Dipole Moment and Electronic Structure Calculations of the Electronic States of the Molecule SiC below 97000cm^{-1}

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Abstract

Beside its importance in the astrophysics, the silicon carbide has a great importance in the industry of semiconductors and ceramics. Because of the absence of theoretical data, extensive *ab initio* calculations of dipole moment and higher excited electronic state have been done for this molecule. These calculations have been performed by using the Complete Active Space Self Consistent Field (CASSCF) with Multireference Configuration Interaction MRCI+Q (singly and doubly excitation with Davidson corrections). The potential energy and the dipole moment curves for the 47 low-lying singlet, triplet and quintet electronic states in the representation $^{2s+1}\Lambda^{(+/-)}$ of the molecule SiC have been calculated. The harmonic frequency ω_e, the internuclear distance R_e, the electronic energy with respect to the ground state T_e, the rotational constants B_e and the permanent dipole moment have been obtained for these electronic states. The comparison between the values of the present work and those available in the literature, for several electronic states, shows a good agreement. In the present work thirteen new electronic states have been investigated here for the first time. These new results may leads to more investigation of new experimental works on this molecule.

Keywords: *ab initio* calculation, permanent dipole moments, electronic structure, spectroscopic constants, potential energy curves

1. Introduction

Since the SiC is an elusive molecule, its experimental detection is extremely difficult in a high temperature in thermodynamic equilibrium. But this problem can be solved by sputtering the SiC in a hollow discharge lamp. By using this technique Bernath et al. (Bernath et al., 1988) detected for the first time the $d^1\Sigma^+$ - $b^1\Pi$ electronic transition. By measuring the millimeter-wave spectrum Cernicharo et al. (Cernicharo et al., 1989) reported detailed study of the ground state $X^3\Pi$ of the molecule SiC. A rovibrational measurement of of the ground state has been done by Mollaaghababa et al. (Mollaaghababa et al., 1990). The $A^3\Sigma^-$-X^3P and $C^3\Pi$-$X^3\Pi$ electronic transition have been detected respectively by Brazier et al. (Brazier et al., 1989) and Ebben et al. (Ebben et al., 1991). From the electronic transition $C^3\Pi$-$X^3\Pi$, the spectroscopic constants of these electronic states have been measured by Butenhoff et al. (Butenhoff et al., 1991). Bauschliecher and Langhoff (Bauschlicher JR, & Langhoff (1987) have reported the spectroscopic parameters for the $^3\Pi$ ground state of SiC molecule along with the $A^3\Sigma^-$ states which is nearly 4000 cm^{-1} above the $X^3\Pi$ ground state. Furthermore, the spectroscopic properties for the three lowest lying electronic states $X^3\Pi$, $A^3\Sigma^-$ and $a^1\Sigma^+$ of the diatomic SiC molecule have been computed based on an augmented coupled cluster and different basis sets methods by (Martin, Francois, & Gijbels, 1990).

The absence of theoretical dipole moment calculation and the electronic structure investigation for higher excited electronic states (up to 97000cm^{-1}) of the silicon carbide molecule SiC stimulates us to investigate, in the present work, more extensive *ab initio* calculation for this molecule. These theoretical calculations, in the present-days, are quite capable of producing, with high accuracy, the required data if they are judiciously applied. The potential energy curves and the spectroscopic constants of the low lying 47 singlet, triplet and quintet electronic states have been calculated where 13 electronic states have been investigated here for the first time. The transition energy with respect to the minimum energy for the ground state T_e, the equilibrium internuclear distance R_e, the harmonic frequency ω_e, and the rotational constant B_e have been calculated in order they can be assigned for experimental electronic transitions that have not been observed yet for the SiC molecule. Since the dipole moment curves are the important ingredients that may help to obtain accurate predictions of the transition

dipoles moments and hence the transition lines intensities the permanent dipole moment have been calculated for the considered electronic states of this molecule.

2. Method

In the present work we investigated the low-lying singlet, triplet and quintet electronic states of the molecule SiC using Complete Active Space Self Consistent Field (CASSCF) procedure followed by a multireference configuration interaction (MRCI+Q with Davidson correction) treatment for the electron correlation. The entire CASSCF configuration space was used as the reference in the MRCI calculations, which were done via the computational chemistry program MOLPRO (MOLPRO package) taking advantage of the graphical user interface GABEDIT (Allouche, 2011). The silicon species is treated as a system of 14 electrons by using the Ahlirchs-PVDZ; c basis set for s, p, and d functions. The 6 electrons of the carbon atom are considered using the aug-cc-pVTZ; c basis set for s, p and d functions. Among the 20 electrons explicitly considered for SiC molecule 7 valence electrons were explicitly treated, corresponding to 15 active orbitals. Being an heteronuclear diatomic molecule, SiC is of $C_{\infty v}$ point group symmetry; however, MOLPRO software can only make use of Abelian point groups which means that $C_{\infty v}$ will be treated using the C_{2v} point group placing the molecule along the + z-axis and keeping Si at the origin.

3. Results

3.1 potential energy curves and spectroscopic constants

The potential energy curves (PECs) for the 47 singlet, triplet and quintet electronic states, in the representation $^{2s+1}\Lambda^{(\pm)}$, of the molecule SiC were generated using the MRCI+Q for 96 internuclear distances calculations in the range $1.1\text{Å} \leq R_e \leq 4.1\text{Å}$ (Figure 1-6).
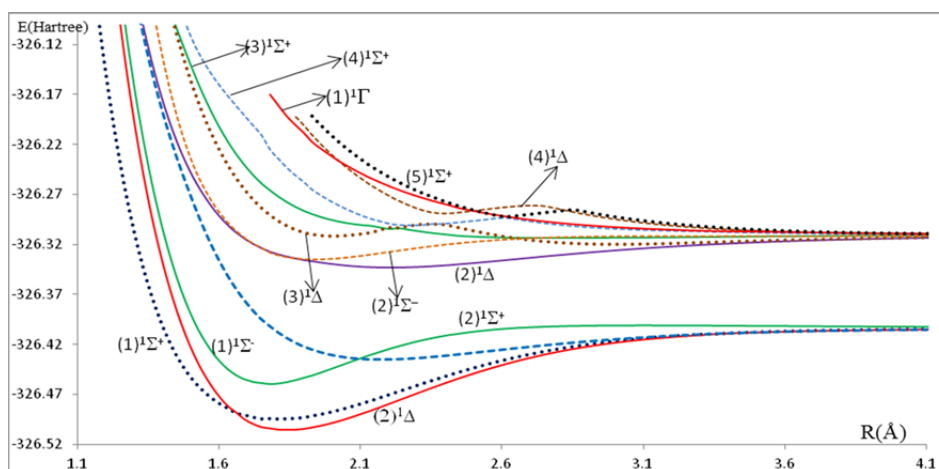

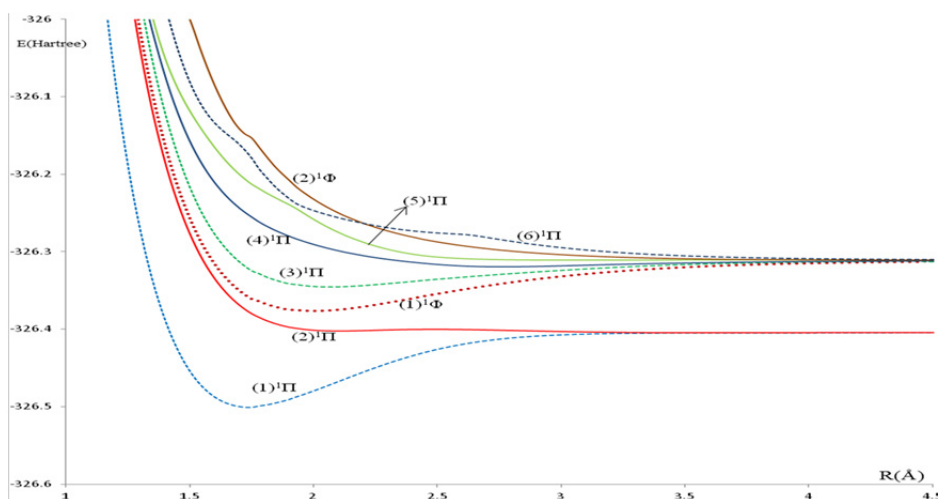Figure 1. Potential energy curves of the $^1\Sigma^{\pm}$ an $^1\Delta$ states of the molecule SiC

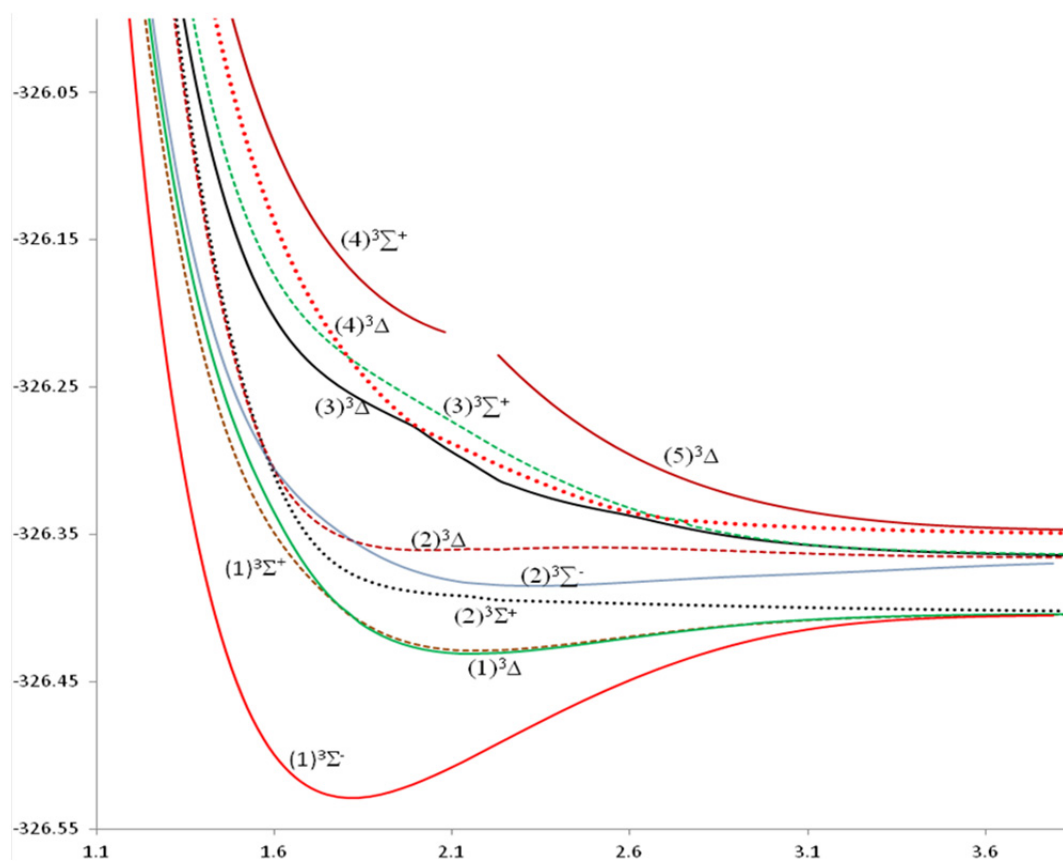Figure 2. Potential energy curves of the $^1\Pi$ ανδ $^1\Phi$ states of the molecule SiC

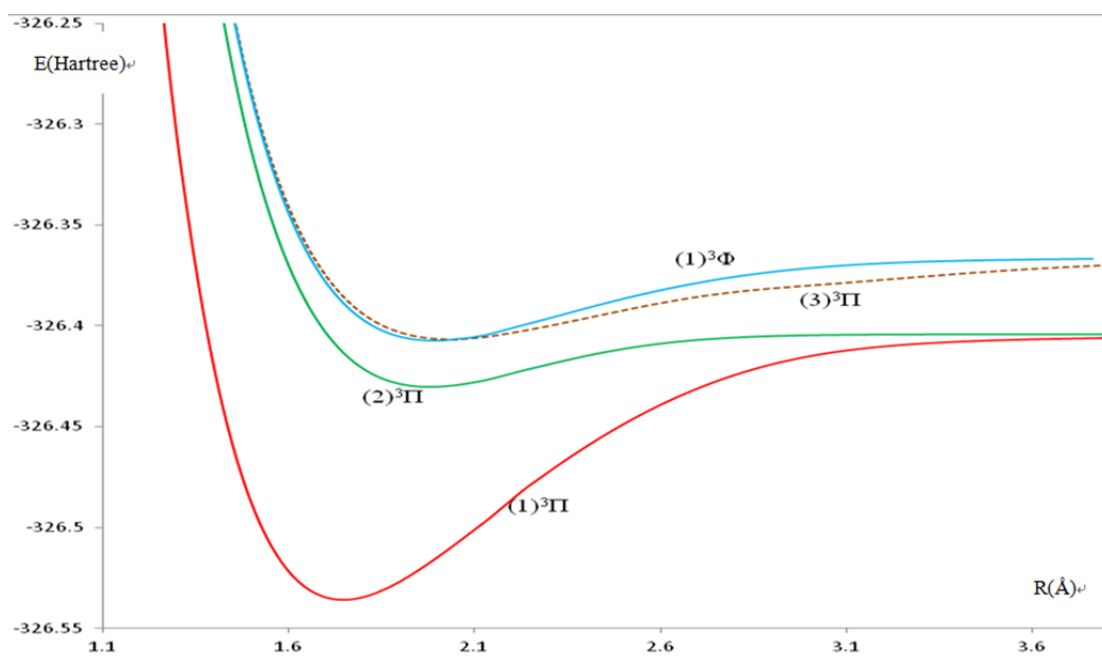Figure 3. Potential energy curves of the $^3\Sigma^\pm$ an $^3\Delta$ states of the molecule SiC

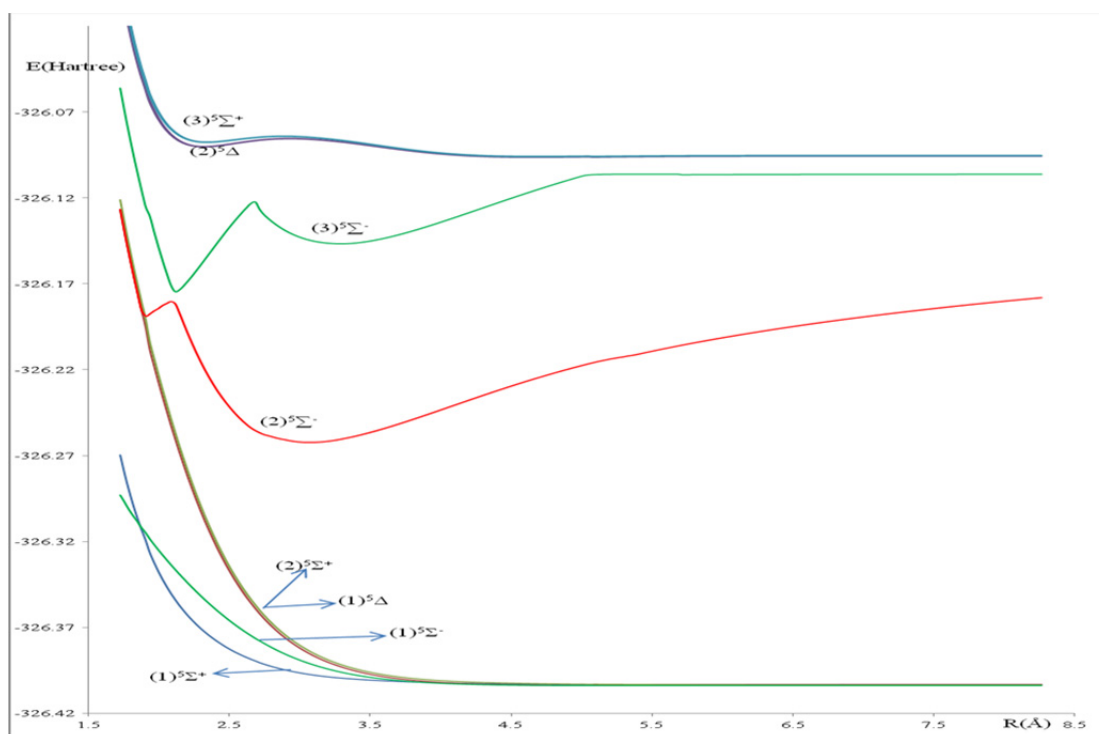Figure 4. Potential energy curves of the $^3\Pi$ and $^3\Phi$ states of the molecule SiC

Figure 5. Potential energy curves of the $^5\Sigma^\pm$ an $^5\Delta$ states of the molecule SiC
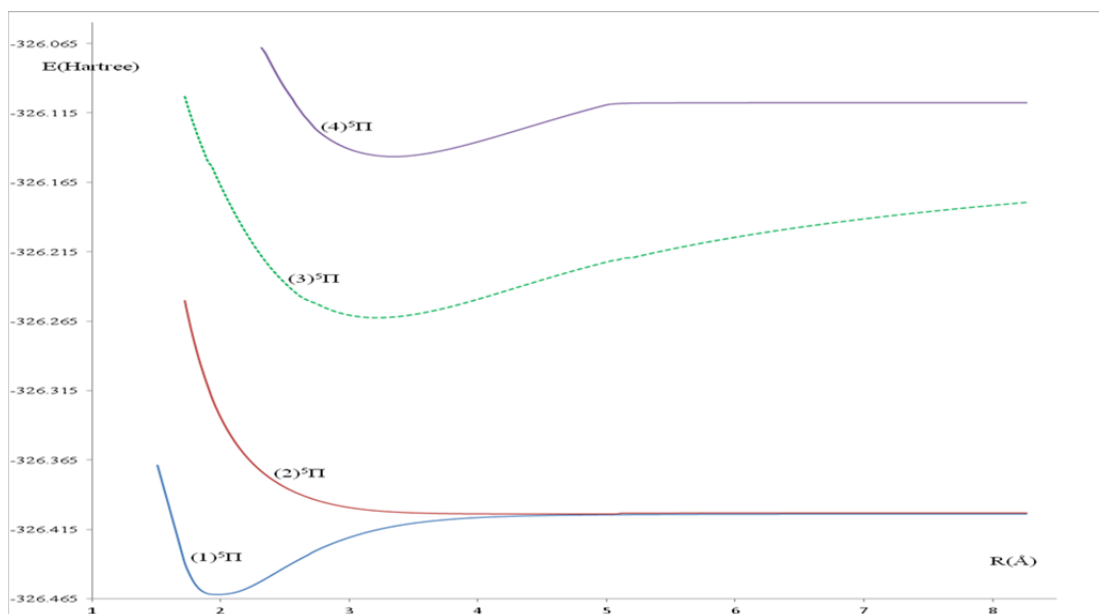
Figure 6. Potential energy curves of the $^5\Pi$ states of the molecule SiC

By fitting the calculated energy values of the different investigated electronic states, into a polynomial in R around the internuclear distance at equilibrium R_e, the harmonic vibrational frequencies ω_e, the relative energy separations T_e, and the rotational constants B_e have been calculated. These values with the available data in literature are given in Table 1.

Table 1. Spectroscopic constants of the silicon carbide molecule SciC

States	T_e (cm^{-1})	ω_e (cm^{-1})	B_e (cm^{-1})	$\alpha_e \times 10^3$	R_e (Å)
$(X)^3\Pi$	0	946.6	0.655	5.502	1.749
		927[a3]			1.722[a6]
		981[b1]	0.679[b1]	6.23[b1]	1.715[b1]
		984[b2]	0.681[b2]	6.24[b2]	1.713[b2]
		979[b3]	0.676[b3]	6.22[b3]	1.719[b3]
		976[b4]	0.676[b4]	6.22[b4]	1.720[b4]
		1033[c1]			1.709[c1]
		958[c2]			1.726[c2]
		947[c3]			1.732[c3]
		934[c4]			1.737[c4]
		923[c5]			1.741[c5]
		906[c6]			1.705[c6]
		917[c7]			1.701[c7]
		944[c8]			1.738[c8]
		1035[c9]			1.709[c9]
		963[c10]			1.726[c10]
		954[c11]			1.730[c11]
		937[c12]			1.737[c12]
		925[c13]			1.741[c13]
		979[d]	0.67502[d]	5.63[d]	
		914[e]			1.75[e]
		965.16[f1]	0.67976[f1]	5.38[f1]	1.7182[f1]
		964.6[f2]			
		954.2[f3]	0.6692[f3]	5.7[f3]	1.732[f3]
		930[g]			1.72[g]
		954[h]			1.726[h]
$(1)^3$	3380	857.1	0.605	5. 358	1.820
	3619[a2].	835[a6]			1.802[a3]
	2076[c1]	904[c1]			1.796[c1]
	3191[c2]	875[2]			1.81^0[c2]
	3909[c3]	870[c3]			1.812[c3]
	2025[c9]	910[c9]			1.798[c9]
	3072[c10]	881[c10]			1.811[c10]
	3798[c11]	877[c11]			1.813[c11]
	3742[c12]	865[c12]			1.82[c12]
	3781[c13]	848[c13]			1.823[c13]
	3831[d]	855[d]	0.60968[d]	5.17[d]	
	5242.3[e]	960[e]			1.82[e]
	4597.5[g]	826[g]			1.82[g]
	3883[h]	860[h]			1.811[h]
$(1)^1$ $^+$	6740	1004.7	0.614		1.805
	5079[a2]	835[a3]			1.802[a3]
	4355[d2]	1053[d2]	0.72299[d2]	0.602[d2]	
	6855.845[b]	1202[e]	0.70977[d]		1.688[d]
	4968[h]	1023[h]			1.656[h]
$(1)^1\Pi$	7679	901.9	0.666	0.793	1.734
	7259[a7]	963[a5]			1.728[a5]
	7662.3[e]	950[e]			1.75[c]
	7661.715[e]	960[e]			1.82[b]
	7027[h]	942[h]			1.741[h]
$(1)^1\Delta$	9008	705.9	0.592	0.379	1.840

	$9094^{(a4)}$	$821^{(a6)}$			$1.821^{(a6)}$
	$10889^{(e)}$	$1202^{(e)}$			$1.68^{(e)}$
	$8397^{(h)}$	$814^{(h)}$			$1.834^{(h)}$
$(1)^3$	15000	450.7	0.424	1.460	2.128
$(2)^1{}^+$	13691	953.9	0.635	0.727	1.776
	$12338^{(a1)}$				$1.794^{(a5)}$
	$12603^{(h)}$	$979^{(h)}$			$1.808^{(h)}$
$(1)^5$	16240	229.9	0.492		1.982
	$16095^{(h)}$	659			1.942
$(2)^3\Pi$	21834	433.4	0.502	4.820	1.995
	22830.4^f	615	0.5450^f	0.12	1.919^f
	$22768^{(h)}$	$594^{(h)}$			$1.911^{(h)}$
$(1)^1{}^-$	22165	446.7	0.424	0.767	2.174
	$24703^{(h)}$	$503^{(h)}$			$2.130^{(h)}$
$(1)^3\Delta$	22975	463.9	0.430	7.960	2.158
	$25489^{(h)}$	$459^{(h)}$			$2.133^{(h)}$
$(1)^3{}^+$	23471	439.3	0.426	7.990	2.168
	$19658^{(h)}$	$1050^{(h)}$			$1.652^{(h)}$
$(3)^3\Pi$	28387	537.7	0.488	9.330	2.025
	$22830.4^{(f1)}$	$615.72^{(f1)}$	$0.5450^{(f1)}$	$6.6^{(f1)}$	$1.919^{(f1)}$
	$22829.46^{(f2)}$	$618.85^{(f2)}$	$0.5474^{(f2)}$	$1.98^{(f2)}$	$1.908^{(f2)}$
	$22768^{(f3)}$	$615.8^{(f3)}$	$0.5511^{(f3)}$	$0.12^{(f3)}$	$1.914^{(f3)}$
	$27080^{(h)}$	$553^{(h)}$			$1.929^{(h)}$
$(2)^1\Pi$	29342	349.6	0.453	2.061	2.103
	$28904^{(h)}$	$540^{(h)}$			$1.963^{(h)}$
$(2)^3{}^-$	33090	325. 8	0.367	1.066	2.330
	$35419^{(h)}$	$385^{(h)}$			$2.218^{(h)}$
$(1)^1$	35061	481.4	0.499	12.210	2.003
$(3)^1\Pi$	41852.0	464.3	0.468	0.580	2.069
$(2)^1\Delta$	42286.4	358.4	0.411	0.536	2.206
$(4)^1\Pi$	47535.7	249.3	0.263	0.645	2.763
	49197.7	621.3	0.496	0.189	2.008
$(5)^1\Pi$	49383.0	2552.9	0.291	0.369	3.075
	60020	248.0	0.194		3.216
	60068	280.0	0.213		3.068
	79329	1733.0	0.441		2.132
$(4)^5$	85471	275.0	0.178		3.352
$(2)^5$ (1st minimum)	97829	407.4	0.374		2.313
(2nd minimum)	96504	114.4	0.907		4.646
$(3)^5{}^+$ (1st minimum)	98364	331.0	0.365		2.341
(2nd minimum)	96533	13.4	0.091		4.713

(a) Bernath et al.: [a1]2MC-ScF+SD, [a2]MR-SOCI, [a3]Davidson correction- MR-SOCI, [a4]HF-SD

   Transition $^1\Delta$-$^3\Sigma^-$, $^1\Pi$-$^3\Pi$, [a5]Davidson correction- 2MC-ScF+SD, [a6]Davidson correction-HF-SD,

(b) Midda et al.: [b1]basis set 6-311G (2df, 2pd), [b2] basis set 6-311G (3df, 3pd), [b3] basis set cc-pVTZ,

   [b4]basis set aug-cc-pVTZ

(c) Bauschlicher, Jr. & Langhoff: [c1]SDCI, [c2]SOCI+Q, [c3]CPF, [c4]MRCI, [c5]MRCI+Q, [c6]MP4 (SDQ)b,

   [c7]MP4 (SDTQ) b, [c8]CClb, [5s4p2d If /4s3p2d If] basis, [c9]SOCI , [c10]SDCI+Q1, [c11]CPF, [c12]MRCI,

   [C13]MRCI+Q

(d) Martin et al.: [d1]QCISD(T)IMC-31IG(2dj), [d2]QCISD(T)IMC-311G(d).

[e]Bruna et al.

[f1]Butenhoff & Rohlfing, [f2]Ebben et al., [f3]Larsson

[g]Andzeim et al.

[h]Borin et al.

The comparison of our calculated values of T_e with those obtained experimentally (Bernath et al. & Ebben et al.) for the electronic states $(1)^1\Delta$ and $(2)^3\Pi$ showed a very good agreement with the relative differences 0.95% and 4.56% respectively. While our calculated value of T_e for the electronic state $(3)^3\Pi$ is larger than those given by (Butenhoff & Rohlfing, Larsson, & Ebben et al.). The different theoretical techniques for the calculation of T_e have large influence on the investigated data for the different excited electronic states. For example, for the electronic state $(1)^3\Sigma^-$ one can find that the calculated values of T_e are 2076 cm^{-1} (Bauschlicher, Jr. and Langhoff/SDCI) and 5242 cm^{-1} (Bruna et al.). Similar results can be found for other excited electronic states. Concerning our calculated values of T_e, they are in good agreement with experimental values and with some theoretical data with the relative differences $\Delta T_e/T_e$= 1.07% $((1)^3\Sigma^-$, Bauschlicher, Jr. and Langhoff/MRCI), $\Delta T_e/T_e$= 1.71% $((1)^1\Sigma^+$, Bruna et al.), $\Delta T_e/T_e$= 0.22% $((1)^1\Pi$, Bruna et al.), $\Delta T_e/T_e$= 0.95% $((1)^1\Delta$, Bernath et al./Transition $^1\Delta$-$^3\Sigma^-$). By comparing our calculated values of T_e with those given by Borin et al., one can find the good agreement with the relative differences 1.4%, 1.49%, 7.04%, 4.6%, 10.9% for the electronic states $(1)^1\Sigma^-$, $(2)^1\Pi$, $(2)^3\Sigma^-$, $(2)^3\Pi$ and $(1)^3\Delta$ respectively. This relative difference becomes larger for the states $(2)^1\Sigma^+$, $(1)^5\Pi$, $(1)^3\Sigma^-$. There is no comparison for the other states since they are given here for the first time.

By comparing our investigated spectroscopic constants for the ground state with those obtained experimentally, one can find a very good agreement with the relative differences $\Delta\omega_e/\omega_e$= 1.6% (Ebben et al.), $\Delta\omega_e/\omega_e$=0.8% (Larsson), $\Delta B_e/B_e$= 3.1%, (Ebben et al.) $\Delta B_e/B_e$= 3.8% (Larsson), $\Delta\alpha_e/\alpha_e$= 1.8% (Ebben et al.), $\Delta\alpha_e/\alpha_e$=0.97% (Larsson) and $\Delta R_e/R_e$= 1.76%, (Ebben et al.), $\Delta R_e/R_e$= 0.97% (Larsson). Also good agreements are obtained by comparing our calculated values of these constants with the experimental data (Ebben et al. & Larsson) for the electronic state $(2)^3\Pi$. The agreement becomes less by comparing our investigated data for the electronic state $(3)^3\Pi$ with the experimental values (Ebben et al. & Larsson). In literature the spectroscopic constants for the molecule SiC have been calculated for different electronic states by different techniques. One can notice the good agreement between these different values for the ground and the first excited state. By comparing our calculated values of these constants for these electronic states with the theoretical data in literature we obtained the very good agreement with the relative differences 0.02%$\leq\Delta\omega_e/\omega_e\leq$12%, 0.77%$\leq\Delta B_e/B_e\leq$3.97%, 2.2%$\leq\Delta\alpha_e/\alpha_e\leq$13.23%, 0.0%$\leq\Delta R_e/R_e\leq$2.29%. While the theoretical investigated values for the spectroscopic constants ω_e depends in the different theoretical techniques of calculation in order one can find a large discrepancy between these values. Concerning our calculated values of this constants, they are in very good agreement with theoretical values with the relative differences 1.82%, 4.46%, 2.63%, 1.06%, 2.84% for the electronic states $(1)^1\Sigma^+$, $(1)^1\Pi$, $(2)^1\Sigma^+$, $(1)^3\Delta$, $(2)^3\Pi$ respectively given by Borin et al. The calculated values of B_e in the present work are in good agreement either with the theoretical values (Bruna et al.) for the electronic states $(1)^1\Sigma^+$ or experimental data (Butenhoff and Rohlfing) for the 2 electronic states $(2)^3\Pi$ and $(3)^3\Pi$. Our calculated values of the internuclear distance R_e are in very good agreement with those given in literature either theoretical or experimental except the investigated values for the electronic states $(1)^1\Sigma^-$, $(1)^3\Delta$, and $(1)^3\Sigma^+$.

3.2 Permanent Dipole Moment

The importance of the calculation of the permanent dipole moment (PMD), which is a fundamental electrostatic property of a neutral molecule, is lying in the description of numerous physical phenomena and in the accurate predictions of transition dipoles and hence intensities. The values of the expectation value of the dipole moment operator depend on the nature of the least energetic and most chemically relevant valence electrons. The calculation of the permanent dipole moment in term of the internuclear distance R have been done by taking the Sc atom at the origin and the carbon atom along the internuclear Z-axis (Figure 7-10).
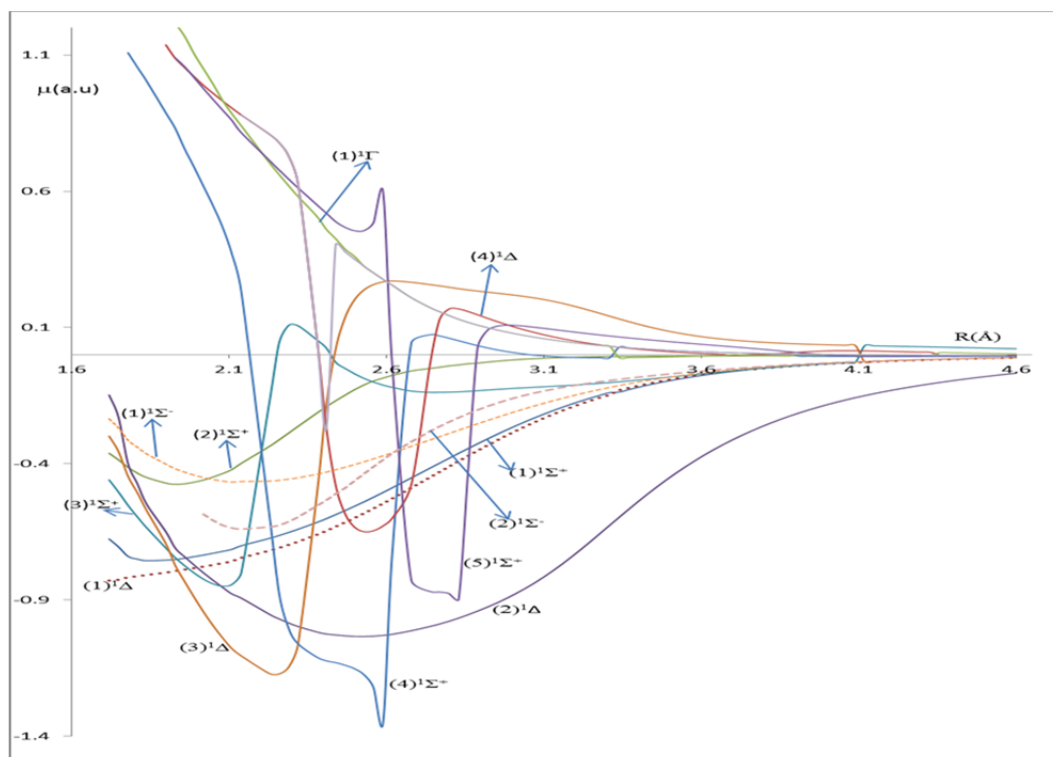
Figure 7. Permanent dipole cuves of the electronic states $^1\Sigma^\pm$, $^1\Delta$ and $^1\Gamma$ of the molecule SiC
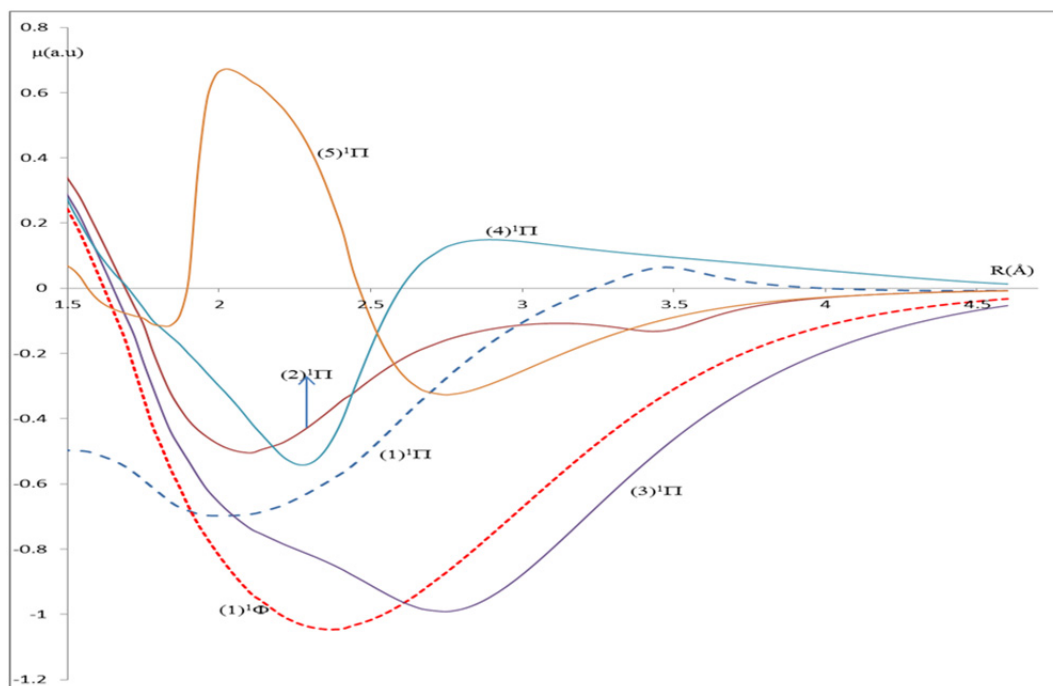

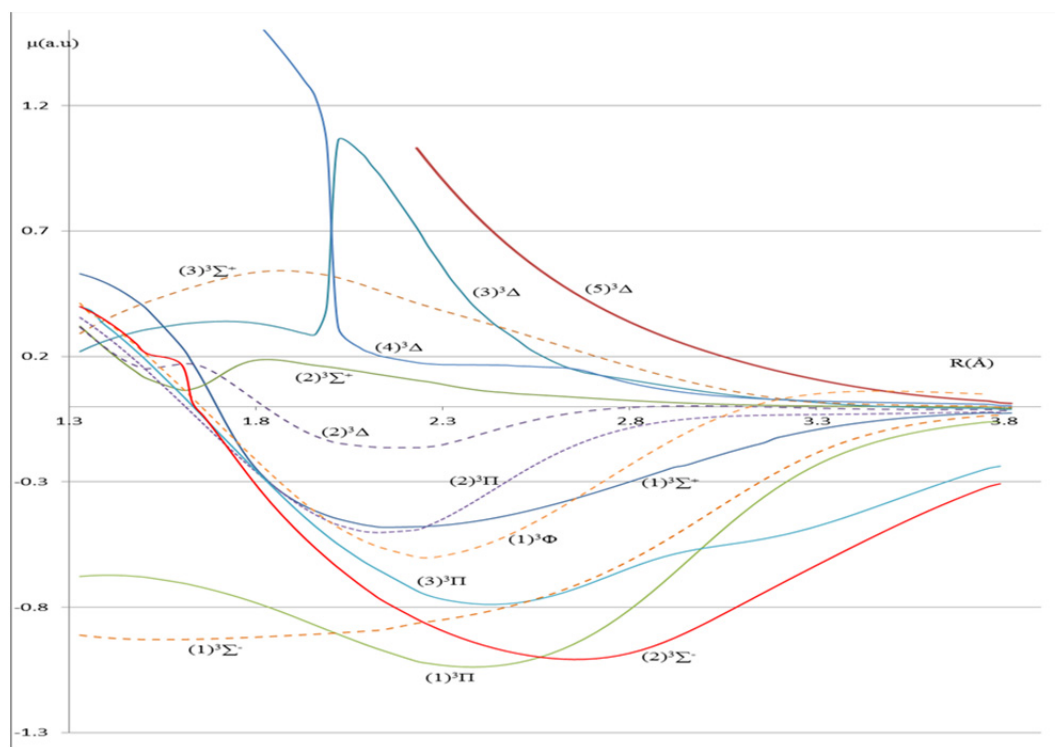Figure 8. Permanent dipole cuves of the electronic states $^1\Pi$ and $^1\Phi$ and of the molecule SiC

Figure 9. Permanent dipole cuves of the electronic states $^3\Sigma^\pm$, $^3\Delta$, $^3\Pi$ and $^3\Phi$ of the molecule SiC
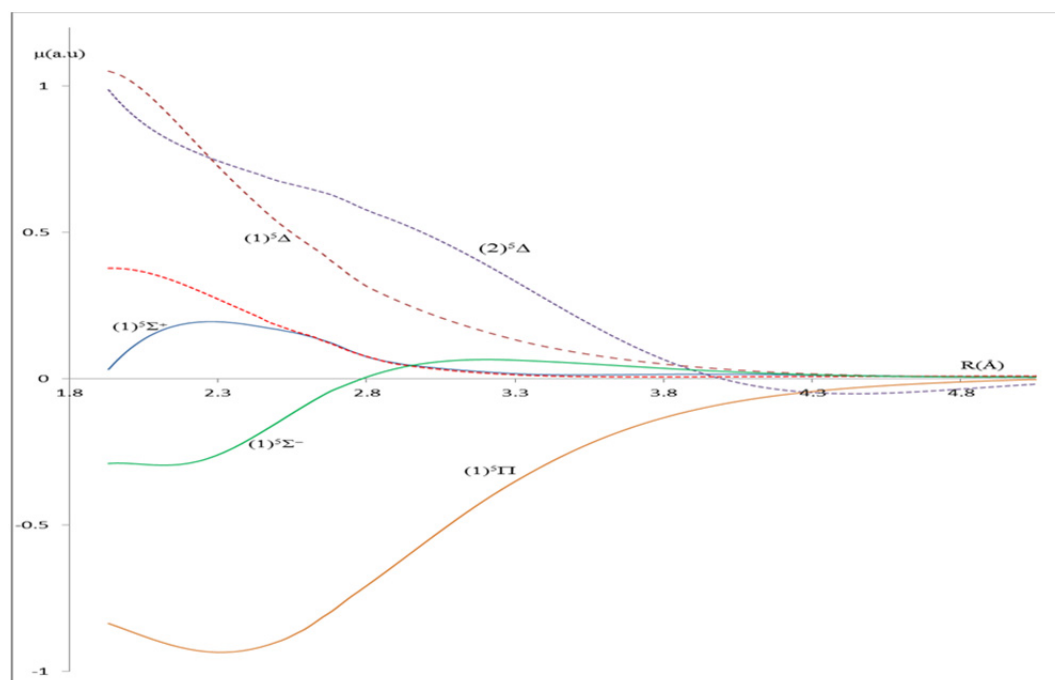

Figure 10. Permanent dipole cuves of the electronic states $^5\Sigma^\pm$, $^5\Delta$ and $^5\Phi$ of the molecule SiC

The investigation of these PDM curves is mainly used to discuss the bond nature, the polarity of the states and their interactions. As the internuclear distance increases one can notice three types of the DMC's for the singlet, triplet and quintet electronic states: *i)* curves in the positive region which are corresponding to an ionic structure of $Si^{\delta-}C^{\delta+}$ type *ii)* curves in the negative region which are corresponding to an ionic structure of $Si^{\delta+}C^{\delta-}$ type *iii)* curves passing from one region to another by changing the ionic structure. It is noticed that at large internuclear distances, the dipole moment curves of all the investigated electronic states tend smoothly to zero which is theoretically the correct behavior for a molecule that dissociates into natural fragments. The sharp change in the

directions of the PDM curves indicate an avoided crossing of the potential energy curves at the same position of the internuclear distance, e.g. $(3)^1\Sigma^+/(4)^1\Sigma^+$ at 2.22Å so that the polarity of the atoms is reversed. This agreement may confirm the validity and the accuracy of the calculation of the studied excited electronic states. No comparison of these values of the PDM with other results in literature since, to the best of our knowledge, they are given here for the first time.

4. Conclusion

From an *ab-initio* MRCI+Q calculation, the permanent dipole moment and the potential energy curves have been investigated for 47 singlets, triplet and quintet electronic states of the molecule SiC. The plots of these curves have been represented and the spectroscopic constants R_e, ω_e, T_e, α_e, and B_e are determined for the investigated electronic states. The spectroscopic constants for 13 states are given here for the first time. In literature there are fragmented experimental data for few electronic states of the molecule SiC. The confirmation of the theoretical investigated data can be done by a future experiment for these electronic states of the molecule SiC

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