

# On the dissociation energy of the CaO, SiO, SiO<sup>+</sup> and VO Astrophysically important diatomic molecules

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## Abstract

The true potential energy curves have been constructed for the different electronic state of the CaO, SiO, SiO<sup>+</sup> and VO molecules by the method of Rydberg-Klein-Rees as modified by Vanderslice et al., (RKR) by curve fitting of the modified form of Lippincott's three parameter empirical potential function. The estimated dissociation energies are found to be  $4.75 \pm 0.06$ ,  $8.25 \pm 0.17$ eV,  $5.75 \pm 0.07$ ,  $6.42 \pm 0.14$  eV respectively.

## 1. Introduction

In recent years, experimental potential energy curves have been constructed for many diatomic species which are of interest in various fields like kinetic mechanisms, spectral phenomena, stellar structure and many associated problems. Detailed knowledge of the spectra and structure of transition metal diatomic oxide is of great astrophysical interest since many of them have been found or proposed to be present in the spectra from M and S-type stars [1-3]. The molecule has large dissociation energy and their cosmic abundance is also relatively high.

The molecule CaO has astrophysical significance, as some of its lines might conceivably appear as interstellar lines. Molecular spectra provide the most useful data for determining the molecular structures and bond energies, and are a key means of verifying the presence of various elements or molecules and monitoring the concentrations of chemical species in laboratory, industrial, atmospheric and interstellar environments. Hultin and Lagerquist [4] have been studied A<sup>1</sup>Σ<sup>+</sup>-X<sup>1</sup>Σ<sup>+</sup> transitions of CaO in 1950 and which a milestone is in understanding and experimental study of perturbations of CaO. Field [5] has been carried out laser experiment on CaO and the vibrational assignment of the levels. High-resolution Fourier transform spectroscopy of the CaO of A<sup>1</sup>Σ<sup>+</sup>-X<sup>1</sup>Σ<sup>+</sup> transition is deeply studied and has presented the new insights into perturbations by the a<sup>3</sup>Π<sub>0</sub><sup>+</sup> and A<sup>1</sup>Π states by Van Groenendael et al [6]. The low resolution of A<sup>1</sup>Σ<sup>+</sup>-X<sup>1</sup>Σ<sup>+</sup> transition of CaO has been recorded by Brewer and Hange [7]. Van Groenendael et al [6] and Focsa et al [8] have been

recorded the spectra of CaO and new  $A^1\Sigma^+ - X^1\Sigma^+$  transition data. The studies on CaO are scanty and it is worth to analyze and evaluate the molecular spectroscopic properties of CaO.

The molecule SiO is of astrophysical importance whose spectra were observed in the sunspots. The absorption spectrum of SiO in the region 1200-1500Å was observed by Lagerqvist et al [9]. The most intense band system designated as  $A^1\Pi - X^1\Sigma^+$  (2000-3000Å) was observed and vibrationally analysed. The  $E^1\Sigma^+ - X^1\Sigma^+$  system in the region 1650-2000Å has been rotationally analyzed by Elander and Lagerqvist [10]. Bredohl et al [11] recorded the spin-forbidden  $a^3\Pi_r - X^1\Sigma^+$  transition band system in the spectral region 2870-3235Å and carried out vibrational and rotational analyses. Bredohl et al [12] reported that there was a change of the vibrational numbering for the system  $c^3\Pi_i - a^3\Pi_r$  of SiO (3900-4500Å).

Rosner et al [13] have been reported the spectral analysis of  $X^2\Sigma_g^+$  and  $A^2\Pi$  states of  $SiO^+$  using fast ion-beam laser spectroscopic method and also expressed the astrophysics significance of the infrared electronic transition frequencies between the  $X^2\Sigma_g^+$  and  $A^2\Pi$  states. From an astrophysical point of view, information about the thermodynamic, spectroscopic and energetic properties of the molecule is required for the chemistry involving dust information processes from the gas phase in circum stellar shells of oxygen-rich stars [14,15].

A study of vanadium oxide (VO) is justified by its importance in astrophysics and also in solid state physics. Astrophysicists have identified the presence of VO in cool M-type stars [16,17-19]. The electronic spectrum of the VO radical appears from the near infrared to the visible in absorption spectra of many cool stars, and provides the basis for the spectral classification of the late M-type stars [19]. These spectra have been utilized as a sensitive probe of the circum stellar environment and are of significant importance in modeling of the stellar atmospheres. VO has great significance in chemical and industrial fields and also finds sample applications in the areas of optical devices, semiconductors, catalysts and coatings [20-25]. Experimental studies confirmed  $X^4\Sigma^-$  is the ground state for VO. Three strong transitions of VO have been identified in the near IR and Visible regions which have been assigned as  $A^4\Pi - X^4\Sigma^-$ ,  $B^4\Pi - X^4\Sigma^-$  and  $C^4\Sigma^- - X^4\Sigma^-$  [25-31]. Two more quartet-quartet transitions of VO have been identified in the near IR that originate from the  $D^4\Delta$  state and terminate on the  $A^4\Pi$  state and another low-lying  $A^4\Phi$  state [32]. Ram and Bernath [33] have identified a new  $2\Delta - 1^2\Delta$  transition of VO in the 21000-22100  $cm^{-1}$  region using a Fourier Transform Spectrometer.

## 2. Potential energy curves

The RKR method is a Wentzel – Kramers – Brillouin approximation with which one obtains reliable potential energy curves from the measured vibrational and rotational constants of the diatomic molecules. Experimentally determined vibrational levels are used to construct the potential energy curve. The RKR method [34] and [35] has been used for obtaining the classical turning points,  $r_{\max}$ ,  $r_{\min}$  of the vibrational motion. The turning points are given in terms of functions  $f$  and  $g$  as follows:

$$r_{\max} = \left[ \frac{f}{g} + f^2 \right]^{\frac{1}{2}} + f, \quad r_{\min} = \left[ \frac{f}{g} + f^2 \right]^{\frac{1}{2}} - f$$

$$f = \left( \frac{8\pi^2 \mu c}{h} \right)^{\frac{1}{2}} \sum_{i=1}^n (\omega x)_i^{-\frac{1}{2}} \ln W_i$$

$$g = \left( \frac{2\pi^2 \mu c}{h} \right)^{\frac{1}{2}} \sum_{i=1}^n \{ 2\alpha_i (\omega x)_i^{-1} [(U_n - U_{i-1})^{\frac{1}{2}} - (U_n - U_i)^{\frac{1}{2}}] + (\omega x)_i^{-1/2} [2B_i - \alpha_i (\omega x)_i^{-1} w_i] \ln W_i \}$$

d

$$W_i = \left[ \frac{[\omega_i^2 - 4(\omega x)_i U_i]^{\frac{1}{2}} - 2(\omega x)_i^{1/2} [U_n - U_i]^{\frac{1}{2}}}{[\omega_i^2 - 4(\omega x)_i U_{i-1}]^{\frac{1}{2}} - 2(\omega x)_i^{1/2} [U_n - U_{i-1}]^{\frac{1}{2}}} \right]$$

The symbols have their usual significance. Using the least-square method as described by Vanderslice et al., [35], the values of  $\omega_i$ ,  $(\omega x)_i$ ,  $B_i$  and  $\alpha_i$  are determined and used in the construction of the potential energy curve.

## 3. Dissociation energy

In the construction of RKR potential curves, the energies  $U(r)$  are calculated with the empirical potential functions by varying the  $D_e$  value. An average percentage deviation is determined between the calculated  $U(r)$  and the experimental  $G(v)$  values. The dissociation energy from any function is that value of  $D_e$  which gives the smallest deviation. The corresponding function determined the dissociation energy of the molecule. A critical evaluation of the more important of these functions was given by Steele et al., [36], and they have shown that the potential function of Hulburt-Hirschfelder (H-H) fits well with the RKR curves of a large number of diatomic molecules [37-38]. In the present investigation, it is noted that H-H function fits best and reproduce the experimental energy values (Table 4.6 - 4.9). Different  $D_e$  values are used in the H-H function and the  $D_e$  values for which the

best fit of the energy values  $U(r)$  is observed, is taken as the dissociation energy ( $D_e$ ) of the molecule

#### 4. Results and discussion

The turning points of the potential energy curves of different electronic states of the above molecules, for the observed vibrational levels are calculated and the details are given below. The spectroscopic constants required for the construction of potential energy curves are presented in Table 4.1 and are taken from the literature [39-46].

**Table 4.1. Spectroscopic constants of different electronic states of diatomic molecules which are considered in the present investigation.**

Molecule	$\mu$	State	$T_e$ ( $cm^{-1}$ )	$\omega_e$ ( $cm^{-1}$ )	$\omega_e x_e$ ( $cm^{-1}$ )	$B_e$ ( $cm^{-1}$ )	$\alpha_e$ ( $cm^{-1}$ )	$r_e$ ( $\text{\AA}$ )	$D_e$ eV
CaO	11.4229	X	0	732.1	4.81	0.444	0.0033	1.822	4.76
		$A^1\Sigma^+$	11184.77	717.96	1.85	0.408	0.0021	1.899	
		$a^3\Pi_0-$	8082.23	541.87	2.60	0.345	0.0021	2.067	
SiO	10.1767	$X\Sigma^+$	0	1239.5	5.92	0.724	0.0049	1.5097	8.18
		$E^1\Sigma^+$	52859	673.5	4.15	0.546	0.0053	1.7394	
SiO <sup>+</sup>	10.1767	$X^2\Sigma^+$	0	1162.18	6.96	0.720	0.0058	1.5162	4.98
		$A^2\Pi^+$	2242.2	946.28	7.00	0.618	0.0047	1.6365	
		$B^2\Sigma^+$	26029.0	1136.58	6.92	0.713	0.0058	1.5243	
VO	12.1729	$X^4\Sigma^{-k}$	0	1011.3	4.86	0.548	0.0035	1.5893	6.4
		$^2\Pi_{1/2}$	12625	935.948	4.17	0.520	0.0033	1.6314	

$\mu$  = Reduced mass

$T_e$  = Electronic energy above ground state ( $cm^{-1}$ )

$\omega_e$  = Vibrational spacing ( $cm^{-1}$ )

$\omega_e x_e$  = Anharmonic correction to vibrational spacing ( $cm^{-1}$ )

$B_e$  = Rigid rotator rotational spacing ( $cm^{-1}$ )

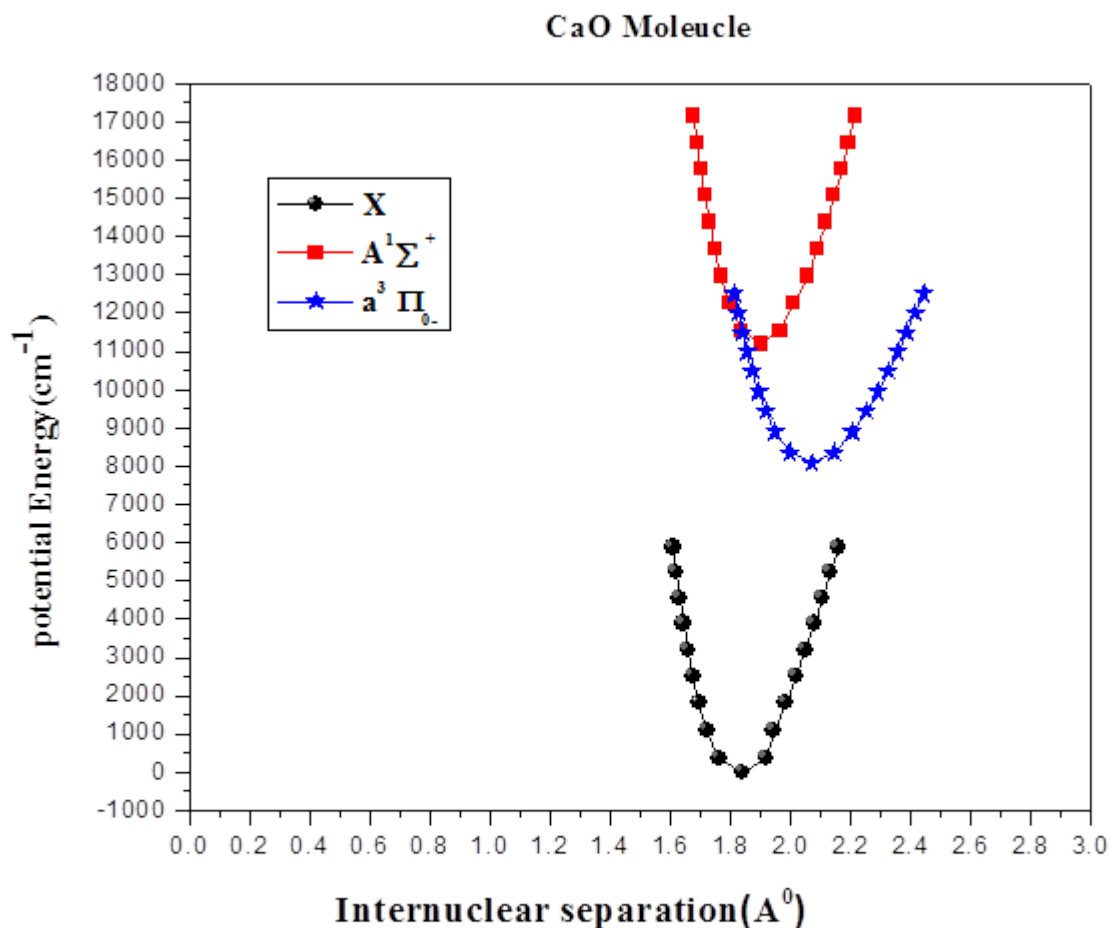
$\alpha_e$  = Non rigid rotator correction to  $B_e$  ( $cm^{-1}$ )

$r_e$  = Equilibrium inter nuclear distance ( $\text{\AA}$ )

#### 4.1. Potential energy curve of CaO, SiO, SiO<sup>+</sup> and VO Molecules

##### 4.1.1. CaO Molecule:

In the present study, the experimental potential energy curves for X,  $A^1\Sigma^+$  and  $a^3\Pi_0-$  states of CaO molecule using RKR method are constructed as shown in Fig (4.1). The molecular constants required in the present work for the evaluation of the turning points are taken from Van Groenendael et al [41]. The maximum and minimum internuclear distances for the observed nine vibrational levels of the ground and excited state have been determined by using Vandervliet et al [47] method. The values obtained by this method are presented in Table [4.2].



**Fig. 4.1** Potential Energy curve of CaO molecule

**Table 4.2:** Turning points of the potential energy curve for different states of CaO molecule.

v	U (cm <sup>-1</sup> )	R min (Å)	R max (Å)
X	State T <sub>e</sub> = 0		
0	364.84	1.761	1.918
1	1087.32	1.721	1.943
2	1800.18	1.695	1.983
3	2503.42	1.675	2.017
4	3197.40	1.658	2.048
5	3881.04	1.643	2.078
6	4555.42	1.630	2.105
7	5220.18	1.618	2.132
8	5875.32	1.608	2.157
A <sup>1</sup> Σ <sup>+</sup>	State T <sub>e</sub> = 11184.77		
0	358.51	1.837	1.965
1	1072.77	1.795	2.010
2	1783.33	1.768	2.056
3	2490.19	1.747	2.089
4	3193.35	1.729	2.117

5	3892.81	1.714	2.144
6	4588.57	1.700	2.169
$a^3\Pi_0-$	State $T_e= 8082.23$		
0	270.28	1.996	2.144
1	806.95	1.948	2.205
2	1338.42	1.917	2.250
3	1864.49	1.893	2.289
4	2385.76	1.872	2.323
5	2901.63	1.855	2.355

#### 4.1.2. SiO Molecule:

In the present study more accurate and reliable vibrational and rotational constants, the turning points for  $X \Sigma^+$  and  $E^1 \Sigma^+$  states of SiO molecule have been calculated to draw the experimental true potential energy curves as shown in Fig (4.2). The molecular constants required for the evaluation of turning points in present work are taken from Grevesse et al [48] and presented in Table 4.3. The turning points for eight levels of the ground state  $X^1 \Sigma^+_g$ , and six vibrational levels of  $E^1 \Sigma^+$  state, have been calculated by Vanderslice et al [47]. The values obtained by these methods are presented in Table [4.3].

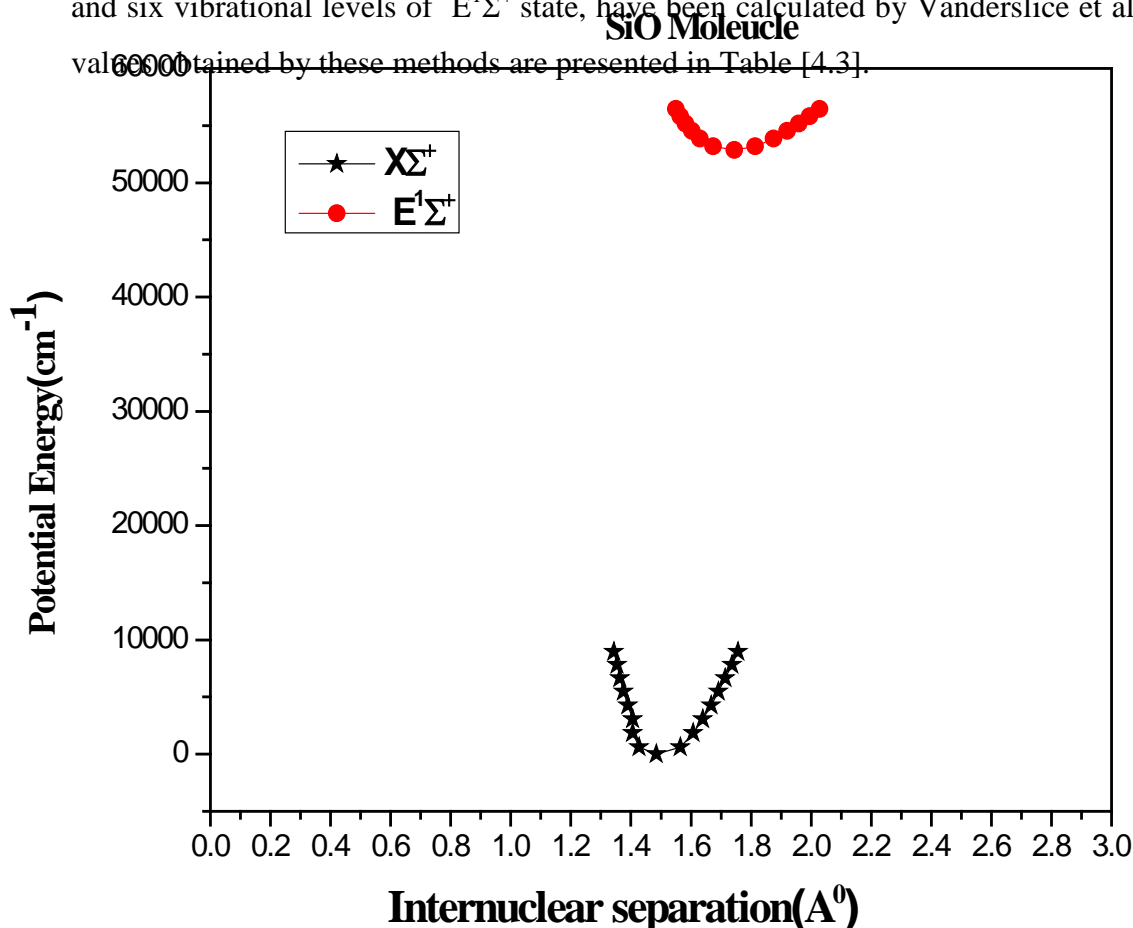


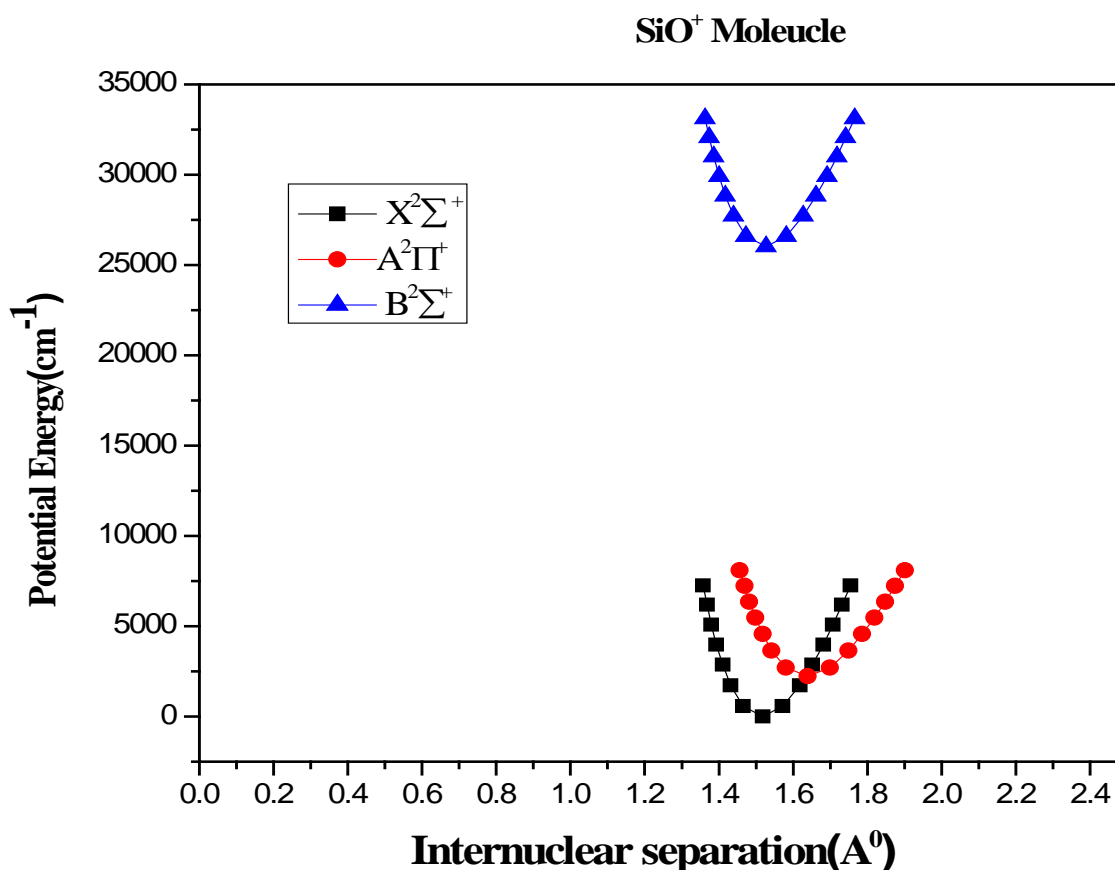
Fig. 4.2 Potential Energy curve of SiO molecule

**Table 4.3: Turning points of the potential energy curve for different states of SiO**

v	U (cm <sup>-1</sup> )	R min (Å)	R max (Å)
X <sup>1</sup> Σ <sup>+</sup>	State T <sub>e</sub> = 0		
0	619.2	1.406	1.564
1	1848.9	1.427	1.607
2	3066.5	1.406	1.639
3	4272.3	1.389	1.667
4	5466.1	1.375	1.691
5	6648.0	1.364	1.714
6	7818.0	1.353	1.736
7	8976.0	1.344	1.756
E <sup>1</sup> Σ <sup>+</sup>	State T <sub>e</sub> = 52859		
0	336.7	1.673	1.814
1	1003.8	1.630	1.875
2	1662.5	1.602	1.920
3	2312.8	1.581	1.959
4	2954.7	1.564	1.994
5	3588.2	1.549	2.027

#### 4.1.3. SiO<sup>+</sup> Molecule:

In the present study the experimental potential energy curves for the X <sup>2</sup>Σ<sup>+</sup>, A <sup>2</sup>Π<sup>+</sup> and B <sup>2</sup>Σ<sup>+</sup> of SiO<sup>+</sup> molecule using RKR method [47] is constructed as shown in Fig (4.3). The spectroscopic constants required in the present study for the evaluation of the r<sub>max</sub> and r<sub>min</sub> points are taken from Huber and Herzberg et al [49] are presented in Table 4.4.



**Fig. 4.3** Potential Energy curve of SiO<sup>+</sup> molecule

**Table 4.4: Turning points of the potential energy curve for different states of SiO<sup>+</sup> molecule.**

v	U (cm <sup>-1</sup> )	R min (Å)	R max (Å)
X <sup>2</sup> Σ <sup>+</sup>	State T <sub>e</sub> = 0		
0	579.3	1.465	1.572
1	1727.5	1.432	1.618
2	2861.8	1.410	1.652
3	3982.2	1.393	1.681
4	5088.6	1.379	1.707
5	6181.1	1.368	1.732
6	7259.7	1.357	1.755
A <sup>2</sup> Π	State T <sub>e</sub> = 2242.2		
0	471.3	1.580	1.699
1	1403.6	1.542	1.749
2	2321.9	1.518	1.786
3	3226.1	1.498	1.819
4	4116.4	1.482	1.848
5	4992.6	1.469	1.875
6	5854.8	1.456	1.901
B <sup>2</sup> Σ <sup>+</sup>	State T <sub>e</sub> =26029		
0	566.4	1.473	1.581
1	1688.9	1.439	1.627
2	2797.6	1.417	1.661
3	3892.4	1.400	1.691
4	4973.4	1.386	1.718
5	6040.6	1.374	1.742

The maximum and minimum internuclear separations for seven vibrational levels of the ground state X<sup>2</sup>Σ<sup>+</sup> state, seven vibrational levels of A<sup>2</sup>Π<sup>+</sup> state and six vibrational levels of B<sup>2</sup>Σ<sup>+</sup> state have been determined by using Vanderslice et al [47] method. The values obtained by this method are presented in Table (4.4). From fig. (4.3) it is interesting to note that there are crossings of potential curves of X<sup>2</sup>Σ<sup>+</sup> and A<sup>2</sup>Π<sup>+</sup> states. These crossings indicate the possible perturbations and pre-dissociations. A<sup>2</sup>Π<sup>+</sup> curve is found to cross the X<sup>2</sup>Σ<sup>+</sup> curve between the vibrational levels 3 and 4. The r<sub>e</sub> value for the ground state X<sup>2</sup>Σ<sup>+</sup> and the excited state B<sup>2</sup>Σ<sup>+</sup> almost the same. So, the important feature of the potential curves is that they are laying approximately one above the other, indicating that the structure of the molecule in the ground state and the excited state should be nearly the same.



#### 4.1.4. VO molecule:

In the present work using more accurate and reliable vibrational and rotational constants, the turning points for the  $X^4 \Sigma^-_k$  and  $E^1 \Pi_{1/2}$  states of VO molecule have been calculated to draw experimental true potential energy curves as shown in fig(4.4). The molecular constants required in the present work for the evaluation of the turning points are taken from Ram et al [50] and presented in Table 4.5.

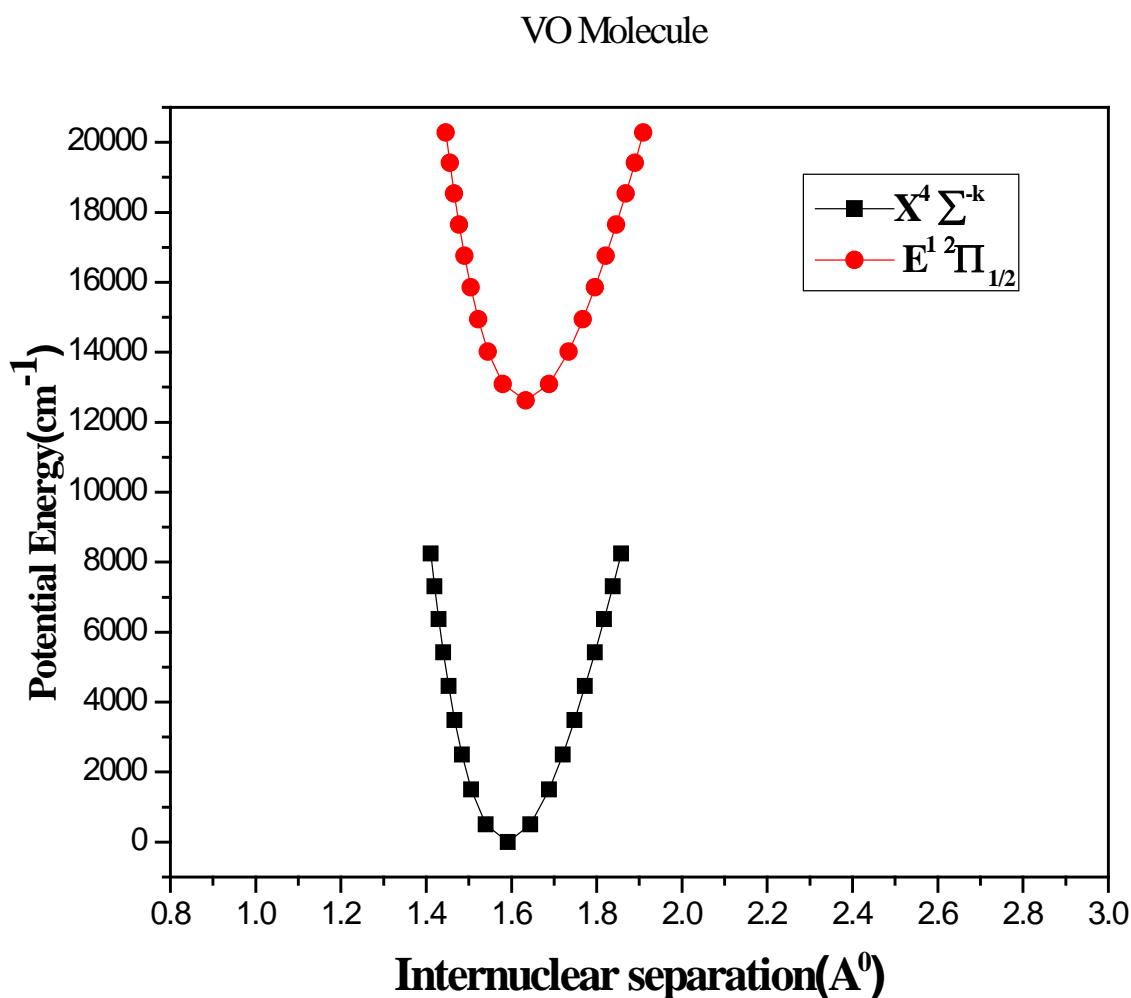


Fig. 4.4 Potential Energy curve of VO molecule

#### 4.5: Turning points of the potential energy curve for different states of VO Molecule

v	U (cm <sup>-1</sup> )	R min (Å)	R max (Å)
<b>X<sup>4</sup>Σ<sup>-k</sup></b>	State T <sub>e</sub> = 0		
0	504.43	1.539	1.644
1	1506.01	1.505	1.688
2	2497.87	1.484	1.720
3	3480.01	1.467	1.747
4	4452.43	1.452	1.772
5	5415.13	1.440	1.795
6	6368.11	1.429	1.817
7	7311.37	1.419	1.838
8	8244.91	1.410	1.857
<b>1<sup>2</sup>Π<sub>1/2</sub></b>	State T <sub>e</sub> = 12625		
0	466.93	1.579	1.688
1	1394.53	1.544	1.734
2	2313.78	1.522	1.767
3	3224.69	1.504	1.796
4	4129.24	1.489	1.821
5	5021.46	1.477	1.845

The turning points for the observed nine vibrational levels of X<sup>4</sup>Σ<sup>-k</sup>, and <sup>2</sup>Π<sub>1/2</sub> state have been determined by using RKR method [47]. The values obtained by this method are presented in Table (2.10). The equilibrium internuclear distance (r<sub>e</sub>) value for the excited states X<sup>4</sup>Σ<sup>-k</sup> and <sup>2</sup>Π<sub>1/2</sub> are not the same. The potentials are wide and the molecule will not behave like a harmonic oscillator.

#### 4.2. Dissociation energies of CaO, SiO, SiO<sup>+</sup> and VO molecules

##### 4.2.1. CaO Molecule

Accurate evaluation of dissociation energy from curve fitting requires a good empirical potential function. The Hulbert–Hirschfelder (H-H) [51] function has been shown to reproduce well RKR curves over a wide range of energies and for a number of diatomic molecules.

**Table 4.6. Energy values obtained from Hulburt–Hirschfelder (H-H) function for the X electronic state of CaO molecule**

r (Å)	U (cm <sup>-1</sup> )	U(r)cm <sup>-1</sup>		
		D <sub>e</sub> =4.72eV	D <sub>e</sub> =4.75eV	D <sub>e</sub> =4.77eV
1.889	364.84	360.45	364.26	368.06
1.943	1087.32	1074.58	1085.92	1097.25
1.983	1800.18	1780.40	1799.18	1817.95
2.047	2503.42	2478.31	2504.45	2530.59
2.048	3197.04	3168.73	3202.15	3235.58
2.077	3881.04	3852.17	3892.81	3933.44
2.105	4555.42	4528.94	4576.71	4624.48
2.132	5220.18	5199.51	5254.35	5309.20
2.157	5875.32	5864.31	5926.17	5988.03
1.761	364.84	3603.17	364.11	367.91
1.721	1087.32	1073.75	1085.08	1096.41
1.695	1800.18	1777.36	1796.11	1814.85
1.675	2503.42	2471.25	2497.32	2523.38
1.658	3197.04	3155.61	3188.89	3222.18
1.643	3881.04	3830.52	3870.93	3911.33
1.630	4555.42	4496.24	4543.67	4591.09
1.618	5220.18	5152.93	5207.29	5261.64
1.607	5875.32	5800.77	5861.96	5923.15
Average percentage deviation		1.04	0.27	0.83

For the RKR  $r \pm$  values, the energies  $U(r \pm)$  are calculated with the empirical potential function by varying the  $D_e$  value. An average percentage deviation is determined between the calculated  $U(r \pm)$  and the experimental  $G(v)$  values. The dissociation energy from which least deviation is considered as the best  $D_e$ . The function leading to the smallest deviation determines the dissociation energy of the molecule. The dissociation energy referred to  $v=0$  level is given by  $D_0 = D_e - G(v)$ .

This procedure is applied to determine the adequacy of the potential functions to represent the electronic ground state of CaO molecule. In the present case, it is found that H-H function [52] fits the curve but when  $D_e = 4.75$  eV. Relevant results of  $U(r \pm)$  are given in Table 4.6 combining the errors involved in the curve fitting with 2 percent inherent to the H-H function, the dissociation is estimated to be  $D_0 = 4.75 \pm 0.06$  eV. This value is in agreement with the thermo-chemical method value 4.76 eV given by Huber and Herzberg [53]. The estimated  $D_e$  value is reliable because it is evaluated using the true potential energy based on experimental data.

#### 4.2.2 SiO molecule

In the curve fitting procedure, an empirical potential function which gives the best reproduction of RKR curve is chosen. In this potential function, the turning points evaluated by the RKR potential energy curve are substituted with different values of  $D_e$ . By this procedure, energy values  $U(r)$  for various vibrational levels are calculated. These values are compared with experimental energy values  $G(v)$ . The value of  $D_e$  for which the best fit is obtained is taken to be the value of dissociation energy for that state of the molecule. In the present study, the five parameter Hulbert –Heirshfelder [51] function is chosen to estimate  $D_e$  value of SiO, as this function is seen to be superior to other functions. The deviation of the calculated energy from the experimentally observed values is found to be minimum (0.11), only when the above potential function is chosen (Table 4.7). The estimated dissociation energy with this function in this study is  $8.25 \pm 0.17$  eV. This value is in fair agreement with the value 8.28 eV recommended by Lide et al. [54] and slightly higher than the value 7.4 eV given by Herzberg [55].

**Table 4.7. Energy values obtained from Hulbert–Hirschfelder (H-H) function for the  $X^2\Sigma^+$  electronic state of SiO molecule.**

r (Å)	U (cm <sup>-1</sup> )	U(r)cm <sup>-1</sup>		
		$D_e = 8.23\text{eV}$	$D_e = 8.25\text{eV}$	$D_e = 8.28\text{eV}$
1.4606	619.2	621.0	619.2	617.3
1.4276	1848.9	1854.1	1848.6	1843.0
1.4063	3066.5	3075.2	3066.9	3056.7
1.3893	4272.3	4284.4	4271.5	4258.7
1.3759	5466.1	5481.6	5465.2	5448.8
1.3640	6648.0	6667.1	6647.1	6627.1
1.3535	7818.0	7840.8	7817.3	7793.8
1.3440	8976.0	9003.0	8976.0	8949.1
1.5641	619.2	621.0	619.1	617.3
1.6076	1848.9	1854.2	1848.6	1843.1
1.6396	3066.5	3075.6	3066.4	3057.2
1.6670	4272.3	4285.3	4272.5	4259.6
1.6916	5466.1	5483.3	5466.9	5450.5
1.7145	6648.0	6669.8	6649.8	6629.8
1.7361	7818.0	7844.6	7821.1	7797.7
1.7568	8976.0	9007.8	8980.9	8953.9
Average percentage deviation		0.31	0.11	0.30

#### 3.9.5. SiO<sup>+</sup> Molecule

Silicon is believed to have a complex chemistry and it is observed in interstellar clouds and also in hot materials surrounding star – forming regions [56]. The Energy values

using (H-H) function for the  $X^2\Sigma^+$  electronic state of  $\text{SiO}^+$  molecule is given in Table 4.8. The dissociation energy obtained in the present study  $D_e(\text{SiO}^+) = 5.75\text{eV}$ . There are different methods to test the reliability of the estimated dissociation energies. If a few experimental values for  $(v+1) - v$  transitions are available, linearly extrapolating the equation (as described earlier)

$$G(v) = \frac{1}{2}[G(v+1) - G(v-1)] = \omega_e - 2\omega_e X_e (v + \frac{1}{2}) \quad \text{to } G(v)=0 \text{ gives } v=v_c; \quad v_c \text{ may be obtained from } v_c = (\omega_e / 2\omega_e X_e) - \frac{1}{2}$$

This value is inserted in the following equation

$$G(v) = \omega_e (v_c + \frac{1}{2}) - \omega_e X_e (v_c + \frac{1}{2})^2 + \dots$$

This  $G(v)$  value is equal to the dissociation energy of the concerned molecule.  $D_0$  value obtained for  $\text{SiO}^+$  from this method is 6.01 eV. The dissociation energy mentioned by Huber and Herzberg [53] is 4.98 eV. The deviation may be due to the strong ionic bonding expected in this molecule. Using  $D_e$  values of SiO (8.28 eV) [52]  $\text{SiO}^+$  (5.75 eV) and Ionization potential of Si (8.15 eV)[52],  $I(\text{SiO})$  can be calculated from the cycle given by Gaydon[52]. i.e.,

$$\begin{aligned} I(\text{SiO}) &= I(\text{Si}) + D_e(\text{SiO}) - D_e(\text{SiO}^+) \\ &= 8.15 + 8.28 - 5.75 \\ &= 10.68 \text{ eV} \end{aligned}$$

which is in good agreement with the value 11.42 eV given by Huber and Herzberg [53]

**Table 4.8. Energy values obtained from Hulburt–Hirschfelder (H-H) function for the X  $^2\Sigma^+$  ground states of SiO $^+$  molecule.**

r (A $^\circ$ )	U (cm $^{-1}$ )	U(r)cm $^{-1}$		
		D $_e$ =5.72eV	D $_e$ =5.74eV	D $_e$ =5.77eV
1.572	579.3	576.7	579.2	581.7
1.618	1727.5	1720.2	1727.7	1735.1
1.652	2861.8	2850.3	2862.7	2875.0
1.681	3982.2	3967.5	3984.7	4001.9
1.707	5088.6	5071.9	5093.9	5115.9
1.732	6181.1	6163.8	6190.6	6217.3
1.755	7259.7	7243.5	7274.8	7306.2
1.465	579.3	576.7	579.2	581.7
1.432	1727.5	1719.5	1726.9	1734.4
1.410	2861.8	2848.1	2860.4	2872.8
1.393	3982.2	3962.2	3979.4	3996.6
1.379	5088.6	5061.8	5083.7	5105.7
1.368	6181.1	6146.8	6173.4	6200.0
1.357	7259.7	7217.2	7248.4	7279.7
Average percentage deviation		0.43	0.07	0.43

### 3.9.8. VO molecule

The study of experimental potential energy curves is fundamentally important in computing the precise dissociation energy of a diatomic molecule, the another has taken up this investigation to find the dissociation energy of the VO molecule as it is astrophysically important and its spectra were observed in M-type stars[57].

The bond dissociation energy of a diatomic molecule is the most direct measure of the strength of the bond, and therefore, of the stability of the chemical combination between the constituent atoms, that is the very existence of the molecule. For a molecular species to form and remain stable against dissociating influence in any environment, astronomical, chemical and so on. The temperature must be sufficiently low and other energetic interactions must be sufficiently mild that the probability of breaking the chemical bond, once formed, is low. Since the dissociation energy is a prime factor in such phenomena, astrophysicist, chemists and spectroscopists are concerned with the determination of reliable values of dissociation energy for the diatomic molecules.

The curve fitting method has been found to yield reliable values for the dissociation energy of a large number of diatomic molecules [58]. The procedure involved in this method is already highlighted many times, the only estimated U(r) for a particular De (6.42±0.14 eV)

is presented in Table 4.9 and the obtained dissociation energy of VO molecule is in agreement with the value (6.41 eV) quoted by Huber and Herzberg [53].

**Table 4.9. Energy values obtained from Hulburt–Hirschfelder (H-H) function for the X  $^4\Sigma^-K$  electronic state of VO molecule.**

r (Å°)	U (cm <sup>-1</sup> )	U(r)cm <sup>-1</sup>		
		D <sub>e</sub> =6.37eV	D <sub>e</sub> =6.39eV	D <sub>e</sub> =6.42eV
1.644	504.43	499.23	501.17	503.11
1.688	1506.01	1490.69	1496.49	1502.29
1.720	2497.87	2473.13	2482.76	2492.38
1.747	34801.01	3446.80	3460.21	3473.63
1.772	4452.43	4411.82	4428.99	4446.16
1.795	5415.13	5367.35	5388.23	5409.11
1.817	6368.11	6316.93	6341.51	6366.09
1.838	7311.37	7257.33	7285.57	7313.81
1.857	8244.91	8189.95	8221.82	8253.68
1.539	504.43	499.15	501.09	503.03
1.505	1506.01	1490.09	1495.89	1501.69
1.484	2497.87	2471.05	2480.67	2490.28
1.467	3480.01	3441.92	3455.31	3468.70
1.452	4452.43	4402.73	4419.98	4436.99
1.440	5415.13	5353.37	5369.04	5395.03
1.429	6368.11	6293.81	6318.30	6342.79
1.419	7311.37	7224.09	7252.20	7280.31
1.410	8244.91	8144.18	8175.87	8207.56
Average percentage deviation		1.00	0.62	0.25

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