Theoretical Study with Rovibrational and Dipole Moment Calculation of the SiO Molecule

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ABSTRACT

Via CASSCF/MRCI and RSPT2 calculations (single and double excitation with Davidson correction) the potential energy curves of 20 electronic states in the representation $^{2S+1}\Lambda^{(\pm)}$ of the molecule SiO have been calculated. By fitting these potential energy curves to a polynomial around the equilibrium internuclear distance r_e , the harmonic frequency ω_e , the rotational constant B_e , and the electronic energy with respect to the ground state T_e have been calculated. For the considered electronic states the permanent dipole moment μ have been plotted versus the internuclear distance r . Based on the canonical functions approach, the eigenvalues E_v , the rotational constant B_v and the abscissas of the turning points $r_{\min}$ and $r_{\max}$ have been calculated. The comparison of these values to the experimental and theoretical results available in the literature is presented. In the present work 8 higher electronic states have been studied theoretically for the first time.

Keywords: *Ab Initio* Calculation; SiO Molecule; Potential Energy Curves; Spectroscopic Constants; Dipole Moment; Rovibrational Calculation

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, and shocked gas [1]. Because of the interaction between high velocities jets emerging from a young star and the surrounding molecular environment a large fraction of the silicon monoxide relative to hydrogen molecule are found in the high velocity gas components of molecular outflows [2]. This abundance of SiO comes from the sputtering of dust grains in shocked regions and the subsequent release of Si-bearing material into the gas phase [3-7].

In recent years silica nanoparticles has attracted considerable attention due to their potential applications in many fields including ceramics, chromatography, catalysis and chemical mechanical polishing [8], nanodevices and mesoscopic research [9]. Altman *et al.* [9] probed the behavior of light absorption of silica nanoparticles at high temperatures in the Urbach region, and compare it with that in bulk materials. They assumed that, the SiO vapor emission does not contribute significantly to the flame radiation in visible. This can be easily justified by considering that the lower state of a SiO molecule in-

involved in transitions in visible light is not a ground state of the SiO molecule, but a highly excited one [10].

By studying the published data in literature on the molecule SiO, one can notice the large discrepancy between these values either theoretical or experimental. The values of the electronic transition energy T_e with respect to the ground state $X^1\Sigma^+$ vary as

$$24115 \text{ cm}^{-1} \leq T_e \leq 24031 \text{ cm}^{-1},$$

$$25509 \text{ cm}^{-1} \leq T_e \leq 24031.82 \text{ cm}^{-1} \quad [12],$$

and $32978.9 \text{ cm}^{-1} \leq T_e \leq 45135 \text{ cm}^{-1}$ [12] respectively for the electronic states $(1)^3\Sigma^+$, $(1)^3\Sigma^+$, $(2)^3\Sigma$. Similar data can be found for different spectroscopic constants of different electronic states. Stimulated by these discrepancies, the important connection between energy relations of solids and molecules [13], and based on our previous theoretical calculation [14-23], we performed an *ab initio* study of the low-lying electronic states of the molecule SiO below $132,500 \text{ cm}^{-1}$. In this work, we investigate the potential energy curves (PECs), the electric dipole moment and spectroscopic constants for the 20 $^{2S+1}\Lambda^{(\pm)}$ low-lying electronic states of this molecule obtained by MRCI and RSPT2 calculations. Taking advantage of the electronic structure of the investigated electronic states of the SiO molecule and by using the canonical functions approach [24-26], the eigenvalues E_v , the rotational

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constant B_v and the abscissas of the turning points $r_{\min}$ and $r_{\max}$ have been calculated up to the vibrational level $v = 52$.

2. Computational Approach

2.1. *Ab Initio* Calculation

The PECs of the lowest-lying electronic states of SiO molecule have been investigated via CASSCF method. MRCI and RSPT2 calculations (single and double excitations with Davidson corrections) were performed. Silicon atom is treated in all electron schemes where the 14 electrons of the silicon atom are considered using the cc-PVTZ basis set including s, p, d and f functions [27]. The oxygen atom is treated in all electron schemes where the 8 electrons of the oxygen atom are considered using the DGAUSS-a2-Xfit basis set including s, p and d functions [28]. Among the 22 electrons explicitly considered for the SiO molecule (14 electrons for Si and 8 for O), 18 inner electrons were frozen in subsequent calculations so that 4 valence electrons were explicitly treated. This calculation has been performed via the computational chemistry program MOLPRO [29] taking advantage of the graphical user interface GABEDIT [30].

The PECs for the 20 electronic states in the representation $2S+1\Lambda^{(\pm)}$ obtained from MRCI calculation have been obtained for 222 internuclear distances in the range $1.06 \text{ \AA} \leq r \leq 4.00 \text{ \AA}$. These potential energy curves for the singlet, triplet and quintet electronic states in the different symmetries are given, respectively in **Figures 1-3**.

The spectroscopic constants such as the vibration harmonic constants ω_e and $\omega_e x_e$, the internuclear distance at equilibrium r_e , the rotational constant B_e , and the electronic transition energy with respect to the ground state T_e have been calculated by fitting the energy values around the equilibrium position to a polynomial in terms of the internuclear distance. These values are given in **Table 1** together with the available values in the literature either theoretical or experimental. The comparison of our MRCI calculated values of $r_e \omega_e$, and B_e for the ground state $X^1\Sigma^+$ with those given in literature, either theoretical or experimental, shows an excellent agreement with the relative differences

$$0.05\% \left({}^{(\text{Fit})} \text{Ref.}[6] \right) \leq \frac{\delta r_e}{r_e} \leq 2.9\% \left({}^{(\text{SCF})} \text{Ref.}[35] \right),$$

$$0.6\% \left({}^{(\text{MSCF30})} \text{Ref.}[35] \right) \leq \frac{\delta \omega_e}{\omega_e} \leq 10.7\% \left({}^{(\text{MP2-1})} \text{Ref.}[33] \right),$$

Figure 1. Potential energy curves of the lowest singlet and triplet Σ and Δ -states of the molecule SiO.

Figure 2. Potential energy curves of the lowest singlet and triplet Σ and Δ -states of the molecule SiO.

Figure 3. Potential energy curves of the lowest quintet states of the molecule SiO.

Table 1. Spectroscopic constants for the electronic states of the molecule SiO.

States	$T_e(\text{cm}^{-1})$	$\Delta T_e/T_e\%$	$r_e(\text{\AA})$	$\Delta r_e/r_e\%$	$\omega_e(\text{cm}^{-1})$	$\Delta\omega_e/\omega_e\%$	$B_e(\text{cm}^{-1})$	$\Delta B_e/B_e\%$	$\omega_e x_e(\text{cm}^{-1})$	$\Delta\omega_e x_e/\omega_e x_e\%$		
$X^1\Sigma^+$	0.0		1.5237 ^{a1} 1.5328 ^{a2}		1270.03 ^{a1}							
					1230.75 ^{a2}							
							1241.6 ^b	2.2				
							1216.3 ^{c1}	4.2	0.7124 ^{a1}		5.07 ^{a1}	
							1245.4 ^{c2}	1.9	0.7041 ^{a2}		2.26 ^{a2}	
							1240.5 ^{c3}	2.3				
							1179.9 ^{c4}	7.1				
							1176.0 ^{c5}	7.4				
							1181.8 ^{c6}	6.9				
			1.5098 ^{b,d}	0.91	1242 ^{b,d}	2.2	0.727 ^{b,d}	2.0	5.97 ^{b,d}	17.7		
			1.5273 ^{e1}	0.24	1231 ^{e1}	3.0	0.709 ^{e1}	0.5	8.00 ^{e1}	58		
			1.5230 ^{e2}	0.05	1154 ^{e2}	9.1	0.713 ^{e2}	0.1	6.34 ^{e2}	25		
			1.4811 ^{f1}	2.8	1406.9 ^{f1}	10.7			5.02 ^{f1}	5.1		
			1.5055 ^{f2}	1.2	1309.2 ^{f2}	3.1			5.17 ^{f2}	2.0		
			1.5192 ^{f3}	0.3	1240.7 ^{f3}	2.3			5.85 ^{f3}	5.0		
			1.496 ^g	1.8	1247.9 ^g	1.6			5.97 ^g	17.7		
			1.479 ^{h1} 1.514 ^{h2}	2.9	1400 ^{h1}	10.2			5.0 ^{h1}	1.4		
			1.515 ^{h3}	0.64	1262 ^{h2}	0.6			5.7 ^{h2}	12.4		
				0.64	1241.7 ^{h3}	2.2			5.84 ^{h3}	15.2		
			1.5097 ^{i,j,k}	0.92	1241.5 ^{i,j,k}	2.2			5.97 ^{i,j,k}	17.7		
			1.5130 ^m	0.70	1242.4 ^m	2.2	0.72358 ^m	1.6				
			1.521 ⁿ	0.18	1216 ⁿ	4.2						
1.509739 ^p	0.92	1241.54394 ^p	2.2	0.726752 ^p	2.0	5.974370 ^p	17.7					
1.509733 ^{ac}	0.92	1241.54304 ^{ac}	2.2	0.726752 ^{ac}	2.0	5.973907 ^{ac}	17.7					
1.5166 ^q	0.46	1242.1 ^q	2.2	0.720 ^q	1.1	6.9 ^q	36.1					
1.5100 ^{ad}	0.89	1238.98 ^{ad}	2.44	0.726482 ^{ad}	2.0	5.96702 ^{ad}	17.7					
$(1)^3\Sigma^+$	30065.93 ^{a1} 25968.19 ^{a2} 24115.85 ^{r1} 37827.19 ^{r2} 32324.65 ^x 35810.82 ^{s1} 33630 ^b 33 568 ⁿ 33657.11 ^{ad}	19.8 25.8 7.5 19.1 11.8 11.6 11.9	1.86 ^{r1} 1.74 ^{r2} 1.70 ^x 1.70 ^{s2} 1.70 ^b 1.7081 ⁿ 1.7128 ^{ad}	8.7 1.7 0.6 0.6 0.6 0.1 0.15	661 ^{r1} 790 ^b 821 ⁿ 792.13 ^{ad}	23.7 8.9 5.3 8.6	0.56 ^{r1} 0.565584 ^{ad}	0.9 0.10				

Continued

(1) ³ Δ	32857.67 ^{a1}		1.7192 ^{a1}		844.56 ^{a1}		0.560 ^{a1}	
	30729.55 ^{r1}	6.5	1.88 ^{r1}	9.3	625 ^{r1}	26.0	0.48 ^{r1}	14.3
	25809.60 ^{r2}	21.4	1.76 ^{r2}	2.4			0.55 ^{r2}	1.8
	35084.92 ^x	6.8	1.71 ^x	0.5			0.57 ^x	1.8
d ³ Δ			1.71 ^u	0.5				
	36536.72 ^v	11.2			761 ^v	10.0	0.57 ^v	1.8
	36880 ⁿ	12.2	1.717 ⁿ	0.1	797 ⁿ	5.6		
	36487 ^b	11.0	1.715 ^b	0.2	767 ^b	5.6		
					863 ^w	2.2		
(1) ³ Σ ⁻	34819.56 ^{a1}		1.7298 ^a		799.37 ^a		0.553 ^a	
	32987.90 ^{r1}	5.3	1.90 ^{r1}	9.8	596 ^{r1}	25.4	0.16 ^{r1}	
	43473.05 ^{r2}	24.8	1.78 ^{r2}	2.9			0.32 ^{r2}	
	36536.72 ^x	4.9	1.78 ^x	2.9			0.55 ^x	0.5
e ³ Σ ⁻	38311.13 ^v	10.0	1.72 ^v	0.6	718 ^v	10.2	0.56 ^v	1.3
	37848 ⁿ	8.7	1.738 ⁿ	0.5	785 ⁿ	18.0		
	38309 ^b	10.0	1.726 ^b	0.2	748 ^b	6.4		
					803 ^w	0.4		
	35433.8 ^{a1}		1.7265 ^{a1}				0.5544 ^{a1}	
(1) ¹ Σ ⁻			1.746 ^g	1.1	703.3 ^g			
	34842.96 ^{r1}	1.7	1.96 ^{r1}	13.5	513 ^{r1}		0.48 ^{r1}	13.4
	44924.84 ^{r2}	26.8	1.83 ^{r2}	5.6			0.49 ^{r2}	11.6
	37343.26 ^x	5.4	1.77 ^x	2.5				
	38633.75 ^v	9.0	1.75 ^v	1.4	740 ^v		0.54 ^v	2.3
	37920 ⁿ	7.0	1.743 ⁿ	0.9	725 ⁿ			
	38624 ^b	9.0	1.727 ^b	0.0	740 ^b			
					735 ^w			
(1) ¹ Δ	38606.70 ^{ad}	8.2	1.7314 ^{ad}	0.3	743.72 ^{ad}	5.7	0.553178 ^{ad}	0.22
	35637.35 ^{a1}		1.7289 ^{a1}		938.37 ^{a1}		0.5527 ^{a1}	
	34580.78 ^{a2}		1.7190 ^{a2}		887.47 ^{a2}		0.5598 ^{a2}	
	35407.54 ^{r1}	0.6	1.98 ^{r1}	14.5			0.42 ^{r1}	24.0
	46457.28 ^{r2}	36.4	1.85 ^{r2}	7.0			0.48 ^{r2}	13.1
	37181.96 ^x	4.3	1.79 ^x	3.5			0.52 ^x	5.9
D ¹ Δ	38795.05 ^v	8.9	1.78 ^v	2.9	780 ^v	16.9		
	38955 ⁿ	9.3	1.744 ⁿ	0.9	723 ⁿ	22.9		
	38823 ^b	8.9	1.729 ^b	0.0	730 ^b	22.2		
					798 ^w	15.5		

Continued

3Π	57708.29 ^{a1}		1.7683 ^{a1}		583.90 ^{a1}		0.5286 ^{a1}	
³ Π(III)	65007.93 ^x	12.6	1.64 ^x	7.3			0.61 ^x	15.4
	59604.05 ^z	3.3	1.70 ^z	3.9	482 ^z	17.4	0.57 ^z	7.8
(2) ¹ Σ ⁺	60430.60 ^{a1}		1.6544 ^{a1}		935.16 ^{a1}		0.6049 ^{a1}	
	65311.28 ^{a2}		1.6499 ^{a2}		947.04 ^{a2}		0.6076 ^{a2}	
	68718.06 ^{r1}	13.7	2.29 ^{r1}	38.4			0.32 ^{r1}	
F ¹ Σ ⁺	63878.76 ^x	5.7	1.62 ^x	2.1	1934 ^x		0.63 ^x	4.1
	68395.44 ^{ab}	13.2	1.60 ^{ab}	3.3	1105 ^{ab}	18.2	0.64 ^{ab}	5.8
(1) ¹ Π	60679.12 ^{a1}		1.7500 ^{a1}		750.77 ^{a1}		0.5392 ^{a1}	
	58794.03 ^{a2}		1.8160 ^{a2}		491.22 ^{a2}		0.5010 ^{a2}	
A ¹ Π			1.644 ^g	6.1	813.5 ^g	8.3		
	43863 ⁿ	27.7	1.650 ⁿ	5.7	813 ⁿ	8.3		
	42835.4 ^b	29.4	1.6206 ^b	7.4	852.8 ^b	13.4		
	42961.96 ^{ad}	7.3	1.6229 ^{ad}		851.99 ^{ad}	0.63 ^{ad}		5.73 ^{ad}
	62668.94 ^{r1}	3.3	2.10 ^{r1}	20.0	803 ^{r1}	6.9	0.37 ^{r1}	
G ¹ Π	65169.24 ^x	7.4	1.59 ^x	9.1	733 ^x	2.4	0.66 ^x	22.4
	69443.96 ^y	14.4	1.62 ^y	7.4	863 ^y	14.9	0.63 ^y	16.8
(2) ³ Δ	65452.41 ^{a2}		2.2928 ^{a2}		444.52 ^{a2}		0.3143 ^{a2}	
(1) ³ Γ	65602.38 ^{a2}		2.3971 ^{a2}		583.8 ^{a2}		0.2878 ^{a2}	
(1) ¹ Γ	76322.36 ^{a2}		3.7182 ^{a2}		187.11 ^{a2}		0.1195 ^{a2}	
(3) ¹ Γ	82511.00 ^a		1.8508 ^{a2}		1338.96 ^{a2}		0.4829 ^{a2}	
			1.779 ^g	3.9	620.0 ^g			
(3) ³ Π	88538.96 ^{a1}		1.6667 ^{a1}		887.135 ^{a1}		0.5958 ^{a1}	
(2) ¹ Π	89827.23 ^{a1}		1.6592 ^{a1}		873.72 ^{a1}		0.6015 ^{a1}	
(1) ¹ Φ	96905.19 ^{a1}		1.6286 ^{a1}		1003.01 ^{a1}		0.6237 ^{a1}	
(2) ⁵ Π	113278.88 ^{a1}		2.1573 ^{a1}		484.12 ^{a1}		0.3554 ^{a1}	
(1) ⁵ Σ ⁻	122498.94 ^{a1}		2.5163 ^{a1}		340.09 ^{a1}		0.2612 ^{a1}	
(1) ⁵ Δ	123876.23 ^{a1}		2.9340 ^{a1}		148.81 ^{a1}		0.1922 ^{a1}	
(2) ⁵ Σ	132432.98 ^{a1}		2.6970 ^{a1}		128.29 ^{a1}		0.2254 ^{a1}	

^{a1}For present work with MRCI calculation; ^{a2}For present work with RSPT2 calculation; ^bRef.[10]; ^{c1}(experimental)Ref. [31]; ^{c2}(B3-LYP1)Ref.[31]; ^{c3}(B3-LYP2)Ref.[31]; ^{c4}(BP86)Ref.[31]; ^{c5}(MP2.1)Ref.[31]; ^{c6}(MP2.2)Ref.[31]; ^dRef.[32]; ^{e1}(MRCI+Q)Ref.[6]; ^{e2}(Fit)Ref.[6]; ^{f1}(SCF)Ref.[33]; ^{f2}(CI-SD)Ref.[33]; ^{f3}(CEPA-1)Ref.[33]; ^g(SCF+CI)Ref.[34]; ^{h1}(SCF)Ref.[35]; ^{h2}(MCSCF30)Ref.[35]; ^{h3}(MCSCF-CI)Ref.[35]SCF; ⁱ(exp)Ref.[36]; ^j(exp)Ref.[37]; ^k(exp)Ref.[38]; ^mRef.[39]; ⁿRef.[40]; ^pRef.[44]; ^{r1}Ref.[11]; ^{r2}Ref.[11]; ^{s1}Ref.[45]; ^{s2}Ref.[45]; ^tRef.[46]; ^uRef.[47]; ^vRef.[48]; ^wRef.[49]; ^xRef.[50]; ^yRef.[51]; ^zRef.[52]; ^qRef.[53]; ^{ab}Ref.[54]; ^{ac}Ref.[55]; ^{ad}Ref.[56]; N.B experimental value c1 (Ref.[31]) is in solid methane.

$$0.1\% \left(\text{Ref. [6]} \right) \leq \frac{\delta B_e}{B_e} \leq 2.0\% \left(\text{Refs. [10, 32, 44, 55]} \right).$$

The agreement becomes less by comparing our calculated value of ω_e with the experimental values of literature [10,32,36-38,44,55] where the relative difference $\frac{\delta\omega_e}{\omega_e} = 17.7\%$. One can notice that, the theoretical value of ω_e published in literature varies between 5.0 cm^{-1} and 8.0 cm^{-1} for the ground state [6,33-35]. The comparison of our calculated values by using the RSPT2 and MRCI techniques with those available in literature for the spectroscopic constants r_e , ω_e and B_e shows the average values

$$\left(\frac{\delta r_e}{r_e} = 0.97\% \right)_{\text{MRCI}}, \left(\frac{\delta r_e}{r_e} = 1.54\% \right)_{\text{RSPT2}},$$

$$\left(\frac{\delta\omega_e}{\omega_e} = 4.0\% \right)_{\text{MRCI}}, \left(\frac{\delta\omega_e}{\omega_e} = 3.0\% \right)_{\text{RSPT2}},$$

$$\left(\frac{\delta B_e}{B_e} = 1.33\% \right)_{\text{MRCI}}, \left(\frac{\delta B_e}{B_e} = 2.37\% \right)_{\text{RSPT2}}.$$

From these results one can find that, the RSPT2 technique may give better value for ω_e while MRCI technique gives better values for r_e and B_e for the ground state of the molecule SiO.

By comparing our calculated values of T_e for the states $(1)^3\Sigma^+$, $(1)^3\Sigma$, $(1)^3\Sigma^-$, $(1)^1\Sigma^-$, $(1)^1\Sigma$, $(2)^1\Sigma$ with those obtained experimentally in literature one can find an overall acceptable agreement with relative difference

$$8.9\% \leq \frac{\delta T_e}{T_e} \leq 11.8\% \text{ in Refs. [10,36] and larger relative difference for the states } (1)^3\Sigma^+, (2)^1\Sigma \text{ given in Refs. [33, 39,43] with relative difference } 13.2\% \leq \frac{\delta T_e}{T_e} \leq 19.1\%.$$

One can notice that, the comparison of our calculated value of T_e , for the considered electronic states, with those calculated in literature shows an excellent agreement by using one technique of calculation with

$$\frac{\delta T_e}{T_e} = 0.6\% \text{ (Ref. [11]) and disagreement by using another technique with } \frac{\delta T_e}{T_e} = 36\% \text{ (Ref. [11]) for the}$$

same state $(1)^1\Sigma$. Concerning the assignment of our calculated value of the $^1\Sigma$ state, it is in good agreement with the calculated values of $G^1\Sigma$ state [32,38] and acceptable agreement with the experimental value given in Ref. [39]. The comparison of our values of T_e with the newly published theoretical work by using the MRCI approach [56] shows an acceptable agreement for the 2 excited electronic states $(1)^3\Sigma^+$ and $(1)^1\Sigma^-$ with relative differences

11.9% and 8.2% respectively.

The comparison of our calculated values of r_e , ω_e , and B_e , for the excited states, with those given in literature experimentally [10,48,51,54] shows that, our values of r_e and B_e are in very good agreement for all the investigated states with

$$0.0\% \left(\text{Ref. [10]} \right) \leq \frac{\delta r_e}{r_e} \leq 7.4\% \left(\text{Ref. [51]} \right) \text{ and}$$

$$1.3\% \left(\text{Ref. [48]} \right) \leq \frac{\delta B_e}{B_e} \leq 2.3\% \left(\text{Ref. [48]} \right) \text{ except the}$$

value of B_e for the state G^1 where $\frac{\delta B_e}{B_e} = 16.8\%$. Our

values of ω_e are also in very good agreement with the experimental values for the electronic states with $T_e \leq 35434 \text{ cm}^{-1}$ and becomes larger for the other investigated electronic states with

$$14.9\% \left(\text{Ref. [51]} \right) \leq \frac{\delta\omega_e}{\omega_e} \leq 22.2\% \left(\text{Ref. [10]} \right).$$

Similarly, by comparing our calculated values of r_e , ω_e , and B_e with those calculated in literature, one can notice that an excellent agreement by using one technique of calculation with relative differences $\frac{\delta r_e}{r_e} = 0.1\%$ for the

state $(1)^3\Sigma^+$ (Ref. [40]), $\frac{\delta\omega_e}{\omega_e} = 2.2\%$ for the state $(1)^3\Sigma$

(Ref. [49]), and $\frac{\delta B_e}{B_e} = 0.5\%$ for the state $(1)^3\Sigma^-$ (Ref.

[50]) and disagreement by using another technique with

$$\frac{\delta r_e}{r_e} = 38.41\% \text{ for the state } (2)^1\Sigma^+ \text{ (Ref. [11]),}$$

$$\frac{\delta\omega_e}{\omega_e} = 26.0\% \text{ for the state } (1)^3\Sigma \text{ (Ref. [11]), and}$$

$$\frac{\delta B_e}{B_e} = 24.0\% \text{ for the state } (1)^1\Sigma \text{ (Ref. [11]). These discrepancies in the theoretical results can be referred to the}$$

basis used in this calculation, the number of valence electron, the software used, the bad assignment of a stateetc. While the comparison with the recent results of Ref. [56] for the 2 states $(1)^3\Sigma^+$ and $(1)^1\Sigma^-$ by using an approach similar to that we used in the present work shows an excellent agreement for the values of r_e and B_e and good agreement for ω_e . For the state $^1\Sigma$, there is an excellent agreement with the value of ω_e and good agreement with the values of r_e and B_e . The SiO molecule possesses sizable dipole moments of 3.0982 D [41]. Such magnitudes of the dipole moment should be sufficient for sustaining dipole-bound states (DBSs). Extensive experimental and computational studies [42,43] of an extra-electron attachment to a number of polar molecules

have shown the critical value of the dipole moment required to support a DBS to be 2.5 D. The electric dipole moment is also of great utility in the construction of molecular orbital based models of bonding and helping in the search for an understanding of the macroscopic properties of imperfect gases, liquids and solids. The expectation value of this operator is sensitive to the valence electrons and the general predictive quality of the computational methodology.

For the investigated electronic states, we calculated in the present work the permanent dipole $\mu(r)$ for $1.2 \text{ \AA} \leq r \leq 4 \text{ \AA}$ (Figures 4 and 5). Each time an adiabatic state loses its ionic character, it becomes again neutral and the corresponding dipole moment tends towards zero.

2.2. The Vibration-Rotation Calculation

Within the Born-Oppenheimer approximation, the vibra-

tion rotation motion of a diatomic molecule in a given electronic state is governed by the radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} (E_{vJ} - U(r)) - \frac{\lambda}{r^2} \right] \Psi_{vJ}(r) = 0 \quad (1)$$

where r is the internuclear distance, v and J are respectively the vibrational and rotational quantum numbers, $\lambda = J(J+1)$, E_{vJ} and Ψ_{vJ} are respectively the eigenvalue and the eigenfunction of this equation. In the perturbation theory these functions can be expanded as

$$E_{vJ} = \sum_{n=0} e_n \lambda^n \quad (2)$$

$$\Psi_{vJ}(r) = \sum_{n=0} \Phi_n(r) \lambda^n \quad (3)$$

with $e_0 = E_v$, $e_1 = B_v$, $e_2 = -D_v \dots$, ϕ_0 is the pure vibration

Figure 4. Permanent dipole moment curves of the lowest singlet and triplet and Δ -states of the molecule SiO.

Figure 5. Permanent dipole moment curves of the lowest singlet and triplet Σ and Δ -states of the molecule SiO.

wave function and ϕ_n its rotational corrections. By replacing Equations (2) and (3) into Equation (1) and since this equation is satisfied for any value of λ , one can write [24-26]

$$\phi_0''(r) + [e_0 - U(r)]\phi_0(r) = 0 \quad (4)$$

$$\phi_1''(r) + [e_0 - U(r)]\phi_1(r) = -[e_1 - R(r)]\phi_0(r) \quad (5-1)$$

$$\begin{aligned} \phi_2''(r) + [e_0 - U(r)]\phi_2(r) \\ = -[e_1 - R(r)]\phi_1(r) - e_2\phi_0(r) \end{aligned} \quad (5-2)$$

$$\begin{aligned} \phi_n''(r) + [e_0 - U(r)]\phi_n(r) \\ = R(r)\phi_{n-1} - \sum_{m=1}^n e_m \phi_{n-m}(r) \end{aligned} \quad (5-n)$$

where $R(r) = 1/r^2$, the first equation is the pure vibrational Schrödinger equation and the remaining equations are called the rotational Schrödinger equations. One may project Equations (7) onto ϕ_0 and find

$$\langle \phi_0 | \phi_0 \rangle e_1 = \langle \phi_0 | \frac{1}{r^2} | \phi_0 \rangle \quad (6-1)$$

$$\langle \phi_0 | \phi_0 \rangle e_2 = \langle \phi_0 | \frac{1}{r^2} | \phi_1 \rangle - e_1 \langle \phi_0 | \phi_1 \rangle \quad (6-2)$$

$$\langle \phi_0 | \phi_0 \rangle e_n = \langle \phi_0 | \frac{1}{r^2} | \phi_{n-1} \rangle - \sum_{m=1}^{n-1} e_m \langle \phi_{n-m} | \phi_0 \rangle \quad (6-n)$$

Once e_0 is calculated from Equation (4), $e_1, e_2, e_3, \dots$ can be obtained by using alternatively Equations (5) and (6). By using the canonical functions approach [24-26] and the cubic spline interpolation between each two consecutive points of the PECs obtained from the *ab initio* calculation of the SiO molecule, the eigenvalue E_v , the rotational constant B_v , the distortion constant D_v , and the abscissas of the turning point $r_{\min}$ and $r_{\max}$ have been calculated up to the vibration level $v = 52$. These values for the state $X^1\Sigma^+$, $(1)^1\Delta$, $(1)^3\Sigma$, $(1)^3\Pi$, $(2)^3\Pi$ and $(2)^1\Pi$ (as illustration) are given in **Table 2**. The comparison of our calculated values of E_v , B_v , $r_{\min}$ and $r_{\max}$ with the experimental data of Ref.[55] for the ground state $X^1\Sigma^+$ shows an excellent agreement for the 35 considered vibrational levels. Similar results are obtained by comparing our calculated values of B_v with the calculated Shi *et al.* [56] for the considered states.

Table 2. Values of E_v , B_v , D_v and $r_{\min}$ and $r_{\max}$ of the SiO molecule.

v	$X^1\Sigma^+$					$(1)^1\Delta$					$(1)^3\Delta$				
	E_v (cm ⁻¹)	$B_v \times 10$ (cm ⁻¹)	$D_v \times 10^7$ (cm ⁻¹)	$r_{\min}$ (Å)	$r_{\max}$ (Å)	E_v (cm ⁻¹)	$B_v \times 10$ (cm ⁻¹)	$D_v \times 10^7$ (cm ⁻¹)	$r_{\min}$ (Å)	$r_{\max}$ (Å)	E_v (cm ⁻¹)	$B_v \times 10$ (cm ⁻¹)	$D_v \times 10^7$ (cm ⁻¹)	$r_{\min}$ (Å)	$r_{\max}$ (Å)
0	633.9305* 619.3920**	7.10 7.242338	8.97	1.47494 1.4606053	1.5772 1.564163	482.1	5.56	8.81	1.664	1.789	422.8	5.56	10.4	1.660	1.788
1	1893.198 1849.0065	7.06 7.192007	8.96	1.44213 1.42765	1.61988 1.6076	1366.2	5.58	7.67	1.622	1.832	1232.0	5.52	9.83	1.621	1.842
2	3141.771 3066.7266	7.01 7.141723	8.95	1.42083 1.4063274	1.6511 1.6396929	2282.6	5.58	7.56	1.594	1.859	2043.9	5.48	10.5	1.595	1.882
3	4379.93 4272.5878	6.97 7.091488	8.93	1.40424 1.3897700	1.67767 1.6670194	3210.5	5.55	10.2	1.572	1.893	2843.2	5.44	8.70	1.575	1.914
4	5607.947 5466.6258	6.93 7.041300	8.88	1.39039 1.3759916	1.70143 1.6916551	4074.9	5.45	10.1	1.555	1.925	3652.0	5.41	9.37	1.558	1.942
5	6826.139 6648.8761	6.88 6.991159	8.89	1.3784 1.3640855	1.72348 1.7145082	4911.1	5.42	8.08	1.540	1.955	4459.1	5.39	9.42	1.544	1.968
6	8034.551 7819.3743	6.84 6.941067	8.85	1.36776 1.3535482	1.74435 1.7360834	5755.1	5.43	5.90	1.527	1.973	5260.6	5.33	10.4	1.531	1.995
7	9233.604 8978.156	6.80 6.891022	8.58	1.35817 1.3440662	1.76367 1.7566958	6620.5	5.42	7.36	1.515	1.991	6048.5	5.30	10.2	1.519	2.019
8	10426.17 10125.257	6.76 6.841025	8.28	1.34938 1.335287	1.78219 1.7765575	7491.5	5.41	9.27	1.504	2.018	6826.6	5.25	8.72	1.509	2.044
9	11614.53 11260.712	6.73 6.791076	8.19	1.34125 1.327486	1.80026 1.7958198	8350.0	5.34	10.1	1.494	2.035	7601.8	5.21	10.2	1.499	2.067
10	12799.35 12384.558	6.70 6.741174	7.56	1.33367 1.3201275	1.81658 1.8145948	9183.0	5.31	6.32	1.485	2.052	8367.3	5.18	8.73	1.490	2.091
11	13985.65 13496.83	6.68 6.691321	6.67	1.32653 1.3132685	1.83127 1.8329686	10024.6	5.31	8.76	1.476	2.077	9130.4	5.15	7.02	1.482	2.111
12	15179.54 14597.563	6.66 6.641515		1.31974 1.3068427	1.84522 1.8510092	10854.9	5.20	10.9	1.468	2.101	9898.8	5.14	6.67	1.474	2.126

Continued

13	16376.97 15686.793	6.64 6.591756	6.90	1.31328 1.3007972	1.85926 1.8687714	11623.8	5.10	7.34	1.461	2.123	10675.0	5.14	6.24	1.467	2.141
14	17564.86 16764.556	6.59 6.542046	8.35	1.30717 1.2950884	1.87471 1.8862999	12392.8	5.13	5.26	1.454	2.146	11457.1	5.11	11.1	1.459	2.164
15	18729.64 17830.887	6.51 6.492383	10.2	1.30145 1.2896807	1.89247 1.9036325	13170.2	5.06	10.6	1.447	2.168	12221.1	5.02	17.1	1.453	2.187
16	19863.12 18885.821	6.44 6.442768	11.6	1.29612 1.2845439	1.90996 1.920801	13915.0	5.00	7.12	1.441	2.189	12946.6	4.94	9.50	1.447	2.207
17	20969.76 19929.395	6.38 6.3932	11.3	1.2911 1.2796526	1.92678 1.9378326	14659.1	4.99	9.25	1.435	2.210	13663.4	4.93	4.39	1.441	2.228
18	22064.93 20961.645	6.34 6.343681	8.96	1.28632 1.2749849	1.94447 1.954751	15395.5	4.92	10.1	1.430	2.231	14389.7	4.90	12.8	1.435	2.249
19	23154.06 21982.604	6.30 6.294209		1.28172 1.2705220	1.96044 1.9715771	16118.8	4.89	8.64	1.425	2.252	15098.4	4.83	11.1	1.430	2.270
20	24234.74 22992.31	6.27 6.244785	8.05	1.2773 1.2662473	1.97363 1.9883291	16836.7	485	9.91	1.419	2.272	15794.0	4.80	6.02	1.425	2.290
21	25315.7 23990.798	6.25 6.195408	8.66	1.27302 1.2621465	1.98686 2.0050237	17544.8	4.81	8.87	1.415	2.292	16491.2	4.77	11.6	1.420	2.310
22	26398.66 24978.102	6.22 6.14608	6.90	1.26886 1.2582069	2.00346 2.0216754	18246.1	4.77	9.82	1.410	2.312	17176.0	4.72	9.20	1.415	2.330
23	27464.85 25954.26	6.15 6.096799	6.28	1.26487 1.254417	2.02082 2.0382979	18939.0	4.73	9.20	1.406	2.332	17853.6	4.69	8.03	1.411	2.350
24	28503.02 26919.306	6.08 6.047566	10.0	1.2611 1.2507669	2.0345 2.0549033	19624.4	4.69	8.90	1.401	2.352	18526.7	4.65	10.1	1.406	2.370
25	29530.92 27873.277	6.06 5.99838	12.7	1.25746 1.2472474	2.0478 2.0715029	20302.9	4.66	9.37	1.397	2.372	19191.0	4.62	8.71	1.402	2.389
26	30563.92 28816.207	6.04 5.949243	8.91	1.25389 1.2438503	2.06412 2.0881073	20974.0	4.62	9.34	1.393	2.391	19849.8	4.58	9.20	1.398	2.409
27	31582.14 29748.132	5.95 5.900153	5.12	1.25045 1.2405603	2.08297 2.1047262	21637.9	4.58	8.83	1.389	2.411	20501.7	4.54	8.40	1.394	2.428
28	32558.73 30669.088	5.84 5.851111	9.66	1.24723 1.2373947	2.10038 2.1213687	22295.2	4.55	8.87	1.385	2.430	21148.1	4.51	9.21	1.390	2.447
29	33508.62 31579.111	5.80 5.802116	16.7	1.24416 1.2343233	2.11734 2.1380435	22945.8	4.51	8.98	1.382	2.450	21788.2	4.48	8.77	1.387	2.466
30	34457.86 32478.235	5.77 5.753169	13.3	1.24116 1.2313484	2.13487 2.1547588	23590.2	4.48	8.54	1.378	2.469	22422.4	4.44	8.45	1.383	2.485
31	35394.39 33366.498	5.70 5.704270	5.98	1.23825 1.2284650	2.15252 2.1715224	24229.3	4.45	7.09	1.375	2.490	23051.1	4.41	8.32	1.380	2.504
32	36308.34 34243.933	5.63 5.655419	9.95	1.23547 1.2256683	2.17001 2.1883416	24866.1	4.43	5.56	1.372	2.506	23674.5	4.38	8.83	1.376	2.523
33	37209.82 35110.577	5.59 5.606616	13.0	1.23277 1.2229539	2.18763 2.2052239	25504.3	4.42	4.20	1.368	2.518	24292.2	4.34	8.58	1.373	2.542
34	38099.68 35966.466	5.53 5.55786	9.68	1.23016 1.2203178	2.20541 2.2221760	26147.4	4.42	4.69	1.365	2.532	24904.2	4.31	8.51	1.370	2.560
35	38973.71 36811.635	5.48 5.509152	9.69	1.22763 1.2177562	2.22325 2.2392048	26793.2	4.40	9.08	1.362	2.552	25510.3	4.27	8.73	1.367	2.579
36	38100	5.53	11.3	1.230	2.205	27430.7	4.34	10.6	1.359	2.572	26110.0	4.24	9.57	1.364	2.598
37	38974	5.48	10.4	1.228	2.223	28046.1	4.25	1.42	1.356	2.591	26702.2	4.20	10.1	1.361	2.618
38	39834	5.42	10.5	1.225	2.241	28644.7	4.22	3.26	1.353	2.609	27285.6	4.15	10.6	1.358	2.638
39	40682	5.37	10.9	1.223	2.259	29247.1	4.23	4.92	1.350	2.628	27858.8	4.10	11.7	1.355	2.659
40	41515	5.31	10.6	1.220	2.277	29850.0	4.18	10.3	1.348	2.648	28419.6	4.04		1.353	2.682
41	42335	5.26	10.9	1.218	2.296	30438.3	4.12	9.22	1.345	2.666	28964.6	3.97		1.350	2.707

Continued

42	43142	5.20	10.9	1.216	2.315	31019.3	4.11	4.67	1.342	2.685	29488.0	3.87		1.348	2.735
43	43935	5.15	11.1	1.214	2.334	31600.6	4.08	10.0	1.340	2.704	29979.2	3.72		1.346	2.771
44	44714	5.09	11.1	1.212	2.353	32173.2	4.04	8.83	1.337	2.723	30415.2	3.45		1.344	2.828
45	45480	5.03	11.4	1.210	2.372	32739.0	4.01	6.34	1.335	2.742	30756.4	3.00		1.342	2.922
46	46231	4.97	11.5	1.208	2.392	33302.0	3.98	9.57	1.333	2.761					
47	46969	4.91	11.7	1.206	2.412	33858.0	3.95	7.67	1.330	2.779					
48	47692	4.85		1.204	2.432	34409.1	3.92	7.37	1.328	2.798					
49	48400	4.79		1.203	2.453	34956.0	3.89	7.90	1.326	2.817					
50	49093	4.73		1.201	2.475	35497.9	3.87	6.76	1.324	2.836					
51	49770	4.66		1.199	2.497										
52	50432	4.60		1.198	2.519										
			(1) ³					(2) ³					(2) ¹		
0	263.3	5.17	20.6	1.707	1.868	440.6	5.93	10.0	1.610	1.731	444.7	5.99	9.90	1.601	1.721
1	775.3	5.08	18.3	1.662	1.938						1374.6	5.96	8.90	1.564	1.769
2	1290.2	5.01	20.1	1.635	1.995						2322.9	5.94	8.95	1.539	1.804
3	1787.5	4.89	21.6	1.614	2.047										
4	2264.3	4.81	16.5	1.598	2.097										
5	2740.5	4.74	17.6	1.584	2.130										
6	3211.3	4.68	19.6	1.572	2.175										
7	3666.0	4.53	31.6	1.561	2.222										
8	4082.1	4.41	1.68	1.552	2.267										

*First entry for the present work; **Second entry Refs. [51,54].

3. Conclusion

In the present work, the *ab initio* investigation for the 20 low-lying singlet and triplet electronic states of the SiO molecule has been performed via CAS-SCF/MRCI method. The potential energy and the dipole moment curves have been determined along with the spectroscopic constants T_e , r_e , ω_e , $\omega_e x_e$ and the rotational constant B_e for the lowest-lying electronic states. The comparison of our results, for the ground and excited states, with those obtained experimentally in literature shows an overall very good agreement, while the agreement with the theoretical data depends on the technique of calculation. By using the canonical functions approach [24-26], the eigenvalue E_v , the rotational constant B_v , and the abscissas of the turning points $r_{\min}$ and $r_{\max}$ have been calculated up to the vibrational level $v = 52$ with an excellent agreement by comparing with the available results in literature. Eight electronic states have been investigated in the present

work for the first time. These newly obtained results maybe confirmed by the investigation of new experimental works on this molecule.

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