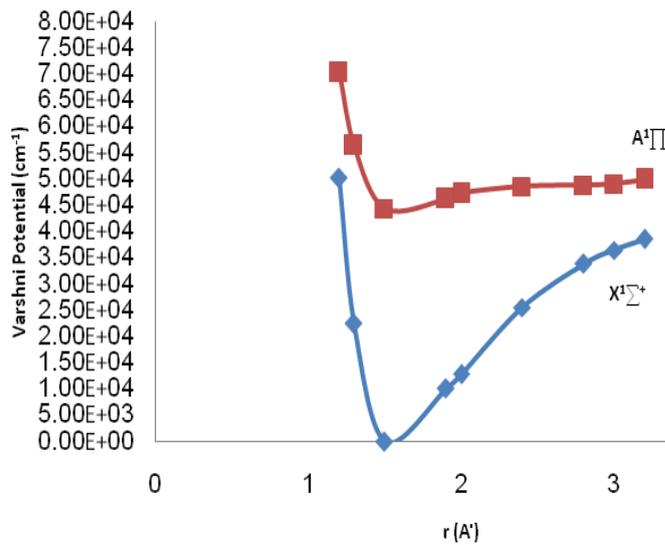
To calculate Varshni potential for SiO molecule (eq. 4) is used for the ground state $X^1\Sigma^+$ and the excited state $A^1\Pi$, and here are the results in table (3) and figure (1).

The calculations appear the maximum value of varshni potential is at ($r = 1.2 \text{ Å}$) that mean the minimum value of bond length give us maximum potential in ground state of SiO molecule. At bond length ($r = 1.5 \text{ Å}$), 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 $A^1\Pi$ of this molecule except the potential don't equal zero at the equilibrium bond length but equal to (44363 cm^{-1}) which is also minimum value of the potential.

Table 3: Varshni Function for Ground State $X^1\Sigma^+$ and Exited State $A^1\Pi$

r (Å)	$X^1\Sigma^+$ $U_{\text{Varsh}}(x)$ cm^{-1}	$A^1\Pi$ $U_{\text{Varsh}}(x)$ cm^{-1}
1.2	50220	70358
1.3	22518	56462
1.5	0	44363
1.9	10121	46285
2	12814	47335
2.4	25632	48656
2.8	33875	48925
3	36522	49112
3.2	38614	50021

**Figure 1: Calculated Varshni Potential Curves for $X^1\Sigma^+$ and $A^1\Pi$ States**

RESULTS OF HUA POTENTIAL FUNCTION

To calculate Hua potential for SiO molecule eq. (6) 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 [6], 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 (4) and figure (2).

The calculations appear the maximum value of Hua potential is (40330 cm^{-1}) in ground state of SiO molecule at ($r = 1.2 \text{ Å}$) which is the minimum value of bond length. At bond length ($r = 1.5 \text{ Å}$), 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 (38652 cm^{-1}) which is also minimum value of the potential.

The $X^1\Sigma^+$ potential-curves from the Varshni and Hua calculations are compared with the experimental RKR curve of Timothy and Hinry [7] as in table (5) and Figure (3). Both of the theoretical curves are in quantitative agreement with experiment. The Varshni and Hua potential curves for the $A^1\Pi$ state are compared with the corresponding experimental RKR curve in table (6) and Figure (4). As can be seen, the computed and experimental shape are in general agreement [7]. Therefore behavior results of Hua potential is similar to behavior results of varshni potential with simple different but the results are in good agreement with experimental values.

Table 4: Hua Potential Function for Ground State $X^1\Sigma^+$ and Exited State $A^1\Pi$

r (Å)	$X^1\Sigma^+$ $U_{\text{Hua}}(r)$ cm^{-1}	$A^1\Pi$ $U_{\text{Hua}}(r)$ cm^{-1}
1.2	40330	112924
1.3	14518.8	64528
1.5	0	38652
1.9	7255	39523.4
2	12099	41943.2
2.4	29844.2	43556.4
2.8	37542	44363
3	40330	44422
3.2	41943.2	44412

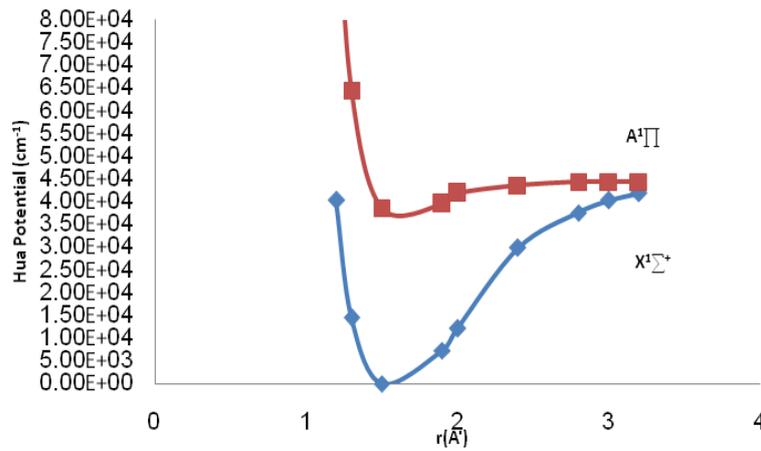


Figure 2: Calculated Hua Potential Curves for $X^1\Sigma^+$ and $A^1\Pi$ States

Table 5: Comparing Hua Function and Varshni and Experimental for Ground State $X^1\Sigma^+$

r (Å)	Varshni Potential	Hua Potential	Experimental Potential [7]
1.2	50220	54481.6	50396
1.3	22518	22793	16938.6
1.5	0	0	0
1.9	10121	14764.2	12099
2	12814	18834.1	14518.2
2.4	25632	32514	30037
2.8	33875	39751	37652.4
3	36522	41231	39341
3.2	38614	41352	40221.1

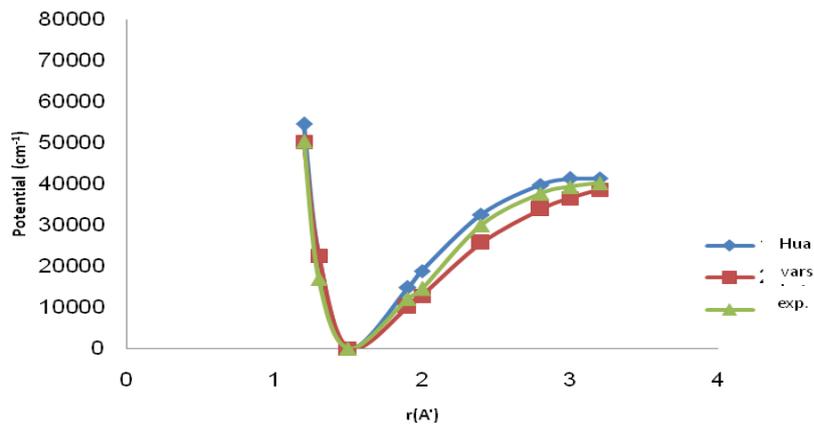


Figure 3: Theoretical Potential Calculated by Varshni Potential and Hua Potential Compare with Experimental Curves for Ground States $X^1\Sigma^+$

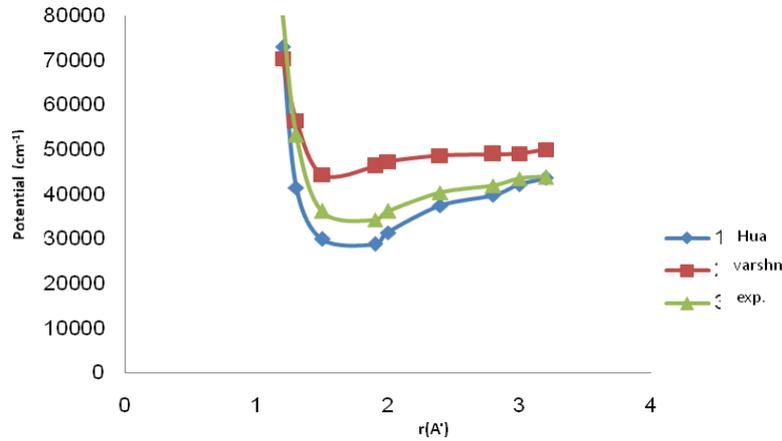


Figure 4: Theoretical Potential Calculated by Varshni Potential and Hua Potential Compare with Experimental Curves for Excited States $A^1\Pi$

Table 6: Comparison Hua Function and Varshni and Experimental for Ground State $A^1\Pi$

r (\AA°)	Varshni Potential	Hua Potential	Experimental Potential [7]
1.2	70358	72950.8	80254
1.3	56462	41485.7	53235.5
1.5	44363	29976.2	36254.4
1.9	46285	28800.1	34297.1
2	47335	31428.2	36225.1
2.4	48656	37428.3	40330
2.8	48925	39845.4	41943.1
3	49112	42114	43521
3.2	50021	43556	43888

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 Varshni function and 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.

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