# Theoretical electronic structure with rovibrational and dipole moment calculation of SiN Molecule

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**Abstract**. Atomic and molecular data are at the origin of the atmospheres of planetary and stellar objects discoveries. Based on the laboratory astrophysics and the computational molecular spectroscopy, the interpretation of this data can give the chemical compositions and temperatures of these astrophysical systems. The detection and the identification of the SiN radical in the interstellar medium has drawn the attention to the gas phase chemistry and the evidence of a link between the interstellar chemistry of silicon and that of nitrogen. The quantum chemistry methods used to predict the spectroscopic properties of the SiN molecule can be calibrated with some available experimental results. In order to obtain reliable theoretical data that may help in the interpretation of interstellar or laboratory spectra concerning the SiN molecule, we performed theoretical calculation of 31 low-lying electronic state, below 66000 $cm^{-1}$, of the molecule SiN by using the Complete Active Space Self Consistent Field (CASSCF) method followed by the Multi Reference Configuration Interaction with Davidson correction MRCI+Q. The potential energy along with the dipole moment curves of these states have been calculated along with the spectroscopic constants $R_e$, $\omega_e$, $B_e$, and $T_e$. The Rotation-vibration lines for the considered electronic states of SiN molecule were obtained by direct solution of the nuclear motion Schrödinger equation using the canonical approach with program Rovib-1. By comparing our investigated values of the calculated vibrational energy $E_v$, the rotational constant $B_v$ and the turning points $R_{min}$ and $R_{max}$. with those available in literature shows a very good agreement. To the best of our knowledge nine new electronic states have been studied here for the first time that have not been observed yet.

## 1. introduction

The remarkable interest of silicon nitride resides in many properties such as strength, hardness, chemical inertness, good resistance to corrosion, high thermal stability, and good dielectric properties [1]. In literature, many spectroscopic investigations have been focused on the ground and the first excited states where some spectroscopic constants have been obtained [2-12]. The spectroscopic constants $R_e$, $\omega_e$, $\omega_e x_e$ and the electronic energy with respect to the ground state $T_e$ have been investigated by different theoretical techniques for the doublet and quartet electronic states where the ground state is proved to be $X^2\Sigma^+$ and the first excited state is $A^2\Pi$ [13-38]. Recently Xing *et al*. [39] determined the spectroscopic parameters and the potential energy curves (PECs) of thirteen $^{2s+1}\Lambda^{(\pm)}$electronic states using the complete active space self-consistent field method followed by the internally contracted multireference configuration interaction approach with the Davidson modification (MRCI+Q).

By using an *ab initio* calculation, we investigate in the present work, the PEC's for 31 doublet and quartet electronic states of the SiN molecule along with the corresponding spectroscopic parameters. The comparison of these results with those reported in literature showed a very good agreement. Taking advantage of the electronic structure of the investigated electronic states of the molecule SiN and by using the canonical functions approach, the eigenvalue $E_v$, the rotational constant $B_v$, and the turning points $R_{min}$ and $R_{max}$ have been calculated for several vibrational levels of the considered doublet and quartet electronic states.

## 2. Method of calculations

The low-lying doublet and quartet electronic states of the molecule SiN have been studied by using state averaged complete active space self-consistent field (CASSCF) procedure followed by a multireference configuration interaction (MRDSCI with Davidson correction) treatment for the electron correlation. The entire CASSCF configuration space was used as the reference in the MRDSCI calculations, which were done via the computational chemistry program MOLPRO [40] taking advantage of the graphical user interface GABEDIT [41]. This software is intended for the higher level of accuracy correlated *ab initio* calculations. MOLPRO has been run on a PC-computer with LUNIX-type operating systems. The 14 electrons of the silicon atom are considered using the aug-cc-pV5Z basis set for s, p, d and f functions. The nitrogen species is treated as a system of 7 electrons by using the same basis set for s, p, and d functions. Among the 21 electrons explicitly considered for the SiN molecule (14 electrons for Si and 7 for N) 10 inner electrons were frozen in subsequent calculations so that 11 valence electrons were explicitly treated. The corresponding active space contains $7\sigma(Si:3s,3p_0,4s;N:1s,2s,2p_0,3s)$ and $2\pi(Si:3p_{\pm1};N:2p_{\pm1})$ orbitals, which correspond to 11 active molecular orbitals distributed into irreducible representation $a_1$, $b_1$, $b_2$ and $a_2$ in the following way: $7a_1$, $2b_1$, $2b_2$, 0, noted [7, 2, 2, 0].All computations were performed in the $C_{2v}$point group. The 15 doublet and 16 quartet low-lying electronic states of the molecule SiN were generated using the MRSDCI calculation for61 internuclear distances in the range $1Å \le R_e \le 3Å$ in the representation $^{2s+1}\Lambda^{(+/-)}$ where we assumed that, the SiN molecule is mainly ionic around the equilibrium position. These potential energy curves are given in Figs1-4.

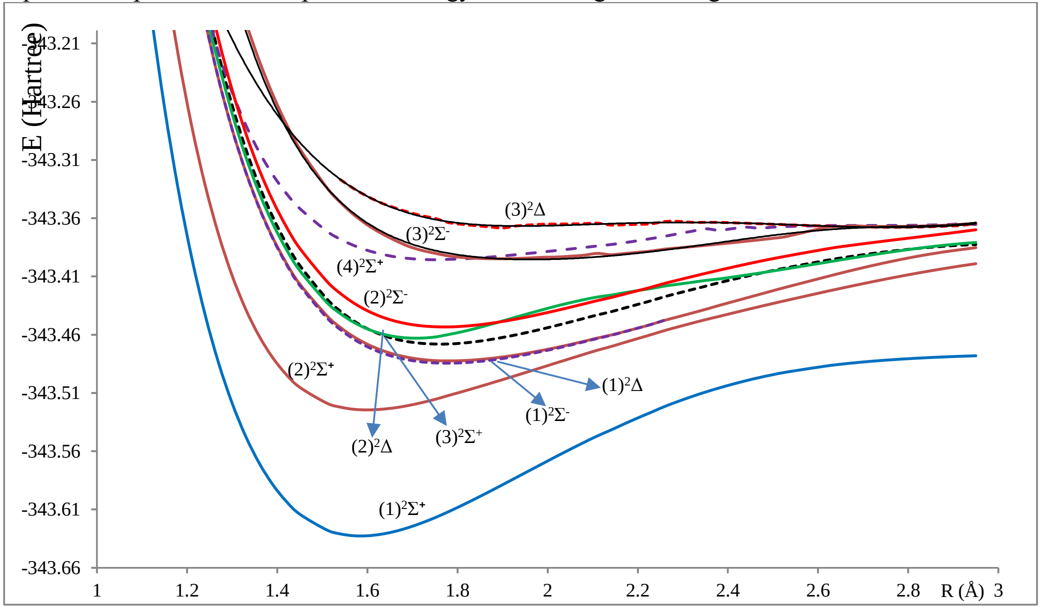

Fig. 1: Potential energy curves of the electronic states $^2\Sigma^{\pm}$ and $^2\Delta$ of the molecule SiN

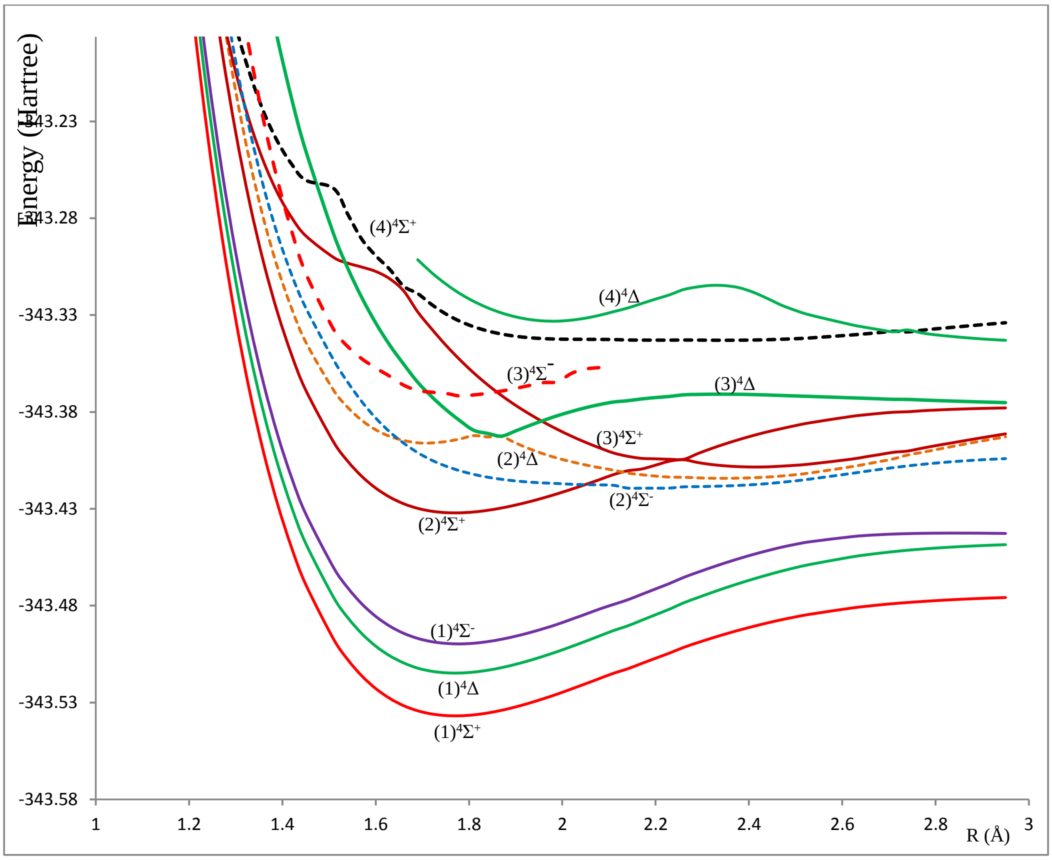

Fig. 2: Potential energy curves of the states $^4\Sigma^\pm$ and $^4\Delta$ of the molecule SiN

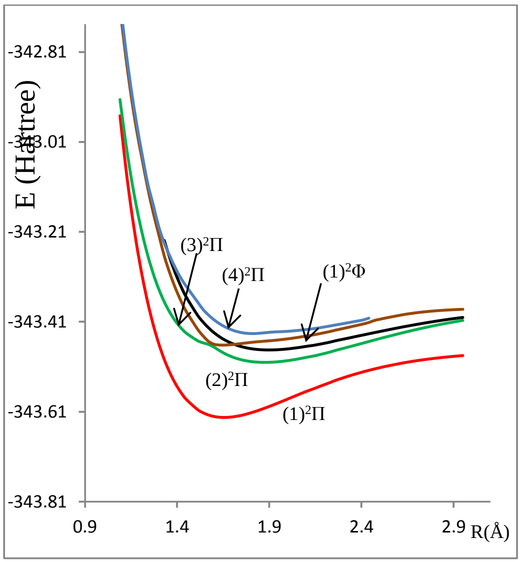

Fig. 3: Potential energy curves of the states $^2\Pi$ and $^2\Phi$ of the molecule SiN

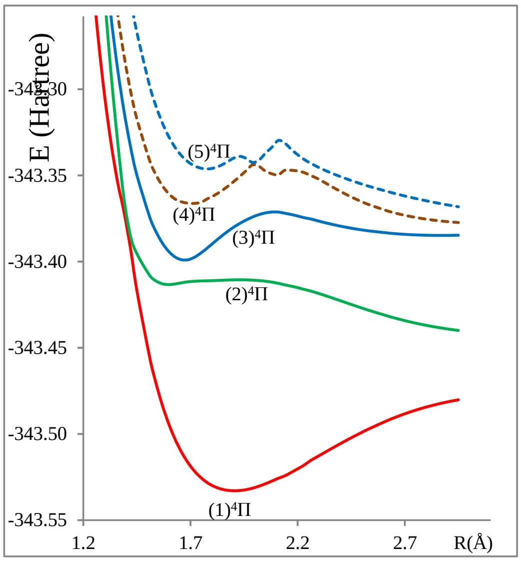

Fig. 4: Potential energy curves of the states $^4\Pi$ of the molecule SiN

In the considered range of R, some crossings and avoided crossings occur between the potential energy curves of different symmetries at large values of the internuclear distance. The positions of these crossings and avoided crossings are given in Table 1.

Table 1: Positions of the crossings and avoided crossing between the different electronic states of the molecule SiN

| State(1)/state(2) | Crossing between ($n_1$) state1/($n_2$) state2 | $R_c$(Å) | |
|---|---|---|---|
| $^2\Sigma^+/^2\Delta$ | 3/2 | 1.60 | |
| | 3/2 | 2.47 | |
| | 3/2 | 2.77 | |
| | 4/3 | 2.53 | |
| $^2\Sigma^+/^2\Sigma^-$ | 3/2 | 1.87 | |
| | 3/2 | 2.17 | |
| | 4/3 | 1.84 | |
| | 4/2 | 1.30 | |
| | 4/3 | 2.62 | |
| $^2\Pi/^2\Phi$ | 3/1 | 1.69 | |
| | 4/1 | 1.33 | |
| $^4\Sigma^+/^4\Delta$ | 2/2 | 2.11 | |
| | 3/3 | 1.93 | |
| | 3/3 | 1.51 | |
| | 4/3 | 1.45 | |
| | 3/2 | 1.18 | |
| | 4/4 | 2.71 | |
| $^4\Sigma^+/^4\Sigma^-$ | 2/2 | 2.05 | |
| | 2/3 | 1.84 | |
| | 3/3 | 1.30 | |
| | 4/3 | 1.33 | |
| | 3/2 | 1.30 | |
| $^4\Sigma^-/^4\Delta$ | 3/2 | 1.72 | |
| | Avoided crossing between ($n_1$) state1/($n_2$) state2 | $R_{AC}$(Å) | $\Delta E_{AC}$ (cm$^{-1}$) |
| $^2\Pi/^2\Pi$ | 2/3 | 1.57 | 1502.54 |
| $^4\Pi/^4\Pi$ | 1/2 | 1.39 | 1710.32 |
| $^4\Pi/^4\Pi$ | 4/5 | 1.90 | 298.85 |
| $^4\Pi/^4\Pi$ | 2/3 | 1.24 | 746.45 |
| | 2/3 | 1.66 | 2922.87 |
| $^4\Delta/^4\Delta$ | 2/3 | 1.84 | 402.46 |
| $^4\Sigma^+/^4\Sigma^+$ | 2/3 | 2.23 | 1201.18 |
| | 2/3 | 2.14 | 1356.353 |
| | 3/4 | 1.63 | 1069.41 |

$R_{AC}$ and $\Delta E_{AC}$ are respectively the internuclear distance and the energy difference at the avoided crossing between the two corresponding states.

The existence of the avoided crossing phenomena constellated to the interaction between the adiabatic potential curves of the corresponding states. The crossing between 2 potential energy curves of two electronic states and their wavefunctions are adiabatic solutions of the Schrödinger equation. But if these wavefunctions belong to the same symmetry, they will mix with each other to give two adiabatic solutions, which no longer cross between the corresponding PECs and the crossing becomes avoided.

This avoided crossing causes an important change in the dipole moment of the two states where the electronic characteristics interchanged in this region and the polarity of the atoms is reversed which is the cause of the abrupt gradient change of the DMS's at the same position of the avoided crossing. In Fig.5 we give the crossing of the DMC's at the positions of the avoided crossing of the PECs given in Table 1, which can confirm the accuracy of our calculated data.

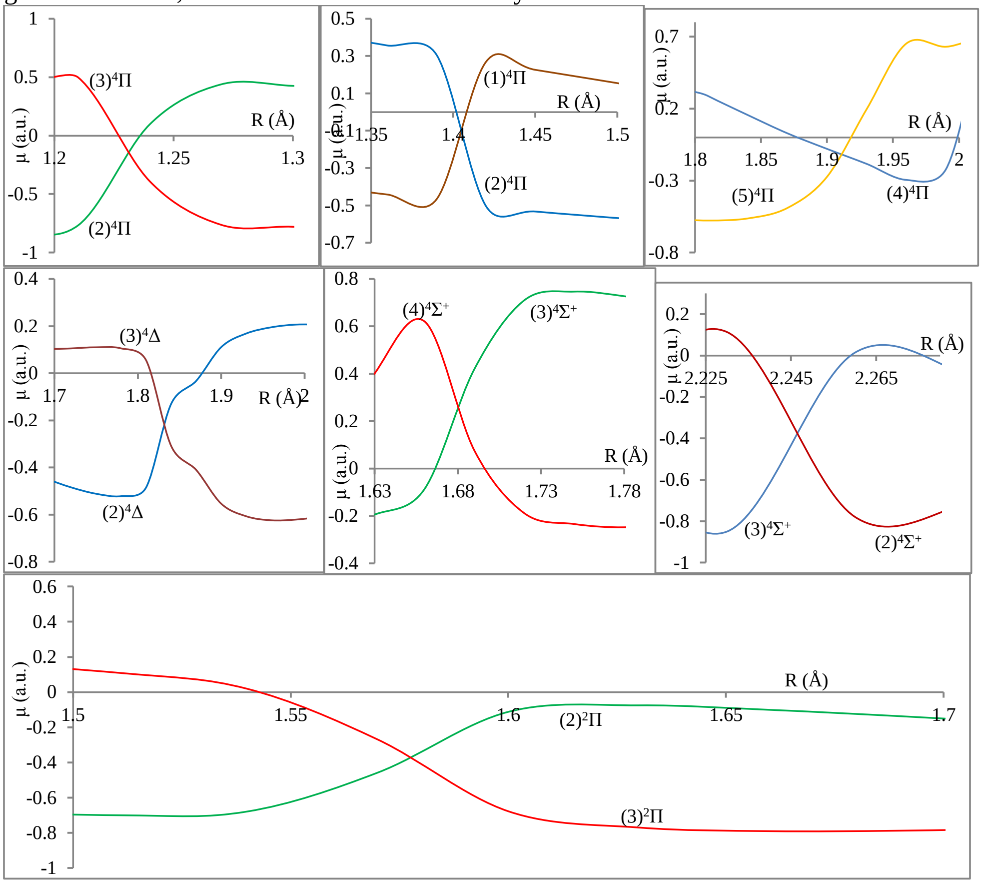

Fig. 5: Dipole moment curves at the positions of the avoided crossings.

For the investigated bound electronic states, the transition energy with respect to the energy minimum for the ground state $T_e$, the equilibrium internuclear distance $R_e$, the harmonic frequency $\omega_e$ and the rotational constant $B_e$ have been calculated. These values are given in Table 2.

Table 2: Spectroscopic constants of the molecule SiN.

| $^{2S+1}\Lambda^{(\pm)}$ states | $T_e$ (cm$^{-1}$) | $\Delta T_e/T_e$ % | $R_e$ (Å) | $\Delta R_e/R_e$ % | $B_e$ (cm$^{-1}$) | $\Delta B_e/Be$ % | $\omega_e$ (cm$^{-1}$) | $\Delta\omega_e/\omega_e$ % |
|---|---|---|---|---|---|---|---|---|
| $X^2\Sigma^+$ | 0.0(a) | | 1.585(a) | | 0.717(a) | | 1115.77(a) | |
| | 0.0(b) | | 1.572(b) | 0.82 | 0.73(b) | 1.78 | 1155(b) | 3.39 |
| | 0. 0[c] | | 1.593(c) | 0.50 | | | 1124(c) | 0.73 |
| | 0.0(d) | | 1.566(d) | 1.21 | | | | |
| | 0.0(e) | | 1.582(e) | 0.18 | | | | |
| | 0. 0(f) | | 1.568(f) | 1.08 | | | 1167(f) | 4.38 |
| | 0. 0(g) | | 1.568(g) | 1.08 | | | 1189(g) | 6.15 |
| | 0.0(h) | | | | | | 1151(h) | 3.06 |
| | 0. 0(i) | | 1.578(i) | 0.44 | | | 1162(i) | 3.97 |
| | 0.0(j) | | 1.589(j) | 0.25 | | | | |
| | 0.0(k) | | 1.571(k) | 0.89 | 0.731(k) | 1.91 | 1151.36(k) | 3.09 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $0.\,0^{(l)}$ | | $1.572^{(l)}$ | 0.82 | $0.73^{(l)}$ | 1.78 | | |
| | $0.0^{(m)}$ | | | | | | $1151.3^{(m)}$ | 3.09 |
| | $0.0^{(n)}$ | | | | $0.73^{(n)}$ | 1.78 | $1151.2^{(n)}$ | 3.07 |
| | $0.0^{(s)}$ | | $1.58^{(s)}$ | 0.31 | $0.722^{(s)}$ | 0.69 | $1152^{(s)}$ | 3.14 |
| $(1)^2\Pi$ | $1999.3^{(a)}$ | | $1.654^{(a)}$ | | $0.658^{(a)}$ | | $1004.02^{(a)}$ | |
| | $2053^{(b)}$ | 2.60 | $1.639^{(b)}$ | 0.91 | $0.672^{(b)}$ | 2.08 | $1044^{(b)}$ | 3.82 |
| | $4785^{(e)}$ | 58.20 | $1.646^{(e)}$ | 0.48 | | | | |
| | $633^{(f)}$ | | $1.64^{(f)}$ | 0.85 | | | $1046^{(f)}$ | 4.01 |
| | | | $1.693^{(j)}$ | 2.30 | | | | |
| | | | $1.635^{(k)}$ | 1.16 | | 2.51 | $1044.41^{(k)}$ | 3.86 |
| | $2032.15^{(m)}$ | 1.61 | | | | | | 2.67 |
| | $2031.37^{(n)}$ | 1.57 | | | $0.67^{(n)}$ | 1.79 | $1031.65^{(m)}$ | 2.70 |
| | | | | | | | $1031.94^{(n)}$ | |
| | $2032.4^{(p)}$ | 1.62 | $1.641^{(p)}$ | 0.79 | $0.67^{(p)}$ | 1.79 | | |
| | $2099^{(s)}$ | 4.74 | $1.65^{(S)}$ | 0.24 | $0.66^{(s)}$ | 0.30 | $1025^{(S)}$ | |
| $(1)^4\Sigma^+$ | $20724.4^{(a)}$ | | $1.770^{(a)}$ | | $0.575^{(a)}$ | | $745.88^{(a)}$ | |
| | $18551^{(r)}$ | 11.71 | $1.783^{(r)}$ | 0.72 | | | | |
| | $22195^{(s)}$ | 6.62 | $1.756^{(s)}$ | 0.79 | $0.585^{(s)}$ | 1.70 | $799^{(s)}$ | 6.64 |
| $(1)^4\Pi$ | $21892.42^{(a)}$ | | $1.900^{(a)}$ | | $0\,.496^{(a)}$ | | $605.92^{(a)}$ | |
| | $20890^{(r)}$ | 4.79 | $1.892^{(r)}$ | 0.422 | | | | |
| | $22809^{(s)}$ | 4.01 | $1.893^{(s)}$ | 0.36 | $0\,.504^{(s)}$ | 1.58 | $639^{(s)}$ | 5.17 |
| $(2)^2\Sigma^+$ | $23745.1^{(a)}$ | | $1.599^{(a)}$ | | $0.705^{(a)}$ | | $952.25^{(a)}$ | |
| | $24122^{(c)}$ | 1.56 | $1.612^{(c)}$ | 0.80 | | | $958^{(c)}$ | 0.6 |
| | $24299.21^{(k)}$ | 2.28 | $1.579^{(k)}$ | 1.26 | $0.723^{(k)}$ | 2.48 | $1031.03^{(k)}$ | 7.64 |
| | $24299.19^{(m)}$ | 2.28 | | | | | | 7.64 |
| | | | | | | | $1031.02^{(m)}$ | |
| | $24861^{(s)}$ | 4.48 | $1.59^{(s)}$ | 0.56 | $.714^{(s)}$ | 1.26 | $1025^{(s)}$ | 7.09 |
| $(1)^4\Delta$ | $25567.0^{(a)}$ | | $1.770^{(a)}$ | | $0.575^{(a)}$ | | $746.10^{(a)}$ | |
| | $24197^{(r)}$ | 5.66 | $1.78^{(r)}$ | 0.56 | 0.584 | 1.54 | $779^{(s)}$ | 4.22 |
| | $27172^{(s)}$ | 5.9 | $1.757^{(s)}$ | 0.74 | | | | |
| $(1)^4\Sigma^-$ | $28878.3^{(a)}$ | | $1.770^{(a)}$ | | $0.571^{(a)}$ | | $721.18^{(a)}$ | |
| | $27020^{(r)}$ | 6.87 | $1.784^{(r)}$ | 0.78 | | | | |
| | $30236^{(s)}$ | 4.49 | $1.763^{(s)}$ | 0.39 | $0.581^{(s)}$ | 1.72 | $760^{(s)}$ | 5.107 |
| $(2)^2\Pi$ | $28887.6^{(a)}$ | | $1.875^{(a)}$ | | $0.512^{(a)}$ | | $680.08^{(a)}$ | |
| | $27865.63+a^{(k)}$ | | $1.857^{(k)}$ | 0.969 | $0.523^{(k)}$ | 2.1 | $699.33^{(k)}$ | 2.75 |
| | $28859.55^{(m)}$ | 0.10 | | | | | $699.32^{(m)}$ | 2.75 |
| | $28859.55^{(q)}$ | 0.10 | | | | | $699.32^{(q)}$ | 2.75 |
| | $29652^{(s)}$ | 2.57 | $1.869^{(s)}$ | 0.32 | $0.517^{(s)}$ | 0.97 | $705^{(s)}$ | 3.53 |
| $(1)^2\Sigma^-$ | $32547.9^{(a)}$ | | $1.776^{(a)}$ | | $0.571^{(a)}$ | | $711.93^{(a)}$ | |
| | $33847^{(s)}$ | 3.84 | $1.768^{(s)}$ | 0.45 | $0.577^{(s)}$ | 1.04 | $755^{(s)}$ | 5.82 |
| $(1)^2\Delta$ | $32978.4^{(a)}$ | | $1.780^{(a)}$ | | $0.568^{(a)}$ | | $693.76^{(a)}$ | |
| | $34489^{(s)}$ | 4.38 | $1.776^{(s)}$ | 0.22 | $0.572^{(s)}$ | 0.69 | $739^{(s)}$ | 6.12 |
| $(1)^2\Phi$ | $34943.4^{(a)}$ | | $1.897^{(a)}$ | | $0.5^{(a)}$ | | $641.7^{(a)}$ | |
| | $38752^{(s)}$ | 9.82 | $1.724^{(s)}$ | 10.03 | $0.607^{(s)}$ | 17.62 | $1247^{(s)}$ | 48.54 |
| $(2)^2\Delta$ | $36144.8^{(a)}$ | | $1.760^{(a)}$ | | $0.582^{(a)}$ | | $763.69^{(a)}$ | |
| | $37592^{(s)}$ | 3.84 | $1.753^{(s)}$ | 0.39 | $0.587^{(s)}$ | 0.85 | $797^{(s)}$ | 4.17 |
| $(3)^2\Sigma^+$ | $37258.8^{(a)}$ | | $1.700^{(a)}$ | | $0.62^{(a)}$ | | $993.30^{(a)}$ | |
| | $38713^{(s)}$ | 3.75 | $1.71^{(s)}$ | 0.58 | $0.617^{(s)}$ | 0.48 | $941^{(s)}$ | 5.55 |
| $(2)^2\Sigma^-$ | $39378.1^{(a)}$ | | $1.770^{(a)}$ | | $0.575^{(a)}$ | | $743.93^{(a)}$ | |
| $(4)^2\Pi$ | $42949.4^{(a)}$ | | $1.806^{(a)}$ | | $0.552^{(a)}$ | | $913.38^{(a)}$ | |
| | $44861^{(s)}$ | 4.26 | $1.801^{(s)}$ | 0.27 | $0.566^{(s)}$ | 2.47 | $989^{(s)}$ | 7.64 |
| $(2)^4\Sigma^+$ | $(F)43718.1^{(a)}$ | | $1.769^{(a)}$ | | $0.576^{(a)}$ | | $700.37^{(a)}$ | |
| | $(S)48916.7^{(a)}$ | | $2.41^{(a)}$ | | $0.309\ ^{(a)}$ | | $453.21^{(a)}$ | |
| | $44895^{(s)}$ | 2.62 | $1.759^{(a3)}$ | 0.56 | $0.583^{(s)}$ | 1.20 | $738^{(s)}$ | 5.09 |
| $(2)^4\Sigma^-$ | $46511.2^{(a)}$ | | $2.190^{(a)}$ | | $0.372^{(a)}$ | | $463.65^{(a)}$ | |
| $(2)^4\Pi$ | $48149.6^{(a)}$ | | $1.599^{(a)}$ | | $0.703^{(a)}$ | | $803.39^{(a)}$ | |
| | $49282^{(s)}$ | 2.29 | $1.59^{(s)}$ | 0.56 | $0.714^{(s)}$ | 1.54 | $968^{(s)}$ | 17.0 |
| $(2)^4\Delta$ | $47638.1^{(a)}$ | | $2.340^{(a)}$ | | $0.326^{(a)}$ | | $334.23^{(a)}$ | |
| | $50063^{(s)}$ | 4.84 | $2.35^{(s)}$ | 0.42 | $0.326^{(s)}$ | 0.00 | $358^{(s)}$ | 6.63 |
| $(3)^4\Pi$ | $51277.7^{(a)}$ | | $1.673^{(a)}$ | | $0.644^{(a)}$ | | $1139.63^{(a)}$ | |
| | $53266^{(s)}$ | 3.73 | $1.695^{(s)}$ | 1.00 | $0.628^{(s)}$ | 2.54 | $1134^{(s)}$ | 0.49 |
| $(4)^2\Sigma^+$ | $52051.9^{(a)}$ | | $1.750^{(a)}$ | | $0.587^{(a)}$ | | $623.01^{(a)}$ | |
| $(3)^2\Sigma^-$ | $52208.2^{(a)}$ | | $1.877^{(a)}$ | | $0.509^{(a)}$ | | $584.33^{(a)}$ | |
| $(3)^4\Sigma^-$ | $57066.5^{(a)}$ | | $1.785^{(a)}$ | | $0.564^{(a)}$ | | $644.88^{(a)}$ | |
| $(3)^2\Delta$ | $58169.5^{(a)}$ | | $1.870^{(a)}$ | | $0.509^{(a)}$ | | $831.98^{(a)}$ | |
| $(4)^4\Pi$ | $58464.5^{(a)}$ | | $1.699^{(a)}$ | | $0.624^{(a)}$ | | $857.13^{(a)}$ | |
| $(5)^4\Pi$ | $62861.3^{(a)}$ | | $1\,.776^{(a)}$ | | 0.57 | | $928.82^{(a)}$ | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | 64362$^{(s)}$ | 2.33 | 1.766$^{(s)}$ | 0.56 | 0.578$^{(s)}$ | 1.38 | 879$^{(s)}$ | 5.66 |
| $(4)^4\Sigma^+$ | 63275.3$^{(a)}$ | | 2.340$^{(a)}$ | | 0.349$^{(a)}$ | | 46.97$^{(a)}$ | |
| $(4)^4\Delta$ | 65431.8$^{(a)}$ | | 1.978$^{(a)}$ | | 0.460$^{(a)}$ | | 737.46$^{(a)}$ | |

(a)Present work, (b)Ref.[22], (c)Ref. [29], (d)Ref. [14], (e)Ref.[13], (f)Ref. [18] , (g)Ref.[21], (h)Ref.[16], (i)Ref.[20],(j)Ref.[17], (k)Ref.[3], (l)Ref.[4], (m)Ref.[9], (n)Ref.[10], (o)Ref.[12] , (p)Ref.[8], (q)Ref.[5], (r)Ref.[15], (s)Ref. [32].F and S represent the first and the second minima respectively.

## 3. Results and discussions

By comparing our calculating values with those obtained experimentally for the 4 states $X^2\Sigma^+$, $(1)^2\Pi$, $(2)^2\Sigma^+$, and $(2)^2\Pi$, available in literature, one can find an excellent agreement for $T_e$, $R_e$, $B_e$ with the relative differences 0.1%(Refs.[5,9]$(2)^2\Pi$)$\leq\Delta T_e/T_e\leq$2.28% (Refs.[3,9]$(2)^2\Sigma^+$), 0.79% (Ref.[8] $(1)^2\Pi$) $\leq \Delta R_e/R_e \leq$ 1.26% (Ref.[3] $(2)^2\Sigma^+$), 1.78% (Refs. [4,10] $X^2\Sigma^+$) $\leq \Delta B_e/B_e \leq$ 2.48% (Ref.[3]$(2)^2\Sigma^+$) respectively and a good agreement for the value of $\omega_e$ with the relative difference 2.67% (Refs.[10]$(1)^2\Pi$)$\leq\Delta\omega_e/\omega_e\leq$7.64% (Refs.[3,9]$(2)^2\Sigma^+$).The comparison of these constants, calculated in the present work, with the theoretical values published in literature shows also good agreements. The corresponding relative differences are 1.56% (Ref.[29]$(2)^2\Sigma^+$)$\leq$ $\Delta T_e/T_e$ $\leq$9.82% (Ref.[32] $(1)^2\Phi$), 0.18%(Ref.[13] $X^2\Sigma^+$) $\leq\Delta R_e/R_e$ $\leq$10.03% (Ref.[32]$(1)^2\Phi$), 0.00%(Ref.[32]$(2)^4\Delta$)$\leq\Delta B_e/B_e\leq$2.47% (Ref.[32]$(4)^2\Pi$) and 1.56%(Ref.[29]$(2)^2\Sigma^+$)$\leq$ $\Delta\omega_e/\omega_e$ $\leq$9.82% (Ref.[32] $(1)^2\Phi$). A larger relative differencesis noticed by comparing our values of $T_e$ with those given in Refs. [13, 18] for the states $(1)^2\Pi$ and $(1)^4\Sigma$ and the values $B_e$ and $\omega_e$ for the state $(1)^2\Phi$ calculated by Cai *et al.* [32] at CMRCI level. From this over all good agreement with the experimental and theoretical data in literature, we can pretend the accuracy of the results concerning the new investigated electronic states in the present work, which can be confirmed by new experiments on this molecule.

## 4. The vibration rotation calculation.

By using the canonical functions approach [42-45] and the cubic spline interpolation between each two consecutive points of the PECs obtained from the *ab initio* calculation of the SiN molecule, the eigenvalue $E_v$, the rotational constant $B_v$, and the abscissas of the turning point $R_{min}$ and $R_{max}$ have been calculated for the considered electronic states up to the vibrational levels v = 27. These values for the different electronic states are given in Table 3. The absence of the comparison with other results is

Table 3: Values $E_v$, $B_v$ and the abscissas of the turning points for the vibrational levels of electronic states of the molecule SiN.

| | $X^2\Sigma^+$ | | | | $(2)^2\Sigma^+$ | | | | $(1)^2\Delta$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| V | $E_v$ ($cm^{-1}$) | $B_v$ ($cm^{-1}$) | $R_{min}$ (Å) | $R_{max}$ (Å) | $E_v$ ($cm^{-1}$) | $B_v$ ($cm^{-1}$) | $R_{min}$ (Å) | $R_{max}$ (Å) | $E_v$ ($cm^{-1}$) | $B_v$ ($cm^{-1}$) | $R_{min}$ (Å) | $R_{max}$ (Å) |
| 0 | 519.15 | 0.728 | 1.531 | 1.645 | 472.81 | 0.701 | 1.542 | 1.667 | 334.38 | 0.564 | 1.713 | 1.859 |
| 1 | 1618.92 | 0.723 | 1.495 | 1.693 | 1400.95 | 0.691 | 1.505 | 1.722 | 1012.56 | 0.558 | 1.670 | 1.922 |
| 2 | 2708.91 | 0.717 | 1.472 | 1.729 | 2317.80 | 0.682 | 1.483 | 1.763 | 1688.25 | 0.552 | 1.642 | 1.969 |
| 3 | 3785.07 | 0.711 | 1.454 | 1.760 | 3216.64 | 0.673 | 1.466 | 1.800 | 2353.47 | 0.547 | 1.620 | 2.010 |
| 4 | 4848.85 | 0.705 | 1.439 | 1.787 | 4094.16 | 0.662 | 1.452 | 1.836 | 3012.23 | 0.540 | 1.603 | 2.046 |
| 5 | 5903.17 | 0.700 | 1.426 | 1.814 | 4940.23 | 0.651 | 1.440 | 1.870 | 3665.01 | 0.535 | 1.587 | 2.079 |
| 6 | 6938.23 | 0.693 | 1.415 | 1.838 | 5769.07 | 0.643 | 1.430 | 1.902 | 4311.22 | 0.530 | 1.574 | 2.111 |
| 7 | 7963.64 | 0.687 | 1.404 | 1.862 | 6577.03 | 0.633 | 1.420 | 1.933 | 4947.38 | 0.524 | 1.562 | 2.144 |
| 8 | 8973.67 | 0.682 | 1.395 | 1.885 | 7367.44 | 0.625 | 1.412 | 1.963 | 5571.93 | 0.518 | 1.551 | 2.173 |
| 9 | 9970.44 | 0.675 | 1.387 | 1.907 | 8141.98 | 0.616 | 1.405 | 1.992 | 6192.96 | 0.515 | 1.541 | 2.201 |
| 10 | 10954.82 | 0.669 | 1.379 | 1.929 | 8900.93 | 0.608 | 1.398 | 2.021 | 6814.94 | 0.511 | 1.532 | 2.228 |
| 11 | 11924.45 | 0.663 | 1.372 | 1.951 | 9645.40 | 0.600 | 1.391 | 2.049 | 7433.31 | 0.506 | 1.523 | 2.251 |
| 12 | 12881.20 | 0.657 | 1.365 | 1.972 | 10375.65 | 0.592 | 1.385 | 2.076 | 8045.19 | 0.502 | 1.515 | 2.277 |
| 13 | 13824.82 | 0.651 | 1.359 | 1.994 | 11089.95 | 0.583 | 1.379 | 2.104 | 8655.43 | 0.497 | 1.508 | 2.305 |
| 14 | 14754.44 | 0.645 | 1.353 | 2.014 | 11788.04 | 0.575 | 1.374 | 2.134 | 9251.10 | 0.490 | 1.501 | 2.330 |
| 15 | 15671.29 | 0.639 | 1.347 | 2.035 | 12468.68 | 0.566 | 1.369 | 2.161 | 9836.75 | 0.487 | 1.494 | 2.356 |
| 16 | 16574.60 | 0.632 | 1.342 | 2.056 | 13136.09 | 0.559 | 1.365 | 2.187 | 10423.22 | 0.483 | 1.488 | 2.379 |
| 17 | 17462.75 | 0.626 | 1.336 | 2.077 | 13798.35 | 0.554 | 1.360 | 2.214 | 11004.16 | 0.478 | 1.482 | 2.404 |
| 18 | 18335.84 | 0.619 | 1.332 | 2.098 | 14451.45 | 0.546 | 1.356 | 2.240 | 11576.38 | 0.474 | 1.476 | 2.429 |
| 19 | 19193.35 | 0.612 | 1.327 | 2.120 | 15090.31 | 0.539 | 1.352 | 2.265 | 12143.10 | 0.469 | 1.470 | 2.453 |
| 20 | 20032.54 | 0.604 | 1.323 | 2.143 | 15720.92 | 0.533 | 1.348 | 2.292 | 12701.66 | 0.464 | 1.465 | 2.477 |
| 21 | 20853.73 | 0.597 | 1.319 | 2.164 | 16338.13 | 0.524 | 1.344 | 2.320 | 13254.95 | 0.461 | 1.460 | 2.501 |
| 22 | 21662.81 | 0.592 | 1.315 | 2.185 | 16936.57 | 0.516 | 1.341 | 2.347 | 13804.31 | 0.456 | 1.455 | 2.525 |
| 23 | 22462.90 | 0.586 | 1.311 | 2.207 | 17524.62 | 0.509 | 1.337 | 2.376 | 14344.11 | 0.451 | 1.451 | 2.549 |
| 24 | 23248.66 | 0.579 | 1.307 | 2.229 | 18100.10 | 0.501 | 1.334 | 2.403 | 14879.30 | 0.447 | 1.446 | 2.574 |
| 25 | 24017.50 | 0.572 | 1.304 | 2.250 | 18662.65 | 0.495 | 1.331 | 2.430 | 15406.81 | 0.442 | 1.442 | 2.598 |
| 26 | 24775.00 | 0.566 | 1.300 | 2.272 | 19217.20 | 0.489 | 1.328 | 2.458 | 15927.84 | 0.438 | 1.438 | 2.622 |
| 27 | 25517.97 | 0.558 | 1.297 | 2.296 | 19763.53 | 0.482 | 1.325 | 2.485 | 16443.37 | 0.434 | 1.434 | 2.646 |

because of the calculation of these values here for the first time.

## 5. Conclusion.

An *ab initio* calculation of 31 doublet and quartet lowest electronic states in the $^{2s+1}\Lambda^{(\pm)}$ representation up to 70000 cm$^{-1}$ has been performed via CASSCF/MRCI methods. The potential energy curves and the spectroscopic constants $T_e$, $R_e$, $B_e$, and $\omega_e$ have been calculated for these electronic states. The comparison of our results with the theoretical and experimental data available in the literature demonstrated a very good agreement which confirms the validity and the accuracy of the investigated new electronic states. By using the canonical functions approach [42-44], the eigenvalue $E_v$, the rotational constant $B_v$, and the abscissas of the turning points $R_{min}$ and $R_{max}$ were calculated up to the vibrational level v=41. New electronic states have been investigated in the present work for the first time.

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