Electronic structure with dipole moment calculations of the high-lying electronic states of BeH, MgH and SrH molecules

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Abstract

By using the complete active space self consistent field (CASSCF) with multi-reference configuration interaction MRCI + Q method including single and double excitations with Davidson correction, the 26, 27 and 25 low-lying doublet and quartet electronic states in the representation \( ^{2S+1} \Lambda^{(+/−)} \) (without spin orbit interaction) of the molecules BeH, MgH and SrH have been investigated. The potential energy curves, the internuclear distance \( R_\text{e} \), the harmonic frequency \( \omega_\text{e} \), the permanent dipole moment \( \mu \), the rotational constant \( B \) and the electronic transition energy with respect to the ground state \( T_\text{r} \) are calculated. Using the canonical approach the eigenvalue \( E_\text{sn} \), the rotational constant \( B \) and the abscissas of the turning points \( R_{\text{min}} \) and \( R_{\text{max}} \) have been calculated for the investigated electronic states. The comparison between the values of the present work and those available in the literature for several electronic states shows very good agreement.

1. Introduction

The mono-hydrides of the alkaline-earth metals are expected to be present in sunspots, stars, nebulae, and the interstellar medium. These species, have received considerable attention from both the experimentalists and the theoreticians, because the molecules SrH, MgH and CaH are relatively easy to synthesize in the gas-phase, have interesting ground states, due to astrophysical significance [1–5] and the apparent simplicity of their electronic structure. Since the excited electronic states of the considered three molecules showed complex spectra their electronic states have been the subject of much interest from both experimental spectroscopists and quantum chemists. Since the collision process between cold atoms allowing high precision measurements with hydrogen isotopes, precise determination of molecular potentials and atomic lifetimes the alkaline-earth-metal hydrides have been the subject of extensive research in the past years. These molecules are ideal candidates for the production of the polar molecules and direct laser cooling [6–16] as well as for the ultracold fragmentation. Moreover, these Hydrides containing alkaline-earth metals offer a wide variety of interesting applications. For example, they are prototypes for hydrogen storage materials. They have been predicted to be stable at pressures that can be achieved in a diamond anvil cell and they are predicted to display high-temperature superconductivity. With small amounts of hydrogen (0.1%–1%) the Hydrides containing alkaline-earth metals are investigated as viable magnetic, thermoelectric or semiconducting materials.

The BeH molecule is less popular for experimentalists because of the toxicity of the Be-containing molecules, while it is extensively studied theoretically by using ab initio method. The early work on the electronic emission spectra of BeH molecule has been done by Watson and Fredrickson [17]. Recently, there is more demanding of this molecule due to the existence of near-degeneracy effects and low-lying states [18] and it is being studied in the surfaces of fusion reactors ITER (International Thermonuclear Experimental Reactor) through the Joint European Torus (JET) of the European Community Fusion Program.

Since the visible emission of MgH was observed in the Sun and then in many stars and because of the relative abundances of the magnesium isotopes in stellar atmospheres, this molecule attracted the attention of the
Table 1. The lowest dissociation limits of BeH, MgH and SrH molecules.

| Dissociation of atomic levels Be + H | Dissociation energy limit of BeH levels (cm⁻¹) | Molecular states of BeH | Total dissociation energy limit of Be + H atoms (cm⁻¹) | Relative error (%) |
|-------------------------------------|-----------------------------------------------|------------------------|-------------------------------------------------------|-------------------|
| Be(1s²2s², 3S) + H(1s, 1S)          | 0⁻                                            | X²Σ⁺                   | 0⁺                                                   | 0.0               |
| Be(1s²2s²2p, 3P) + H(1s, 1S)       | 22 115⁺                                       | (2)²Σ⁺,(1)²Π,(1)¹Σ⁺,(1)¹Π | 21 978⁺                                               | 6.4               |
| Be(1s²2s²2p, 3P) + H(1s, 1S)       | 43 861⁺                                       | (3)²Σ⁺,(2)²Π           | 42 565⁺                                               | 2.9               |
| Be(1s²2s²3s, 3S) + H(1s, 1S)       | 56 412⁺                                       | (4)²Σ⁺                 | 54 677⁺                                               | 3.1               |
| Be(1s²2s²3p, 3P) + H(1s, 1S)       | 60 167⁺                                       | (1)²Σ⁺,(3)²Π,(1)¹Σ⁻,(2)¹Π | 58 907⁺                                               | 2.1               |
| Be(1s²2p², 1D) + H(1s, 1S)         | 60 888⁺                                       | (5)²Σ⁺,(1)²Δ,(4)²Π    | 56 882⁺                                               | 6.6               |

| Dissociation limit of atomic levels Mg + H | Dissociation energy limit of MgH levels (cm⁻¹) | Molecular states of MgH | Total dissociation energy limit of Mg + H atoms (cm⁻¹) | Relative error (%) |
|------------------------------------------|-----------------------------------------------|------------------------|-------------------------------------------------------|-------------------|
| Mg(2p⁵3s², 3S) + H(1s, 1S)              | 0⁻                                            | X²Σ⁺                   | 0⁺                                                   | 0.0               |
| Mg(3s³p, 3P) + H(1s, 1S)               | 20 972⁺                                       | (2)²Σ⁺,(1)²Π,(1)¹Σ⁺,(1)¹Π | 21 850⁺                                               | 4                 |
| Mg(3s³p, 3P) + H(1s, 1S)               | 34 814⁺                                       | (3)²Σ⁺,(2)²Π           | 35 051⁺                                               | 0.7               |
| Mg(3s⁴s, 4S) + H(1s, 1S)               | 43 677⁺                                       | (4)²Σ⁺,(5)²Σ⁺,(2)⁴Σ⁺   | 41 197⁺                                               | 5.7               |
| Mg(3s⁴s, 4S) + H(1s, 1S)               | 48 083⁺                                       | (6)²Σ⁺                 | 43 503⁺                                               | 9.4               |
| Mg(3s³p, 3P) + H(1s, 1S)               | 50 870⁺                                       | (7)²Σ⁺,(3)²Π,(3)¹Σ⁺,(2)¹Π | 47 844⁺                                               | 5.9               |
| Mg(3s³d, 1D) + H(1s, 1S)               | 51 810⁺                                       | (8)²Σ⁺,(1)²Δ,(4)²Π    | 46 403⁺                                               | 10.4              |

| Dissociation of atomic levels Sr + H | Dissociation energy limit of SrH levels (cm⁻¹) | Molecular states of SrH | Total dissociation energy limit of Sr + H atoms (cm⁻¹) | Relative error (%) |
|-------------------------------------|-----------------------------------------------|------------------------|-------------------------------------------------------|-------------------|
| Sr(5s⁵s, 3S) + H(1s, 1S)            | 0⁻                                            | X²Σ⁺                   | 0⁺                                                   | 0.0               |
| Sr(5s³p, 3P) + H(1s, 1S)            | 12 892⁺                                       | (2)²Σ⁺,(1)²Π,(1)¹Σ⁺,(1)¹Π | 14 573⁺                                               | 11.5              |
| Sr(5s⁴d, 1D) + H(1s, 1S)            | 20 645⁺                                       | (3)²Σ⁺,(1)²Δ,(2)²Π    | 18 232⁺                                               | 11.7              |
| Sr(5s³p, 3P) + H(1s, 1S)            | 21 118⁺                                       | (3)²Π,(4)²Σ⁺          | 21 698⁺                                               | 2.7               |
| Sr(5s⁴d, 1D) + H(1s, 1S)            | 21 383⁺                                       | (5)²Σ⁺,(2)²Δ,(4)²Π    | 20 149⁺                                               | 5.8               |

* Present work.
* Experimental values from the NIST atomic spectra Data base.
astrophysical community very early [19–21]. High resolution infrared emission spectra have been measured by Seto et al [22] for MgH molecule with the record of vibration–rotation emission spectrum.

The electronic transition of the strontium hydride molecule SrH has been investigated since the thirties [23–26]. Recently, experimental [27] and theoretical [28–30] studies have been occurred to investigate the low lying electronic sates and to calculate the potential energy curves with the molecular parameters. By using diode laser spectrometer Magg et al [31] and Birk et al [32] recorded three vibration–rotation bands.

In the present work, we employed the ab-initio method to investigate the potential energy curves (PECs) and the static dipole moment curves (DMCs) of the low-lying 26, 27 and 25 doublet and quartet electronic states of the BeH, MgH and SrH molecules respectively. The spectroscopic constants as the equilibrium internuclear distance \( R_0 \), the harmonic frequency \( \omega_0 \), the vibrational constant \( B_0 \), the transition energy with respect to the ground state minimum \( T_e \), and the permanent dipole moment \( \mu \) are calculated for the bound states of these molecules. For the study of the rovibrational problem there are many important theories and techniques in literature with computer programs as LEVEL [33–36] or the Duo program [37]. In order to obtain high order precision there is a need for large order centrifugal distortion constant as \( D_{v,H \nu,L \nu}^{e} \) [38–44]. By using the canonical function approach one can obtain these constants with the high values of vibrational levels even near dissociation by one single and simple routine. This method provides strong evidence for our assumption that the higher-order of \( D_{v,H \nu,L \nu}^{e} \) and the higher vibrationel \( v \) and rotational level \( J \) for any electronic state and any type of potential energy curves (either experimental, empirical or theoretical) are as accurate as the low-order values. In this technique we use the compact form \( e_n = \langle \Phi_0 | R \Phi_{n-1} \rangle \) (R = 1/\( r \)) of a CDC (\( e_1 = B_0, e_2 = D_0, e_3 = H_0, \ldots \)) of any order \( n \) where \( \Phi_n \) is the solution of the differential equation \( \Phi''_n + f(r)\Phi'_n = s(r) \) where \( f(r) \) and \( s(r) \) are given, as well as their initial values at an arbitrary origin. This is done by using a simple method for the computation of the functions \( \Phi_n \) orthogonal to \( \Phi_0 \) (the vibrational wavefunction), and by deriving exact values of \( \Phi_n(r_0) \) and \( \Phi'_n(r_0) \) which are the initial values of \( \Phi_n \) at an arbitrary point \( r_0 \) [38, 45–47].

2. Computational approach

2.1. Ab initio calculation

In the present work an ab initio calculation of the lowest-lying electronic states of BeH, MgH and SrH has been performed via CASSCF and MRCI (single and double excitation with Davidson correction) calculations. Multi-reference CI calculations (MRCI) were performed to determine the correlation effects. The potential energy calculations for the states \( \Sigma^\pm, \Delta \) of the molecules have been carried by using CAS-SCF method. The calculations have been performed via the computational chemistry program MOLPRO [48] taking the advantage of the graphical user interface GABEDIT [49]. This software is intended for high level accuracy correlated ab initio
calculations. MOLPRO has been run on a PC- computer with UNIX-type operating systems. For the three studied molecules BeH, MgH and SrH, the one electron hydrogen atom is treated using for s, p, d, and f functions the correlation-consistent polarized Quadruple-Zeta basis set, augmented with sets of diffuse functions aug-cc-pVQZ \[50\].

Figure 2. Potential energy and dipole moments curves of $^3\Pi$ states of BeH molecule.

Figure 3. Potential energy and dipole moments curves of $^4\Sigma^\pm$ and $^4\Delta$ states of BeH molecule.
In the BeH molecule, the beryllium atom is treated in all electron schemes, the 4 electrons are considered using for $s$, $p$, $d$, and $f$ functions of the triple zeta basis set VTZ [51]. The quality of chosen basis sets for the H, Be, Mg, and Sr isolated atoms is checked by comparing our calculation of the lowest energy values of the asymptotic energy at each dissociative asymptote with those obtained experimentally by NIST Atomic Spectra Database [52] (table 1). This comparison shows a relative difference ranges between $0.7\% \leq \Delta E/E \leq 11.7\%$. For some of the highest electronic states the dissociation limits are not obtained because of the undulation of potential energy curves of these states. For these undulations the short-range electronic interactions are significant at certain energy points. They are related to the singularities in the electronic Hamiltonian operator and giving rise to the Coulomb cusp in the electronic wave function and appearance of cusps in the exact wave function. Also, these undulations are explained by the breakdown of the Born-Oppenheimer (B.O) approximation since the interactions between electronic states are significant at certain energy points, and the responsible term for the so-called ‘non-adiabatic effects’ can be very important and it cannot be neglected. However, the overall good relative error given in table 1 can ensure the accuracy of our calculated data.

An heteronuclear diatomic molecule belong to $C_{\infty v}$ group. Since MOLPRO can handle only Abelian point-groups the linear molecules are treated in $C_2v$ instead of $C_{\infty v}$. The states $\Sigma^+$, $\Pi_x$, $\Delta_0$, and $\Delta_x2–y2$ belong to the irreducible representation number 1, the states $\Pi_{yz}$, $\Delta_{xy}$ belong to the irreducible representation 2, the states $\Pi_y$, $\Delta_{yz}$ belong to the irreducible representation 3, and $\Delta_{zx}$ belong to the irreducible representation 4. Among the 5 electrons explicitly considered for BeH (4 electrons for beryllium and 1 electron for hydrogen) two inner electrons were frozen in subsequent calculations so that 3 valence electrons were explicitly treated. The active space contains 7 $s$ ($Be: 2s, 2p_0, 3s, 3p_0, 4s, 3d_{0,3} H: 1s$), $3\pi$ ($Be: 2p_{0,1}, 3p_{0,1}, 3d_{0,1}$) and $1\delta$ ($Be: 3d_{0,3}$) orbitals which corresponds to 15 active molecular orbitals distributed into irreducible representation $a_1, b_1, b_2, a_2$, noted [1, 3, 8].

For the molecule MgH, the 12 electrons of the magnesium atom are considered using for $s$, $p$, and $d$ functions the cc-pVQZ basis set. Among the 13 electrons of the considered molecule, 10 electrons were frozen in subsequent calculations, so that 3 valence electrons were explicitly treated. The active space contains 7 $\sigma$ ($Be: 2s, 2p_0, 3s, 3p_0, 3d_0, 4s, 3d_{0,3}, H: 1s, 2s, 2p_0), 3\pi$ ($Mg: 3p_{0,1}, 3d_{0,1}; H: 2p_{0,1}), 1\delta$ ($Mg: 3d_{0,3})$ orbitals in the $C_2v$ symmetry; this corresponds to 15 active molecular orbitals distributed into irreducible representation $a_1, b_1, b_2, a_2$ in the following way: $8a_1, 3b_1, 3b_2, 1a_2$, noted [1, 3, 8].

In the molecule SrH, the strontium species is considered using for $s$, $p$, $d$, and $f$ functions the Effective Core Potential ECP28MWB basis set, where 28 electrons are considered as inner electrons and the remaining 10 electrons are considered as valence electrons. Among the 11 electrons, 8 electrons were frozen in subsequent calculations, so that 3 electrons were explicitly treated. The active space contains 2$\sigma$ ($Sr: 4d_{0,3}; H: 1s), 1\pi$($Sr: 4d_{0,3}$),

Figure 4. Potential energy and dipole moments curves of $^4\Pi$ states of BeH molecule.
Table 2. Positions of the crossings and avoiding crossing between the different electronic states of molecules BeH, MgH, and SrH.

| Molecule | State 1 | State 2 | Crossing between (\(n_1\) state1)/(\(n_2\) state2) | R\(_c\) (Å) |
|----------|---------|---------|-----------------------------------------------|----------|
| BeH      | \(1^3\Delta\) | \(6^1\Sigma^+\) | 1/6 | 1.343 |
|          | \(1^3\Delta\) | \(1^3\Sigma^-\) | 1/1 | 2.543 |
|          | \(1^1\Delta\) | \(2^1\Sigma^-\) | 1/2 | 2.383 |
|          | \(2^1\Delta\) | \(2^1\Sigma^-\) | 2/2 | 3.643 |
|          | \(2^1\Delta\) | \(3^1\Sigma^-\) | 2/3 | 1.223 |
|          | \(2^1\Delta\) | \(3^1\Sigma^-\) | 2/3 | 1.983 |
|          | \(2^1\Delta\) | \(3^1\Sigma^-\) | 3/2 | 3.023 |
|          | \(2^1\Delta\) | \(3^1\Sigma^-\) | 3/2 | 3.963 |

Avoiding crossing

| State 1 | State 2 | \(\Delta E\) \(10^{-3}\) | R\(_c\) (Å) |
|---------|---------|-----------------|----------|
| \(2^3\Sigma^+\) | \(3^5\Sigma^+\) | 4.254 83 | 1.323 |
| \(3^3\Sigma^+\) | \(4^3\Sigma^+\) | 30.028 33 | 1.883 |
|          |          | 13.755 58     | 4.963 |
| \(4^3\Sigma^+\) | \(5^3\Sigma^+\) | 12.952 38 | 2.463 |
| \(5^3\Sigma^+\) | \(1^1\Delta\) | 15.724 43 | 2.063 |
| \(5^3\Sigma^+\) | \(6^3\Sigma^+\) | 18.320 91 | 2.023 |
| \(6^3\Sigma^-\) | \(7^5\Sigma^-\) | 3.694 17 | 3.183 |
| \(2^2\Pi\) | \(3^2\Pi\) | 3.459 63 | 1.683 |
| \(3^2\Pi\) | \(4^2\Pi\) | 6.187 56 | 1.283 |
| \(4^2\Pi\) | \(5^2\Pi\) | 8.525 29 | 2.183 |
| \(1^1\Sigma^-\) | \(2^1\Sigma^-\) | 24.930 41 | 1.563 |
| \(1^1\Delta\) | \(2^1\Delta\) | 0.225 74 | 1.623 |
| \(2^2\Pi\) | \(3^2\Pi\) | 11.356 53 | 1.483 |

| State 1 | State 2 | Crossing between (\(n_1\) state1)/(\(n_2\) state2) | R\(_c\) (Å) |
|---------|---------|-----------------------------------------------|----------|
| \(2^3\Sigma^+\) | \(3^5\Sigma^+\) | 1/7 | 1.959 682 |
|          |          | 1/8 | 3.759 682 |
|          |          | 1/8 | 4.179 682 |
|          |          | 1/8 | 7.119 682 |
| \(2^1\Delta\) | \(3^1\Delta\) | 2/1 | 1.939 682 |
| MgH      | \(2^3\Sigma^+\) | \(4^3\Sigma^+\) | 5/1 | 3.799 682 |
|          |          | \(2^1\Delta\) | 5/1 | 6.079 682 |
|          |          | \(2^1\Delta\) | 6/2 | 2.539 682 |

Avoiding crossing

| State | State n + 1/State n | R\(_{AC}\) (Å) | \(\Delta E_{AC}\) (cm\(^{-1}\)) |
|-------|---------------------|----------------|--------------------------|
| \(2^1\Sigma^+\) | 4/3 | 6.179 682 | 187.87 |
|          | 5/4 | 2.799 682 | 2486.88 |
|          | 6/5 | 2.579 682 | 398.72 |
|          | 7/6 | 2.199 682 | 1412.36 |
|          | 7/6 | 4.699 682 | 2068.04 |
|          | 8/7 | 3.799 682 | 278.27 |
|          | 8/7 | 7.259 682 | 452.84 |
| \(2^2\Pi\) | 4/3 | 4.119 682 | 176.06 |
| \(4^3\Sigma^+\) | 2/1 | 1.779 682 | 1552.91 |

| State 1 | State 2 | Crossing between (\(n_1\) state1)/(\(n_2\) state2) | R\(_c\) (Å) |
|---------|---------|-----------------------------------------------|----------|
| \(2^1\Delta\) | \(3^3\Sigma^+\) | 1/3 | 3.183 |
| \(4^1\Delta\) | \(4^3\Sigma^+\) | 2/3 | 3.963 |

Avoiding crossing

| State | State n + 1/State n | R\(_{AC}\) (Å) | \(\Delta E_{AC}\) (cm\(^{-1}\)) |
|-------|---------------------|----------------|--------------------------|
| \(2^1\Sigma^+\) | 1/2 | | |
| \(2^3\Sigma^+\) | 2/3 | | |
| \(2^1\Sigma^+\) | 4/5 | | |
| \(2^3\Sigma^+\) | 5/6 | | |
| \(2^5\Sigma^+\) | 2/3 | | |
| \(4^3\Sigma^+\) | 2/3 | | |
| \(4^2\Pi\) | 2/4 | | |
and $1\delta$ (Sr: 4d±) orbitals in the C\textsubscript{2v} symmetry; this corresponds to 6 active molecular orbitals distributed into irreducible representation a\textsubscript{1}, b\textsubscript{1}, b\textsubscript{2}, a\textsubscript{2} in the following way: 3a\textsubscript{1}, 1b\textsubscript{1}, 1b\textsubscript{2}, 1a\textsubscript{2}, noted [1, 3].

3. Results

3.1. Potential energy curves

For the BeH molecule, the calculations have been performed for 442 internuclear distances in the range $0.67 \, \text{Å} \leq R \leq 7.70 \, \text{Å}$ for 26 electronic states in the representation $\Sigma^{\pm} \Lambda^{(\pm)}$. The number of electronic states obtained in the present work is 14 doublet electronic states (8 in symmetry 1, 5 in symmetry 2 and 1 in symmetry 4), and 12 quartet electronic states (6 in symmetry 1, 3 in symmetry 2 and 3 in symmetry 4). The potential energy with the dipole moment curves of these electronic states are given in figures 1–4 while the complete tables with the figures of these potential energy curves are given in the supplementary materials. In the considered range of R, some crossings and avoided crossings occur between some potential energy curves of at different values of internuclear distances for the doublet and quartet electronic states. The positions of these crossings and avoided crossings are given in table 2.

The calculations for MgH molecule have been performed for 488 internuclear distances in the range $0.80 \, \text{Å} \leq R \leq 8.9 \, \text{Å}$ in the representation $\Sigma^{\pm} \Lambda^{(\pm)}$. The number of electronic states obtained in the present work is 17 doublet states (9 in symmetry one, 6 in symmetry two, and 2 in symmetry four) and 13 quartet electronic states (7 in symmetry one, 4 in symmetry two, and 2 in symmetry four). The potential energy with the dipole moment curves of these electronic states are given in figures 5–8 while the complete tables with the figures of these potential energy curves are given in the supplementary materials. In the considered range R, crossings and avoided crossings occur between some of the investigated potential energy curves. The positions of these crossings and avoided crossings are given in table 2.
The calculations of the SrH molecule have been performed for 649 internuclear distances in the range 1.2 Å ≤ R ≤ 7.3 Å in the representation $^{2S+1} \Lambda \left(\pm\right)$. The number of electronic states obtained in the present work is 10 doublet electronic states (6 in symmetry one and 4 in symmetry two), and 11 quartet states (7 in symmetry one and 4 in symmetry two). The potential energy with the dipole moment curves of these electronic states are depicted in Figures 6 and 7.

Figure 6. Potential energy and dipole moments curves of $^2\Pi$ states of MgH molecule.

Figure 7. Potential energy and dipole moments curves of $^4\Sigma$± and $^4\Delta$ states of MgH molecule.
given in figures 9–12 while the complete tables with the figures of these potential energy curves are given in the supplementary materials. In the considered range $R$, crossings and avoided crossings happen in the doublet and quartet electronic states where their positions are listed in table 2.
3.2. Dipole moment

3.2.1. BeH molecule

The dipole moment operator is among the most reliably predicted physical properties. The expectation value of this operator is sensitive to the nature of the least energetic and most chemically relevant valence electrons. The HF dipole moment is usually large, as the HF wave function over estimates the ionic contribution. To obtain the best accuracy of this operator, multireference configuration interaction (MRCI) wave function were constructed using multi configuration Self-consistent field (MCSCF) active space. All the calculation were performed with...
the MOLPRO [48] program. The variation of the static dipole moment curves in term of the internuclear R are plotted with potential energy curves in the same figures in order to show the agreement between the positions of the avoided crossings of the potential energy curves and the crossing of the dipole moment curves. This agreement, which is represented by vertical lines, is a criteria of the validity and the accuracy of the present work for the titled molecules.

The static dipole moments curves with the potential energy curves for the 3 considered molecules BeH, MgH, and SrH are given as function of the internuclear distance R in figures 1–12 while the complete tables with the figures of these static dipole moments curves are given in the supplementary materials. The dipole moment curves of the electronic states \((4^2\Sigma^+, 4^2\Pi), (4^4\Sigma^+, 4^4\Pi)\) of BeH, \((4^4\Sigma^+, 4^4\Pi)\) of MgH, and \((6^2\Sigma^+, 6^2\Pi)\) of SrH dissociate at infinity as ionic character, while these dipole moment curves of the other electronic states tends to zero at infinity.

4. Comparison and discussion

4.1. BeH molecule
The calculations of the spectroscopic constants such as the vibrational harmonic constant \(\omega_v\), the internuclear distance at equilibrium \(r_0\), the rotation constant \(B_v\), the centrifugal distortion constant \(D_v\), and the electronic transition energy with respect to the ground state \(T_e\) have been done by fitting the energy values around the equilibrium position to a polynomial in terms of the internuclear distance, the degrees of these polynomials are determined from the evaluation of the statistical error for the coefficients. These values are displayed in table 3 together with the available data in literature either theoretical or experimental. Due to the avoided crossing at their minima, we have not carried out the calculations for the spectroscopic constants for the states \((3^2\Sigma^+, 2^2\Pi), (3^2\Pi), (1^4\Delta)\), and \((2^4\Delta)\).

4.1.1. Comparison with the experimental values
As shown in table 3 the comparison of the present values of \(T_e\) for the electronic states \(A^2\Pi, C^2\Sigma^+, \) and \(4^2\Pi\) with the experimental data given by Colin and DeGreef, and Colin et al [54, 64, 60], showed a very good agreement with relative differences \(\delta T_e/T_e = 1.31\%, 0.52\%, 10.36\%\), respectively. Similar very good agreement is obtained by comparing our value of \(T_e\) for the state \(A^2\Pi\) with that given by O’Neil and Schaefer [60, 65, 66] with relative
Table 3. Spectroscopic constants for the lowest electronic states of the molecule BeH.

| state    | \( T_e \) \( (\text{cm}^{-1}) \) | \( \Delta T_e / T_e \% \) | \( R_e \) \( (\text{A}) \) | \( \Delta R_e / R_e \% \) | \( \omega_e \) \( (\text{cm}^{-1}) \) | \( \Delta \omega_e / \omega_e \% \) | \( \omega_e \omega_e \) \( (\text{cm}^{-1}) \) | \( B_e \) \( (\text{cm}^{-1}) \) | \( \Delta B_e / B_e \% \) |
|----------|-------------------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| \( X^2 \Sigma^+ \) | 0.00                          | 0.00             | 1.347            | 2043.93          | 35.8             | 10.255           |               |                 |                 |
|         |                               |                  | 1.343            | 0.3              | 0.25             | 46.15            |               |                 |                 |
|         |                               |                  | 1.345            | 0.1              | 0.82             | 37.326           | 10.266           | 0.1             |
|         |                               |                  | 1.342            | 0.33             | 0.84             | 37.433           | 10.316           | 0.6             |
|         |                               |                  | 1.342            | 0.34             | 2.67             | 10.319           | 0.65            |
|         |                               |                  | 1.340            | 0.44             | 0.37             | 10.191           | 0.62            |
|         |                               |                  | 1.340            | 0.44             | 2.76             | 10.190           | 0.624           |
|         |                               |                  | 1.341            | 0.412            | 0.856            | 10.185           | 0.68            |
|         |                               |                  | 1.342            | 0.34             | 2061.416         | 10.319           | 0.624           |
| \( A^2\Pi \) | 20 267.09                     | 1.338            | 2072.68          |                 |                 |                  |                 | 10.38           | 0.1             |
|         | 20 033                         | 1.15             | 2079             | 1.3377           | 0.37             | 10.39            |                 |                 |
|         | 18 270                         | 9.85             | 2088.58          | 1.3335           | 0.8              | 10.4567          |                 |                 |
|         | 20 647.78                      | 1.87             | 2089.93          | 1.33            | 0.34             | 10.466           | 0.83            |
|         | 20 002.54                      | 1.31             | 2088.38          | 1.333            | 0.75             | 10.467           | 0.83            |
|         | 22 480.97                      | 10.92            | 2088.38          |                 |                 |                  |                 | 10.467           | 0.83            |
|         | 22 496.12                      | 10.92            | 2088.38          |                 |                 |                  |                 |                 |
| \( C^2 \Sigma^+ \) | 30 732.62                     | 2.3              | 100.22           | 3.907            | 4.44             | 3.496            |                 | 0.14            |
|         | 22 367                         | 27.22            | 1053             | 4.44             | 4.44             | 3.511            | 0.28            |
|         | 44 441.13                      | 44.6             | 22.3066          | 5.84             | 17.44            | 1.46             |                 | 0.33            |
|         | 30 407.09                      | 1.06             | 2642.8           | 5.84             |                 |                  | 1.46             |                 |
|         | 30 891.022                     | 0.52             | 1993.23          | 5.84             | 1.75             |                 | 1.46             |                 |
| \( 1^4\Pi \) | 39 551.13                     | 3.907            | 2642.8           | 5.84             | 1.75             |                 | 1.46             |                 |
| \( 1^4 \Sigma^+ \) | 39 551.13                     | 3.907            | 2642.8           | 5.84             | 1.75             |                 | 1.46             |                 |
| \( 3^3 \Sigma^+ (2nd min) \) | 39 551.13                     | 3.907            | 2642.8           | 5.84             | 1.75             |                 | 1.46             |                 |
| \( 4^3 \Sigma^+ (1st min) \) | 39 551.13                     | 3.907            | 2642.8           | 5.84             | 1.75             |                 | 1.46             |                 |
|         | 78 292                         | 39.16            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 49 361.11                      | 12.3             | 1668.15          | 8.71             |                 |                  | 1.46             |                 |
|         | 48 877.17                      | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 62 843                         | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 63 684.76                      | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 89 406                         | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 54 119.78                      | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |
|         | 71 000.08                      | 13.12            | 315.93           | 1.46             | 8.71             |                 | 1.46             |                 |

Notes: (a) \( \geq 0.05 \text{ cm}^{-1} \), (b) \( \geq 1.0 \text{ cm}^{-1} \), (c) \( \geq 2.0 \text{ cm}^{-1} \).
| state       | \(T_e\) (\(\text{cm}^{-1}\)) | \(\Delta T_e/T_e\)% | \(R_e(\text{Å})\) | \(\Delta R_e/R_e\)% | \(\omega_e(\text{cm}^{-1})\) | \(\Delta \omega_e/\omega_e\)% | \(\omega_{5e}(\text{cm}^{-1})\) | \(B_e(\text{cm}^{-1})\) | \(\Delta B_e/B_e\)% |
|------------|-------------------------------|----------------------|---------------------|----------------------|-----------------------------|-------------------------------|-----------------------------|-------------------------|----------------------|
| 4\(^1\)\(\Pi\) | 65 504.48\(^a\) | 1.34\(^a\) | 2939.75\(^a\) | 10.33\(^a\) | | | | | |
| 78 393 | 19.67 | 58 636.48\(^b\) | 10.48 | 58 717.139\(^c\) | 10.36 | | | | |
| 1\(^1\)\(\Sigma^-\) | 66 139.68\(^a\) | 1.51\(^a\) | 1520.22\(^a\) | 8.15 | | | | | |
| 2\(^1\)\(\Sigma^-\) (2nd min) | 77 741.85\(^a\) | 4.77\(^a\) | 1264.53\(^a\) | 0.84\(^a\) | | | | | |
| 1\(^2\)\(\Delta\) | 71 586.74\(^a\) | 1.58\(^a\) | 1294.02\(^a\) | 7.49\(^a\) | | | | | |
| 1\(^3\)\(\Pi\) | 54 603.71\(^b\) | 23.72 | | | | | | | |
| 59 624\(^c\) | 16.71 | | | | | | | | |
| 5\(^3\)\(\Pi\) | 74 423.80\(^a\) | 1.36\(^a\) | 2027.59\(^a\) | 10.05\(^a\) | | | | | |
| 7\(^2\)\(\Sigma^+\) (1st min) | 75 191.15\(^a\) | 1.76\(^a\) | 851.35\(^a\) | 6.01\(^a\) | | | | | |
| (3rd min) | 83 590.39\(^a\) | 5.31\(^a\) | 134.23\(^a\) | 0.75\(^a\) | | | | | |
| 2\(^1\)\(\Pi\) | 77 618.63\(^a\) | 5.42\(^a\) | 20.87\(^a\) | 0.72\(^a\) | | | | | |
| 6\(^2\)\(\Sigma^+\) (3rd min) | 79 666.22\(^a\) | 5.83\(^a\) | 141.82\(^a\) | 0.54\(^a\) | | | | | |
| 3\(^3\)\(\Sigma^+\) (1st min) | 85 242.77\(^a\) | 3.2\(^a\) | 314.98\(^a\) | 1.82\(^a\) | | | | | |
| (2nd min) | 86 083.35\(^a\) | 6.2\(^a\) | 198.46\(^a\) | 0.49\(^a\) | | | | | |
| 3\(^1\)\(\Pi\) | 88 393.12\(^a\) | 2.41\(^a\) | 513.90\(^a\) | 3.2\(^a\) | | | | | |
| 4\(^1\)\(\Sigma^-\) (1st min) | 94 088.65\(^a\) | 2.02\(^a\) | 359.15\(^a\) | 4.71\(^a\) | | | | | |
| (2nd min) | 93 337.84\(^a\) | 5.05\(^a\) | 479.35\(^a\) | 0.73\(^a\) | | | | | |
| 5\(^3\)\(\Sigma^-\) (1st min) | 119 950.46\(^a\) | 1.62\(^a\) | 1106.51\(^a\) | 7.1\(^a\) | | | | | |
| (2nd min) | 120 207.15\(^a\) | 2.2\(^a\) | 923.21\(^a\) | 3.84\(^a\) | | | | | |

\(^a\) The values given in bold are for the present work,
\(^b\) Ref. [53],
\(^c\) Ref. [54],
\(^d\) Ref. [55],
\(^e\) Ref. [56],
\(^f\) Ref. [57],
\(^g\) Ref. [58],
\(^h\) Ref. [59],
\(^i\) Ref. [60],
\(^j\) Ref. [61],
\(^k\) Ref. [62],
\(^m\) Ref. [63].
Table 4. Spectroscopic constants for the lowest electronic states of the molecule MgH.

| State | $T_e$ (cm$^{-1}$) | $\Delta T_e/T_e$ | $R_e$ (Å$^e$) | $\Delta R_e/R_e$ | $\omega_e$ (cm$^{-1}$) | $\Delta \omega_e/\omega_e$ | $\omega_{e\chi_e}$ (cm$^{-1}$) | $\Delta \omega_{e\chi_e}/\omega_{e\chi_e}$ | $\Delta \chi_e/\chi_e$ | $\Delta T_e/Te$ | $\Delta \omega_e/\omega_e$ | $\Delta \omega_{e\chi_e}/\omega_{e\chi_e}$ |
|-------|------------------|------------------|--------------|-----------------|--------------------------|--------------------------|-----------------------------|-----------------------------|-----------------|-----------------|--------------------------|-----------------------------|
| 0.00  | 1.744 23$^a$    | 1.72$^b$         | 1.729 66$^c$ | 1.743$^d$       | 1.726 19$^e$             | 1.724$^f$               | 1.713$^g$                   | 1.730$^h$                   | 1.69$^i$        | 1570.66$^j$     | 32.56$^k$               | 6.03$^l$                        |
|       | 1.72$^b$         | 1.39%            | 1.453 66$^b$ | 0.83%           | 1.495 26$^b$             | 1.495 25$^b$             | 0.58%                       | 31.63$^d$                   | 3.50%           | 21.5$^d$        | 29.67%                   | 2.45%                        |
| 19 130$^a$ | 1.40%            | 1.67$^b$         | 1.679$^b$    | 0.65%           | 1.598 4$^b$              | 1.77%                    | 33.17$^b$                   | 2.98%                       | 1.87%           | 31.4$^b$        | 2.93%                    | 3.22%                        |
| 19 278$^b$ | 0.77%            | 1.69$^b$         | 1.699$^b$    | 0.53%           | 1.561 8$^b$              | 0.56%                    | 1.67$^b$                   | 1.00%                       | 32.1$^b$        | 13.66%          | 3.33%                    | 2.45%                        |
| 19 170$^c$ | 0.21%            | 1.6612$^b$       | 1.70%        | 1.572 02$^b$    | 0.09%                    | 28.046$^b$               | 32.53$^b$                   | 0.07%                       | 6.1913$^d$     | 2.67%           | 6.26$^d$                 | 3.75%                        |
| 14 704$^d$ | 23.14%           | 1.668$^b$        | 1.30%        | 1.599 5$^b$     | 1.84%                    | 32.536$^b$               | 31.2$^b$                    | 1.73%                       | 3.33%           | 3.33%           | 3.33%                    | 2.45%                        |
| 19 216.8$^e$ | 0.45%            | 1.673$^b$        | 1.00%        | 1.692$^b$       | 7.72%                    | 30.0$^b$                 | 7.86%                       | 6.23$^b$                    | 3.33%           | 3.33%           | 3.33%                    | 2.45%                        |
|       | 1.680$^b$        | 0.61%            | 1.598$^b$    | 1.36%           | 31.9$^b$                 | 2.03%                    | 6.178$^b$                   | 2.45%                       | 2.45%           | 2.45%           | 2.45%                    | 2.45%                        |
| 22 174$^f$ | 2.63$^b$         | 812.35$^b$       | 2.63$^b$     | 2.59$^b$        | 1.52%                    | 831.47$^b$               | 2.35%                       | 1.33%                       | 2.45%           | 2.45%           | 2.45%                    | 2.45%                        |
| 22 051$^b$ | 0.55%            | 2.59$^b$         | 2.596$^b$    | 1.29%           | 828.4$^b$                | 1.97%                    | 1.67$^b$                   | 1.00%                       | 32.1$^b$        | 31.2$^b$        | 7.86%                    | 2.45%                        |
| 22 410$^c$ | 1.06%            | 2.622$^b$        | 0.30%        | 818.6$^d$       | 0.77%                    | 2.617$^b$                | 0.49%                       | 2.79%                       | 3.33%           | 3.33%           | 3.33%                    | 2.45%                        |
| 18 414$^d$ | 16.95%           | 2.617$^b$        | 0.49%        | 789.64$^b$      | 2.79%                    | 2.596$^b$                | 1.29%                       | 1.97%                       | 2.45%           | 2.45%           | 2.45%                    | 2.45%                        |
| 32 409$^e$ | 3.96$^b$         | 69.35$^b$        | 3.96$^b$     | 1.71$^h$        | 1483.93$^b$              | 46.38$^b$                | 5.93$^b$                    | 5.93%                       | 3.33%           | 3.33%           | 3.33%                    | 2.45%                        |
| 1st min: | 1.71$^h$         | 1483.93$^b$      | 46.38$^b$    | 5.93$^b$        | 36 251$^i$               | 2.35%                    | 2.59$^b$                   | 1.52%                       | 831.47$^b$      | 2.35%           | 1.33%                    | 2.45%                        |
| (3)$^3\Sigma^+$ | 35 401$^i$ | 2.35%            | 1.67$^b$     | 2.34%           | 1498.43$^b$              | 0.97%                    | 50.33$^b$                   | 8.52%                       | 8.52%           | 8.52%           | 8.52%                    | 8.52%                        |
| 35 551$^i$ | 1.93%            | 1.67$^b$         | 2.34%        | 1445.4$^i$      | 2.60%                    | 392.53$^i$               | 5.34%                       | 1.72$^i$                    | 1.03%           | 1.03%           | 1.03%                    | 1.03%                        |
| 2nd min: | 0.62%            | 4.1$^i$          | 1.22%        | 392.53$^i$      | 5.34%                    | 1.72$^i$                 | 1.03%                       | 1.03%                       | 1.03%           | 1.03%           | 1.03%                    | 1.03%                        |
| 41 325$^i$ | 4.05$^b$         | 371.56$^b$       | 4.05$^b$     | 371.56$^b$      | 5.34%                    | 1.72$^i$                 | 1.03%                       | 1.03%                       | 1.03%           | 1.03%           | 1.03%                    | 1.03%                        |
| 1st min: | 1.72$^i$         | 1763.17$^i$      | 51.44$^d$    | 5.86$^d$        | 40 454$^i$               | 5.86$^d$                 | 3.33%                       | 3.33%                       | 3.33%           | 3.33%           | 3.33%                    | 2.45%                        |
| 38 106$^i$ | 5.80%            | 1.73$^b$         | 0.58%        | 1722.12$^i$     | 2.33%                    | 47.98$^b$                | 6.73%                       | 2.45%                       | 2.45%           | 2.45%           | 2.45%                    | 2.45%                        |
Table 4. (Continued.)

| State | $T_e$ (cm$^{-1}$) | $\Delta T_e/T_e$ | $R_e$(A") | $\Delta R_e/R_e$ | $\omega_e$ (cm$^{-1}$) | $\Delta \omega_e/\omega_e$ | $\omega_{X_e}$ (cm$^{-1}$) | $\Delta \omega_{X_e}/\omega_{X_e}$ | Be | $\Delta$Be/Be |
|-------|----------------|-----------------|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----|-------------|
| (4)$^2\Sigma^+$ | 38 485$^a$ | 4.87% | 1.79$^b$ | 4.07% | 205$^b$ | 0.57$^a$ |
| 2nd min: | 47 211$^b$ | 0.80% | 5.35$^b$ | 2.72% | 218.52$^b$ | 6.60$^b$ |
| 1min: 46 835$^c$ | 1.69$^c$ | 1297.30$^c$ | 32.56$^c$ | 5.98$^c$ |
| (2)$^3\Pi$ | 41 350$^a$ | 9.04% | 1.64$^b$ | 2.96% | 1528.52$^b$ | 17.82% |
| 41 240$^b$ | 9.72% | 1.682$^c$ | 0.47% | 1740$^c$ | 34.12% |
| 2nd min: | 44 883$^a$ | 2.49$^a$ | 461.78$^a$ | 571.9$^a$ | 2.78$^a$ |
| 1st min: | 46 561$^a$ | 1.76$^a$ | 1468.05$^a$ | 5.62$^a$ |
| (5)$^3\Sigma^+$ | 43 138$^a$ | 7.35% | 1.69$^b$ | 3.98% | 1631.23$^b$ | 11.11% |
| 2nd min: | 53 793$^a$ | 2.77$^a$ | 1134.19$^a$ | 1.9$^a$ | 2.25$^a$ |
| 48 973$^b$ | 1.92$^b$ | 1171.26$^b$ | 4.66$^b$ |
| (3)$^3\Pi$ | 42 861$^b$ | 12.48% | 1.67$^b$ | 13.02% | 1466.61$^b$ | 25.22% |
| 42 573$^b$ | 13.07% | 1.68$^b$ | 12.50% | 3.13$^b$ |
| (4)$^2\Pi$ | 49 403$^a$ | 1.89$^a$ | 1768.37$^a$ | 14.54$^a$ | 4.85$^a$ |
| (7)$^3\Sigma^+$ | 57 950$^b$ | 2.34$^a$ | 732.16$^a$ | 335.27$^a$ | 3.13$^a$ |
| 2nd min: | 61 749$^a$ | 4.7$^a$ | 259.82$^a$ | 0.015$^a$ | 0.77$^a$ |
| (1)$^2\Delta$ | 58 211$^a$ | 26.50% | 1.75$^a$ | 6.28% | 1633$^a$ | 29.55% |
| 42 790$^b$ | 1.64$^b$ | 1260.5$^a$ | 5.65$^a$ |
| (6)$^2\Sigma^+$ | 59 187$^b$ | 6.7$^b$ | 7.58$^b$ | 1188.62$^b$ | 0.35$^b$ |
| 2nd min: | 59 309$^a$ | 1.8$^a$ | 1360.3$^a$ | 49.38$^a$ | 5.35$^a$ |
| (3)$^4\Sigma^+$ | 60 623$^a$ | 2.83$^a$ | 491.82$^a$ | 13.47$^a$ | 2.17$^a$ |
| 2nd min: | 61 936$^a$ | 8.12$^a$ | 35 011.7$^a$ | 0.217$^a$ |
| (8)$^3\Sigma^+$ | 60 672$^a$ | 2.13$^a$ | 1403.69$^a$ | 232.54$^a$ | 3.82$^a$ |
| 2nd min: | 62 642$^a$ | 3.77 | 774.04$^a$ | 5.16$^a$ | 1.22$^a$ |
Table 4. (Continued.)

| State   | $T_e$ (cm$^{-1}$) | $\Delta T_e/T_e$ | $\lambda_e$(A°) | $\Delta \lambda_e/\lambda_e$ | $\omega_e$(cm$^{-1}$) | $\Delta \omega_e/\omega_e$ | $\omega_{\chi_e}$(cm$^{-1}$) | $\Delta \omega_{\chi_e}/\omega_{\chi_e}$ | Be     | $\Delta \text{Be}$/Be |
|---------|------------------|------------------|-----------------|-------------------------------|----------------------|-------------------|-----------------------------|--------------------------------|--------|-----------------------|
| (1)$^3\Sigma^-$ | 62 049$^a$ | 1.93$^a$ | 4.56$^b$ | 1010.97$^c$ | 59.33$^d$ | 16.5$^e$ | 6.49$^f$ | 1.42$^g$ |
| (2)$^3\Pi$   | 62 107$^b$ | 3.7$^c$ | 46.9$^c$ | 119.39$^a$ | 46.9$^c$ | 1.25$^h$ | 6.49$^f$ | 1.42$^g$ |
| (4)$^3\Sigma^+$ | 65 913$^c$ | 3.5$^c$ | 6.49$^f$ | 282.73$^a$ | 6.49$^f$ | 1.42$^g$ | 6.49$^f$ | 1.42$^g$ |
| (6)$^2\Pi$   | 66 156$^d$ | 2.4$^e$ | 2.96$^h$ | 560.22$^a$ | 352.85$^a$ | 2.96$^h$ | 2.96$^h$ | 2.96$^h$ |
| 1st min:   | 65 621$^e$ | 3.65$^f$ | 2.46$^g$ | 268.46$^a$ | 4.27$^h$ | 1.3$^i$ | 2.46$^g$ | 1.3$^i$ |
| 2nd min:   | 66 162$^f$ | 2.19$^g$ | 129.56$^a$ | 585.68$^a$ | 129.56$^a$ | 3.6$^h$ | 585.68$^a$ | 3.6$^h$ |
| (9)$^3\Sigma^-$ | 67 353$^g$ | 2.42$^h$ | 2.97$^h$ | 589.82$^a$ | 7.48$^h$ | 2.97$^h$ | 7.48$^h$ | 2.97$^h$ |
| 1st min:   | 67 754$^h$ | 6.18$^i$ | 0.25$^j$ | 682.02$^a$ | 0.25$^j$ | 0.25$^j$ | 682.02$^a$ | 0.25$^j$ |
| 2nd min:   | 73 653$^i$ | 4.85$^j$ | 0.69$^k$ | 508.75$^a$ | 1200.23$^a$ | 0.69$^k$ | 508.75$^a$ | 0.69$^k$ |
| (5)$^5\Sigma^+$ | 76 894$^k$ | 4.05$^k$ | 1.03$^l$ | 680.2$^a$ | 42.27$^m$ | 1.03$^l$ | 42.27$^m$ | 1.03$^l$ |
| (1)$^4\Delta$ | 89 469$^l$ | 1.95$^m$ | 4.55$^n$ | 1042.05$^a$ | 56.08$^n$ | 4.55$^n$ | 56.08$^n$ | 4.55$^n$ |
| (2)$^4\Delta$ | 91 352$^n$ | 2.05$^n$ | 4.1$^o$ | 738.4$^a$ | 118.66$^o$ | 4.1$^o$ | 738.4$^a$ | 4.1$^o$ |

$^a$ Present work,

$^b$ Ref. [39],

$^c$ Ref. [43],

$^d$ Ref. [40],

$^e$ Ref. [44],

$^f$ Ref. [41],

$^g$ Ref. [42],

$^h$ Ref. [42].
Table 5. Spectroscopic constants of the low-lying electronic states of SrH molecule

| State | R_0(A) | % ΔR_0/R_0 | ω_e/(cm^{-1}) | %Δω_e/ω_e | B_e/(cm^{-1}) | % ΔB_e/B_e | T_e/(cm^{-1}) | % ΔT_e/T_e |
|-------|--------|-------------|----------------|-------------|---------------|-------------|--------------|-------------|
| \(X^2\Sigma^+\) | 2.211 | 1166.2 | 3.45 | 0 | 2.210 | 0 | 1167 | 3.45 | 0.6 | 2.160 | 1206.2 | 3.2 | 3.63 | 4.7 | 2.144 | 1207 | 3.3 | 3.67 | 5.8 | 1205.6 | 3.2 |
| \(1\Sigma^+\) | 2.172 | 1214.5 | 3.58 | 13 112 | 5 | 2.160 | 0.5 | 1175 | 3.57 | 0.2 | 13 804 | 5 |
| \(2\Sigma^+\) | 2.121 | 1253.9 | 3.72 | 13 500.6 | 2.8 | 2.117(1) | 2 | 1234.5(1) | 3.73 | 1 | 14 312.7(1) | 2.9 |
| \(1\Delta\) | 2.217 | 1131 | 3.46 | 19 174 | 13.7 | 2.170(1) | 2.1 | 1043 | 3.44 | 0.6 | 16 851 | |
| \(2\Delta\) | 2.178 | 1150 | 3.56 | 21 107 | | 5.081 | | 103.6 | 0.65 | 27 042 | |
| \(1\Pi\) | 2.178 | 1150 | 3.56 | 21 107 | | 8.089 | | 14.17 | 0.26 | 27 054 | |
| \(2\Pi\) | 2.122(1) | 1227(1) | 3.75 | 31 178 | 1 | 3.874(2) | 2 | 290(2) | 1.12 | 34 418(2) |
| \(1\Pi\) | 2.816 | 483 | 2.13 | 33 222 | | 4.57 | | 41.7 | 0.81 | 34 774 |
| \(1\Pi\) | 6.299 | 106.9 | 0.42 | 34 804.7 | | 2.784 | | 342.7 | 2.14 | 34 929 |
| \(2\Delta\) | 4.876 | 78.5 | 0.71 | 35 497 | | 2.531 | | 587.4 | 0.26 | 45 919 |
| \(1\Psi\) | 2.851 | 339.1 | 0.2 | 47 062 | | 2.465 | | 641.6 | 0.27 | 49 809 |

* Present work,
* Ref. [45],
* Ref. [42],
* Ref. [38],
* Ref. [46].

The difference \(\delta T_e/T_e = 1.15\%\). For the \(4\Sigma^+\) state, the comparison between our calculated value of \(T_e\) with that given by Lefebvre-Brion and Colin, and Pitarch-Ruiz et al [56, 67], showed a less agreement with a relative error of \(\delta T_e/T_e = 13.12\%\). The comparison between our calculated values for \(R_e, \omega_e, \delta\), and \(B_e\), for the electronic states \(X^2\Sigma^+, A^2\Pi, \) and \(C^2\Sigma^+, \) with those obtained experimentally by Colin and DeGreef [64], showed a very good agreement with relative differences \(\delta R_e/R_e = 0.33\%, \delta \omega_e/\omega_e = 0.82\%, \) and \(\delta B_e/B_e = 0.6\%\) for \(X^2\Sigma^+, \delta R_e/R_e = 0.34\%, \delta \omega_e/\omega_e = 0.8\%, \) and \(\delta B_e/B_e = 0.74\%\) for \(A^2\Pi, \) and \(\delta R_e/R_e = 0.043\%, \delta \omega_e/\omega_e = 5.25\%, \) and \(\delta B_e/B_e = 0.4\%\).

4.1.2. Comparison with the theoretical values

The comparison between our calculated values of \(T_e\) with the calculated theoretical values given in literature by Matchado et al and Petsalakis et al [55, 68] shows a very good agreements for the electronic states \(A^2\Pi\) and \(C^2\Sigma^+, \) with relative differences 1.87 and 1.06 respectively, and less agreements for the states \(4\Sigma^+, 4\Pi^+, \) and \(5\Sigma^+, \) with the relative differences 12.3, 15.02, and 10.48 respectively. A similar less agreement is obtained by comparing our values of \(T_e\) with those of Cade and Luo [53], Leif et al [58], and Frank et al [59] with relative differences 10.9, 11.0, and 9.8 respectively for the electronic state \(A^2\Pi.\) The agreement deteriorate by comparing our calculated values of \(T_e\) with those given in literature for the electronic states \(1\Sigma^+, 4\Sigma^+, 4\Pi^+, 5\Sigma^+, 4\Pi^+\) [59].

By comparing our calculated values for \(R_e, \omega_e, \) and \(B_e\) for the electronic states \(X^2\Sigma^+, A^2\Pi, \) and \(C^2\Sigma^+, \) with those obtained theoretically by Petsalakis et al [68], one can find an excellent agreement with relative differences \(\delta R_e/R_e = 0.33\%, \delta \omega_e/\omega_e = 0.25\%, \) and \(\delta B_e/B_e = 0.1\%\) for \(X^2\Sigma^+, \delta R_e/R_e = 0.33\%, \delta \omega_e/\omega_e = 0.3\%, \) and \(\delta B_e/B_e = 0.1\%\) for \(A^2\Pi, \) and \(\delta R_e/R_e = 0.28\%, \delta \omega_e/\omega_e = 4.44\%, \) and \(\delta B_e/B_e = 0.14\%\) for \(C^2\Sigma^+.\) Similar excellent agreement is obtained by comparing our values of these constants with those of Focs[61] with the relative differences 0.3 and 0.37 for \(X^2\Sigma^+\) and \(A^2\Pi\) states respectively. The
comparison between the present values for Re and those given by Cade and Huo, and Herzberg and HF methods shows an excellent agreement with the relative differences 0.3% and 0.37% for \( X^2 \Sigma^+ \) and \( A^1 \Pi \) states respectively.

### 4.2. MgH molecule

In the present work, the calculated spectroscopic constants of the molecule MgH are given in table 4 along with those found in the literature either experimentally or theoretically. The comparison of our calculated values of the vibrational harmonic frequency constant \( \omega_e \) for the ground state \( X^2 \Sigma^+ \) with those given in literature shows a very good agreement with the relative differences \( \Delta \omega_e/\omega_e \) equal 2.22% [70], 0.15% [71], 0.54% [72, 73], 0.58% [74].

A less accuracy is obtained for \( \omega_e \) by comparing our values with those given in [73] by using MC and HF methods where \( \Delta \omega_e/\omega_e \) are respectively 6.97% and 7.43%. For the values of Re, there is a very good agreement between our result and those given in [70-75] where 0.07% \( \lesssim \Delta R_e/R_e \lesssim 1.79% \). As for the values of Be, there is also a very good agreement between our result and the ones given in [72, 73, 75] where 1.32% \( \lesssim \Delta B_e/B_e \lesssim 3.32\% \). For the first excited state (1)^1\Pi the comparison of the 5 values of Te the 7 values of Re, the 8 values of \( \omega_e \), and the 4 values of \( B_e \) found in literature [72, 73, 75] with those of the present work showed a very good agreement 0.21% \( \lesssim \Delta T_e/T_e \lesssim 1.4\% \), 0.53% \( \lesssim \Delta R_e/R_e \lesssim 1.7\% \), 0.09% \( \lesssim \Delta \omega_e/\omega_e \lesssim 1.84\% \), 2.45% \( \lesssim \Delta B_e/B_e \lesssim 3.75\% \). A less agreement is noticed by comparing our results with those calculated by using MC and HF methods [73]. The comparison between our results and those found in literature for the excited state (2)^2\Sigma^+ shows also the very good agreement with the relative differences 0.55% \( \lesssim \Delta T_e/T_e \lesssim 1.06\% \) (except for the result given in [75] where the relative error increases to 16.95%), 0.3% \( \lesssim \Delta R_e/R_e \lesssim 1.52\% \), and 0.77% \( \lesssim \Delta \omega_e/\omega_e \lesssim 2.79\% \). No comparison for the value of Be since it is given here for the first time. The comparison of our results with those given by J-M Mestdagh et al [70] for the excited state (3)^2\Sigma^+ shows a very good agreement for the calculated spectroscopic constants where \( \Delta T_e/T_e = 2.35\% \), \( \Delta R_e/R_e = 2.34\% \), and \( \Delta \omega_e/\omega_e = 0.97\% \) for the first minimum. For the second minimum of the same state, we got \( \Delta T_e/T_e = 0.62\% \), \( \Delta R_e/R_e = 1.22\% \), and \( \Delta \omega_e/\omega_e = 5.34\% \). By comparing our results with the experimental ones [74], we get very good results for the first minimum of the same state where \( \Delta T_e/T_e = 1.93\% \), \( \Delta R_e/R_e = 2.34\% \), and \( \Delta \omega_e/\omega_e = 2.6\% \). No comparison for the value of Be since it is given here for the first time also. The same table 4 shows the very close agreement between our work and that obtained by the experimental work [74] and Mestdagh et al [70] for the state (4)^4\Sigma^+ where, for the first minimum, 4.87% \( \lesssim \Delta T_e/T_e \lesssim 5.8\% \), 0.58% \( \lesssim \Delta R_e/R_e \lesssim 4.07\% \), and \( \Delta \omega_e/\omega_e = 2.33\% \). For the second minimum, \( \Delta T_e/T_e = 0.8\% \), \( \Delta R_e/R_e = 2.72\% \), and \( \Delta \omega_e/\omega_e = 6.6\% \).
compared to [70]. The results of $B_e$ are also found for the first time for the considered state. The values obtained for the internuclear distance at equilibrium $R_e$ and the electronic transition energy with respect to the ground states $T_e$ for first minima of both states $(2)^2\Sigma^+$ and $(5)^2\Sigma^+$ shows a good agreement compared to [70], but the accuracy becomes less for the values of the vibrational harmonic constant $\omega_e$ compared to the same reference. The accuracy deteriorates by comparing our results with those given by Mestdagh et al [70] for the states $(3)^2\Pi$ and $(1)^2\Delta$. It was not possible to obtain such constants for some states that made avoided crossing with a neighbor one, these states are given in table 2.
4.3. SrH molecule

The comparison of our calculated values in the present work with those given in literature (table 5) for
the constants $\omega_e$ and $B_e$ for the ground state X$^2\Sigma^+$ shows very good agreement with the relative differences $\Delta \omega_e/\omega_e$ equal $0.0\%$ [76], $3.2\%$ [32], $3.3\%$ [27] and $\Delta B_e/B_e = 0.6\%$ [45], $5.8\%$ [32], $4.7\%$ [27]. The comparison of our results for the state ($1^2\Pi$) with those given theoretically by Leininger and Jeung [64] shows a very good agreement for $T_e$, $\omega_e$ and $B_e$ with the relative difference $\Delta T_e/T_e = 5\%$, $\Delta \omega_e/\omega_e = 3.3\%$, and $\Delta B_e/B_e = 0.2\%$. While the comparison of these constants with those obtained experimentally [27] shows also very good agreement with the relative differences $\Delta T_e/T_e = 2.8\%$, $\Delta \omega_e/\omega_e = 3.1\%$ $\Delta B_e/B_e = 3.7\%$. The comparison between our results and those obtained theoretically in literature for the excited state (2)$^2\Sigma^+$ shows also the very good agreement with the relative difference: $\Delta T_e/T_e = 1.4\%$, $\Delta \omega_e/\omega_e = 7.4\%$ and $\Delta B_e/B_e = 4.3\%$ with the results of Leininger and Jeung [76]. Similar results are obtained by comparing our data with those obtained experimentally [27] with the relative difference $\Delta T_e/T_e = 2.9\%$, $\Delta \omega_e/\omega_e = 3.4\%$ and $\Delta B_e/B_e = 2.9\%$. The spectroscopic constants of the state ($1^2\Delta$) are compared only with the theoretical data given by Leininger and Jeung [76] since there is no experimental data is available yet. It shows a less agreement for $T_e$ with a relative difference $\Delta T_e/T_e = 13.7\%$ which is may be due to an upward displacement in the potential energy. However, the relative error for $\omega_e$ shows somehow a good agreement with a relative difference $\Delta \omega_e/\omega_e = 8.4\%$ and an excellent agreement for $B_e$ with a relative difference $\Delta B_e/B_e = 0.6\%$. The three published values for $R_e$ for the state X$^2\Sigma^+$ shows a very good agreement with our calculated value with relative differences $0.0\%$ [22, 76] $< \Delta R_e/R_e < 3\%$ [27, 32]. For ($1^2\Pi$, ($2^2\Pi$, and ($1^2\Delta$ the calculated values of $R_e$ in the present work are in good agreement with the values in the literature in which the relative difference are $0.5\%$ [76] $< \Delta R_e/R_e < 2.4\%$ [27], $1.8\%$ [17, 22] $< \Delta R_e/R_e < 2\%$ [19, 63] and $\Delta R_e/R_e = 2\%$ [27] respectively. The comparison for the calculated values for the other states is not possible since they are given here for the first time.

Because of the overall good agreement between our calculated data for the three molecules and those given in literature either theoretical or experimental we may confirm the accuracy of these data for the new investigated electronic states. These results may stimulate new experimental works for the high-lying electronic states for these three molecules.

4.4. Transition dipole moment

The transition dipole moment (TDM) between two electronic states is a very useful data as: designing some cooling experiments, to model the electronic spectroscopy of the molecule in all situations and it is then about where the molecules can be found. For the three considered molecules we present in figures 13–15 the TDM between the ground and $^2\Pi$ and $^2\Sigma^+$ excited states. From these figures one can notice, some curves tend to zero due to spin forbidden transitions between two atomic orbitals at the asymptotic limits, while the other curves tend to constant values because of the allowed transitions between the corresponding atomic orbitals. For the readers, it should be noted that there is no guarantee that the relative signs were extracted from MOLPRO correctly and the risk of getting it wrong should be understood. For example, changing the sign of $\langle X|\mu|(2)^2\Sigma^+ \rangle$ (BeH) might be attributed to the phase change of either $|X\rangle$ or $|(2)^2\Sigma^+\rangle$, which should be then propagated to other transition dipole moments consistently.

4.5. The vibration–rotation calculation

For a given electronic state the vibration–rotation motion of a diatomic molecule is governed by the radial Schrödinger equation within the Born–Oppenheimer approximation

$$\frac{d^2\Psi_J(r)}{dr^2} + \left[ k(E_J - U(r)) - \frac{\lambda}{r^2}\right]\Psi_J(r) = 0$$

(1)

where, $r$ is the internuclear distance, $k = 2\mu/\hbar^2$, $2\mu/\hbar^2 v$ and $J$ are respectively the vibrational and rotational quantum numbers, $\lambda = J(J + 1)$. $E_J$ and $\Psi_J$ are the eigenvalue and the eigenfunction of this equation respectively. By using the Rayleigh–Schrödinger perturbation theory, equation (1) can be

$$\phi_{0J}^p(r) + k[e_0 - U(r)]\phi_{0J}(r) = 0$$

(2)

$$\phi_{1J}^p(r) + k[e_0 - U(r)]\phi_{1J}(r) = -k[e_1 - R(r)]\phi_{0J}(r)$$

(3a)

$$\phi_{2J}^p(r) + k[e_0 - U(r)]\phi_{2J}(r) = -k[e_1 - R(r)]\phi_{1J}(R) - k^2\phi_{0J}(r)$$

(3b)

$$\phi_{nJ}^p(r) + k[e_0 - U(r)]\phi_{nJ}(r) = -k[e_1 - R(r)]\phi_{n-1J}(r) - k\sum_{m=2}^n e_m\phi_{n-mJ}(r)$$

(3c)

with $e_0 = E_\nu, e_1 = B_\nu, e_2 = -D_\nu, R(r) = 1/r^2$, $\phi_0$ is the pure vibrational wavefunction and $\phi_n$ are the rotational correction. The first equation is the pure vibrational Schrödinger equation, whereas the remaining equations are the rotational Schrödinger equations. We can project equations (3a)–(3c) onto $\phi_0$ and find...
Table 6. Values of the eigenvalues $E_v$, the abscissas of the turning points $R_{\text{min}}, R_{\text{max}}$, the rotational constants $B_v$, and the centrifugal distortion constants $D_v$ for the different vibrational levels of the investigated electronic states of the BeH molecule.

| $\nu$ | $E_v$ (cm$^{-1}$) | $\Delta E_v / E_v$ | $R_{\text{min}}$ (Å) | $R_{\text{max}}$ (Å) | $B_v$ (cm$^{-1}$) | $\Delta B_v / B_v$ | $D_v \times 10^{-3}$ (cm$^{-1}$) | $\Delta D_v / D_v$ |
|-------|------------------|---------------------|---------------------|---------------------|------------------|---------------------|---------------------|---------------------|
| 0     | 1015.136 a       | 1.224               | 1.496               | 10.09 a             | 1.0094 a         | 1.0272 a           | 1.763               | 2.536               |
|       | 0                | 1.0164 8880 b       | 0.74                | 1.033 d             | 1.026 41 d       | 1.685               |
|       | 0                | 1.10165 613 c       | 0.94                | 1.035 d             | 1.026 41 d       | 1.685               |
| 1     | 1970.1 a         | 1.149               | 1.627               | 9.781 a             | 1.04 a           | 1.285               |
|       | 1986.4442 b      | 0.83                | 9.855 4335 b        | 0.76                | 1.0169 b         | 1.285               |
|       | 1986.416 c       | 0.828               | 9.855 83 c          | 0.76                | 1.04 d           | 1.992               |
|       | 1986.55 d        | 0.836               | 9.874 8 d           | 0.96                | 1.016 24 d       | 1.219               |
|       | 1986.4158 e      | 0.828               | 9.855 737 e         | 0.76                |                   |                     |
| 2     | 3874.2 a         | 1.103               | 1.731               | 9.468 a             | 0.884 a          | 14.706              |
|       | 3896.8785 b      | 0.587               | 9.541 7271 b        | 0.77                | 1.0104 a         | 14.706              |
|       | 3896.871 c       | 0.586               | 9.542 8            | 0.84                | 1.018 d          | 15.158              |
|       | 3897.10 d        | 0.592               | 9.560 1 d           | 0.97                | 1.009 82 d       | 14.23               |
|       | 3896.8702 e      | 0.586               | 9.541 635 e         | 0.77                |                   |                     |
| 3     | 5683.2 a         | 1.069               | 1.825               | 9.143 a             | 0.984 a          | 2.642               |
|       | 5729.2861 b      | 0.812               | 9.220 768 b         | 0.85                | 1.0100 a         | 2.642               |
|       | 5729.260 c       | 0.812               | 9.220 28            | 0.845               | 1.017 d          | 3.354               |
|       | 5729.57 d        | 0.817               | 9.2377 e           | 1.035               | 1.008 85 d       | 2.525               |
|       | 5729.2615 e      | 0.811               | 9.220 120 e         | 0.843               |                   |                     |
| 4     | 7419.3 a         | 1.043               | 1.916               | 8.812 a             | 0.987 a          | 3.04                |
|       | 7480.4528 b      | 0.824               | 8.886 639 b         | 0.84                | 1.0170 a         | 3.04                |
|       | 7480.338 c       | 0.823               | 8.886 74 c          | 0.84                | 1.024 d          | 3.749               |
|       | 7480.68 d        | 0.827               | 8.9033 d           | 1.03                | 1.016 05 d       | 2.943               |
|       | 7480.3404 e      | 0.823               | 8.886 589 e         | 0.84                |                   |                     |
| 5     | 10 086.914 a     | 1.021               | 2.007               | 8.458 a             | 0.951 a          | 9.232               |
|       | (0071 778)       | 0.81                | 8.533 209 b         | 0.89                | 1.0388 a         | 9.232               |
|       | 9145.2834 b      | 0.81                | 8.534 43 d          | 0.9                 | 1.043 d          | 9.674               |
Table 6. (Continued.)

| ν  | Eν (cm⁻¹) | Rmin (Å) | Rmax (Å) | Bν (cm⁻¹) | Dν × 10⁻⁴ (cm⁻¹) |
|----|-----------|----------|----------|-----------|------------------|
| 0  | 509.975   | 2.118    | 2.498    | 3.512d    | 1.74e             |
| 1  | 1504.0759 | 1.989    | 2.662    | 3.505d    | 2.05f             |

C²Σ⁺
### Table 6. (Continued.)

| ν  | E_v (cm\(^{-1}\)) | R_{min} (Å) | R_{max} (Å) | B_v (cm\(^{-1}\)) | D_v \times 10^{-4} (cm\(^{-1}\)) |
|----|-------------------|--------------|--------------|------------------|----------------------------------|
| 0  | 1028.712          | 1.216        | 1.487        | 9.894            | 9.23                             |
| 1  | 3019.358          | 1.142        | 1.618        | 9.570            | 10.44                            |
| 2  | 4928.701          | 1.097        | 1.724        | 9.241            | 10.40                            |
| 3  | 6743.46           | 1.064        | 1.82         | 8.901            | 10.40                            |
| 4  | 8471.263          | 1.038        | 1.913        | 8.553            | 10.43                            |
| 5  | 10 107.237        | 1.017        | 2.007        | 8.185            | 10.52                            |
| 6  | 11 637.393        | 0.999        | 2.104        | 7.796            | 10.78                            |
| 7  | 13 066.186        | 0.984        | 2.205        | 7.388            | 11.04                            |
| 8  | 14 377.417        | 0.971        | 2.315        | 6.931            | 9.66                             |
| 9  | 15 567.101        | 0.96         | 2.437        | 6.433            | 10.68                            |
| 10 | 16 622.653        | 0.95         | 2.578        | 5.879            | 11.23                            |
Table 6. (Continued.)

| ν  | $E_v$(cm$^{-1}$) | $R_{\text{min}}$(Å) | $R_{\text{max}}$(Å) | $B_v$(cm$^{-1}$) | $D_v \times 10^{-4}$(cm$^{-1}$) |
|----|-----------------|----------------------|----------------------|-----------------|---------------------------------|
| 11 | 17 522.448      | 0.943                | 2.745                | 5.237           | 14.34                           |
| 12 | 18 259.058      | 0.937                | 2.961                | 4.492           | 17.72                           |
| 13 | 18 812.258      | 0.932                | 3.264                | 3.611           | 22.17                           |
| 14 | 19 163.321      | 0.93                 | 3.775                | 2.522           | 32.46                           |
|    | (5)$^3\Pi$      |                      |                      |                 |                                 |
| ν  |                |                      |                      |                 |                                 |
| 0  | 994.388        | 1.239                | 1.513                | 9.825           | 0.998                           |
| 1  | 2876.486       | 1.167                | 1.659                | 9.351           | 1.037                           |
| 2  | 4602.088       | 1.125                | 1.785                | 8.832           | 1.072                           |
| 3  | 6157.739       | 1.095                | 1.909                | 8.24            | 1.275                           |
| 4  | 7518.057       | 1.073                | 2.055                | 7.477           | 1.614                           |
| 5  | 8628.675       | 1.057                | 2.239                | 6.656           | 1.191                           |
| 6  | 9644.59        | 1.043                | 2.346                | 6.333           | 0.389                           |
| 7  | 10 688.991     | 1.03                 | 2.462                | 6.312           | 0.985                           |
| 8  | 11 656.943     | 1.019                | 2.585                | 5.871           | 0.94                            |
| 9  | 12 551.498     | 1.01                 | 2.719                | 5.517           | 1.01                            |
| 10 | 13 368.349     | 1.001                | 2.86                 | 5.121           | 0.975                           |
|    | (3)$^3\Pi$      |                      |                      |                 |                                 |
| ν  |                |                      |                      |                 |                                 |
| 0  | 249.1745       | 2.168                | 2.715                | 3.1379          | 5.296                           |
| 1  | 717.0949       | 2.017                | 3.004                | 3.0035          | 5.952                           |
| 2  | 1144.8103      | 1.925                | 3.248                | 2.866           | 6.447                           |
| 3  | 1531.6013      | 1.853                | 3.481                | 2.7219          | 7.97                            |
| 4  | 1879.666       | 1.796                | 3.735                | 2.5741          | 8.506                           |
| 5  | 2195.8466      | 1.741                | 3.948                | 2.4875          | 8.476                           |
| 6  | 2490.621       | 1.684                | 4.207                | 2.3711          | 12.328                          |
| 7  | 2745.8939      | 1.631                | 4.475                | 2.18669         | 10.838                          |
| 8  | 2975.3994      | 1.591                | 4.777                | 2.0428          | 12.997                          |
| 9  | 3171.3209      | 1.564                | 5.124                | 1.8261          | 11.409                          |
| ν  | $\nu_e$ (cm$^{-1}$) | $R_{\text{min}}$(Å) | $R_{\text{max}}$(Å) | $B_{\nu}$(cm$^{-1}$) | $D_{\nu} \times 10^4$(cm$^{-1}$) |
|----|-------------------|------------------|--------------------|----------------|------------------|
| 0  | 752.9479          | 1.369            | 1.685              | 8.0068         | 9.243            |
| 1  | 2203.0035         | 1.284            | 1.843              | 7.7012         | 9.123            |
| 2  | 3577.7376         | 1.233            | 1.971              | 7.3883         | 8.962            |
| 3  | 4869.0617         | 1.196            | 2.092              | 7.0501         | 9.537            |
| 4  | 6078.3775         | 1.167            | 2.212              | 6.695          | 9.465            |
| 5  | 7195.466          | 1.144            | 2.338              | 6.3118         | 9.68             |
| 6  | 8211.4327         | 1.125            | 2.473              | 5.8822         | 10.514           |
| 7  | 9117.2365         | 1.11             | 2.625              | 5.3986         | 11.987           |
| 8  | 9900.9975         | 1.097            | 2.805              | 4.8505         | 13.98            |
| 9  | 10 548.864        | 1.087            | 3.031              | 4.1991         | 16.295           |

\(^a\) The first entry is for the present work,  
\(^b\) Ref.[42]  
\(^c\) Ref.[50]  
\(^d\) Ref. [51],  
\(^e\) Ref.[51].
Table 7. Values of the eigenvalues $E_{\nu}$, the abscissas of the turning points $R_{\text{min}}$ and $R_{\text{max}}$, the rotational constants $B_{\nu}$, and the centrifugal distortion constants $D_{\nu}$ for the different vibrational levels of the investigated electronic states of the molecule MgH.

| $\chi^2 \Sigma^+$ | | | | | |
|------------------|------------------|------------------|------------------|------------------|------------------|
| V                | $E_{\nu}$ (cm$^{-1}$) | $B_{\nu}$ (cm$^{-1}$) | $D_{\nu} \times 10^4$ (cm$^{-1}$) | $R_{\text{min}}$ (Å) | $R_{\text{max}}$ (Å) |
| 0                | 735.527           | 5.644             | 3.41                          | 1.604 69         | 1.913 53         |
| 1                | 2162.260          | 5.471             | 3.42                          | 1.519 06         | 2.063 2          |
| 2                | 3528.592          | 5.293             | 3.45                          | 1.467 09         | 2.182 57         |
| 3                | 4831.647          | 5.107             | 3.51                          | 1.4288           | 2.292 5          |
| 4                | 6066.779          | 4.908             | 3.64                          | 1.398 53         | 2.400 07         |
| 5                | 7227.102          | 4.689             | 3.87                          | 1.373 77         | 2.510 01         |
| 6                | 8302.247          | 4.440             | 4.28                          | 1.353 21         | 2.627 32         |
| 7                | 9276.712          | 4.141             | 5.02                          | 1.336 16         | 2.759 44         |
| 8                | 10 126.418        | 3.757             | 6.48                          | 1.322 32         | 2.920 54         |
| 9                | 11 274.036        | 2.371             | 18.9                          | 1.3049           | 3.554 39         |

| $(1)^2 \Pi$ | | | | | |
|------------------|------------------|------------------|------------------|------------------|------------------|
| V                | $E_{\nu}$ (cm$^{-1}$) | $B_{\nu}$ (cm$^{-1}$) | $D_{\nu} \times 10^4$ (cm$^{-1}$) | $R_{\text{min}}$ (Å) | $R_{\text{max}}$ (Å) |
| 0                | 765.783           | 5.526             | 2.837                         | 1.564 04         | 1.862 47         |
| 1                | 2278.136          | 5.344             | 2.909                         | 1.480 11         | 2.009 73         |
| 2                | 3716.307          | 5.176             | 3.010                         | 1.429 59         | 2.127 44         |
| 3                | 5078.573          | 4.987             | 2.937                         | 1.392 58         | 2.236 02         |
| 4                | 6369.925          | 4.782             | 3.121                         | 1.363 25         | 2.342 89         |
| 5                | 7580.244          | 4.575             | 3.368                         | 1.339 28         | 2.451 73         |
| 6                | 8701.726          | 4.347             | 3.512                         | 1.319 35         | 2.565 94         |
| 7                | 9728.996          | 4.089             | 3.774                         | 1.302 63         | 2.689 77         |
| 8                | 10 653.016        | 3.798             | 4.276                         | 1.288 64         | 2.828 77         |
| 9                | 11 461.810        | 3.469             | 5.045                         | 1.2771           | 2.991 27         |
(5)\( ^3\Pi \)

| V  | \( E_c (\text{cm}^{-1}) \) | \( B_c (\text{cm}^{-1}) \) | \( D_c \times 10^{-4} (\text{cm}^{-1}) \) | \( R_{\text{min}} (\text{Å}) \) | \( R_{\text{max}} (\text{Å}) \) |
|----|-----------------|-----------------|------------------|-----------------|-----------------|
| 0  | 660.514         | 5.704           | 4.446            | 1.6615          | 1.98472         |
| 1  | 1911.384        | 5.400           | 5.186            | 1.5777          | 2.16288         |
| 2  | 3008.085        | 4.988           | 6.814            | 1.5293          | 2.33119         |
| 3  | 3881.927        | 4.272           | 12.597           | 1.49917         | 2.56403         |
| 4  | 4417.931        | 3.236           | 15.178           | 1.48272         | 2.98972         |
| 5  | 4753.634        | 2.761           | 7.988            | 1.47308         | 3.39668         |
| 6  | 5050.765        | 2.552           | 4.186            | 1.46492         | 3.69347         |

(1)\( ^3\Delta \)

| V  | \( E_c (\text{cm}^{-1}) \) | \( B_c (\text{cm}^{-1}) \) | \( D_c \times 10^{-4} (\text{cm}^{-1}) \) | \( R_{\text{min}} (\text{Å}) \) | \( R_{\text{max}} (\text{Å}) \) |
|----|-----------------|-----------------|------------------|-----------------|-----------------|
| 0  | 605.834         | 5.538           | 5.119            | 1.61152         | 1.95231         |
| 1  | 1700.712        | 5.111           | 5.981            | 1.53175         | 2.16250         |
| 2  | 2628.652        | 4.645           | 6.794            | 1.48817         | 2.36209         |
| 3  | 3400.470        | 4.154           | 7.777            | 1.45927         | 2.57736         |
| 4  | 4023.383        | 3.629           | 9.275            | 1.43906         | 2.82695         |
| 5  | 4500.284        | 3.046           | 11.816           | 1.42502         | 3.14204         |
| 6  | 4830.578        | 2.576           | 16.629           | 1.41588         | 3.59004         |
| 7  | 5017.757        | 1.575           | 27.973           | 1.4109          | 4.37853         |

(4)\( ^3\Sigma^- \)

| V  | \( E_c (\text{cm}^{-1}) \) | \( B_c (\text{cm}^{-1}) \) | \( D_c \times 10^{-4} (\text{cm}^{-1}) \) | \( R_{\text{min}} (\text{Å}) \) | \( R_{\text{max}} (\text{Å}) \) |
|----|-----------------|-----------------|------------------|-----------------|-----------------|
| 0  | 479.246         | 5.614           | 7.445            | 1.79132         | 2.16008         |
| 1  | 1431.517        | 5.381           | 7.950            | 1.69225         | 2.36209         |
| 2  | 2301.734        | 5.025           | 8.006            | 1.63534         | 2.53309         |
| 3  | 3093.559        | 4.713           | 9.295            | 1.5951         | 2.70389         |
Table 7. (Continued.)

|   | \( E_i \) (cm\(^{-1}\)) | \( B_i \) (cm\(^{-1}\)) | \( D_i \times 10^{-4} \) (cm\(^{-1}\)) | \( R_{\text{min}} \) (Å) | \( R_{\text{max}} \) (Å) |
|---|----------------|----------------|-----------------|----------------|----------------|
| 4 | 3792.215       | 4.333          | 9.196           | 1.565 13       | 2.885 52       |
| 5 | 4399.337       | 3.890          | 10.740          | 1.542 09       | 3.093 45       |
| 6 | 4901.750       | 3.398          | 13.319          | 1.524 68       | 3.346 13       |
| 7 | 5288.704       | 2.826          | 15.958          | 1.512 12       | 3.662 85       |
| 8 | 5536.126       | 2.115          | 25.873          | 1.503 82       | 4.199 06       |

\((2)^4 \Delta\)

| V | \( E_i \) (cm\(^{-1}\)) | \( B_i \) (cm\(^{-1}\)) | \( D_i \times 10^{-4} \) (cm\(^{-1}\)) | \( R_{\text{min}} \) (Å) | \( R_{\text{max}} \) (Å) |
|---|----------------|----------------|-----------------|----------------|----------------|
| 0 | 489.961        | 5.602          | 7.242           | 1.794 68       | 2.157 15       |
| 1 | 1444.846       | 5.293          | 9.060           | 1.697 65       | 2.372 31       |
| 2 | 2250.033       | 4.769          | 9.315           | 1.645 25       | 2.584 31       |
| 3 | 2939.940       | 4.378          | 10.055          | 1.609 59       | 2.790 42       |
| 4 | 3534.989       | 3.972          | 10.308          | 1.583 17       | 3.006 41       |
| 5 | 4037.954       | 3.502          | 11.330          | 1.563 14       | 3.253 29       |
| 6 | 4442.460       | 2.980          | 13.378          | 1.548 27       | 3.539 97       |
Table 8. Values of the eigenvalues $E_v$, the abscissas of the turning points $R_{\text{min}}$ and $R_{\text{max}}$, the rotational constants $B_v$, and the centrifugal distortion constants $D_v$ for the different vibrational levels of the investigated electronic states of the molecule SrH.

| $v$ | $E_v$ (cm$^{-1}$) | $\tau_{\text{min}}$ (Å) | $\tau_{\text{max}}$ (Å) | $B_v$ (cm$^{-1}$) | $D_v \times 10^{-4}$ (cm$^{-1}$) |
|-----|------------------|-------------------------|-------------------------|-----------------|-------------------------------|
| 0   | 578.290          | 2.0550                  | 2.3990                  | 3.4202          | 1.2152                        |
| 1   | 1711.173         | 1.9561                  | 2.5568                  | 3.3449          | 1.2100                        |
| 2   | 2811.218         | 1.8948                  | 2.6806                  | 3.2667          | 1.2189                        |
| 3   | 3875.929         | 1.8489                  | 2.7905                  | 3.1897          | 1.2008                        |
| 4   | 4908.897         | 1.8118                  | 2.8935                  | 3.1130          | 1.2161                        |
| 5   | 5908.897         | 1.7804                  | 2.9925                  | 3.0360          | 1.1963                        |
| 6   | 6875.019         | 1.7534                  | 3.0896                  | 2.9573          | 1.2124                        |
| 7   | 7808.122         | 1.7297                  | 3.1859                  | 2.8785          | 1.2144                        |
| 8   | 8706.836         | 1.7687                  | 3.2830                  | 2.7952          | 1.2248                        |
| 9   | 9569.535         | 1.6899                  | 3.3821                  | 2.7087          | 1.2823                        |
| 10  | 10 392.835       | 1.6731                  | 3.4850                  | 2.6166          | 1.3382                        |
| 11  | 11 172.865       | 1.6580                  | 3.5941                  | 2.5137          | 1.4411                        |
| 12  | 11 903.129       | 1.6445                  | 3.7137                  | 2.3952          | 1.6436                        |
| 13  | 12 572.684       | 1.6327                  | 3.8514                  | 2.2502          | 1.9925                        |
| 14  | 13 164.454       | 1.6226                  | 4.0233                  | 2.0577          | 2.6266                        |

(1)$^2\Pi$

| $v$ | $E_v$ (cm$^{-1}$) | $\tau_{\text{min}}$ (Å) | $\tau_{\text{max}}$ (Å) | $B_v$ (cm$^{-1}$) | $D_v \times 10^{-4}$ (cm$^{-1}$) |
|-----|------------------|-------------------------|-------------------------|-----------------|-------------------------------|
| 0   | 602.799          | 2.0194                  | 2.3556                  | 3.5433          | 1.2449                        |
| 1   | 1782.832         | 1.9227                  | 2.5108                  | 3.4642          | 1.2402                        |
| 2   | 2928.106         | 1.8627                  | 2.6331                  | 3.3820          | 1.2609                        |
| 3   | 4033.389         | 1.8180                  | 2.7421                  | 3.2975          | 1.2504                        |
| 4   | 5302.187         | 1.7816                  | 2.8447                  | 3.2154          | 1.2649                        |
| 5   | 6133.001         | 1.7514                  | 2.9441                  | 3.1285          | 1.2588                        |
| 6   | 7125.898         | 1.7253                  | 3.0424                  | 3.0415          | 1.2899                        |
| 7   | 8078.442         | 1.7025                  | 3.1412                  | 2.9492          | 1.2971                        |
| 8   | 8989.442         | 1.6823                  | 3.2424                  | 2.8515          | 1.3710                        |
Table 8. (Continued.)

|    |  \( E_v \) (cm\(^{-1}\)) |  \( r_{min} \) (Å) |  \( r_{max} \) (Å) |  \( B_v \) (cm\(^{-1}\)) |  \( D_o \times 10^{-4} \) (cm\(^{-1}\)) |
|----|-----------------|----------------|----------------|-----------------|------------------|
| 0  | 568.788         | 2.0221         | 2.3686         | 3.5164          | 1.3774           |
| 1  | 1673.552        | 1.9253         | 2.5341         | 3.4168          | 1.3975           |
| 2  | 2730.187        | 1.8664         | 2.6692         | 3.3082          | 1.4647           |
| 3  | 3730.161        | 1.8230         | 2.7937         | 3.1941          | 1.4779           |
| 4  | 4677.083        | 1.7874         | 2.9157         | 3.0763          | 1.5633           |
| 5  | 5566.155        | 1.7603         | 3.0385         | 2.9521          | 1.5760           |
| 6  | 6399.075        | 1.7365         | 3.1645         | 2.8234          | 1.6310           |
| 7  | 7176.556        | 1.7161         | 3.2935         | 2.6990          | 1.6095           |
| 8  | 7904.279        | 1.6984         | 3.4236         | 2.5812          | 1.5031           |
| 9  | 8591.328        | 1.6827         | 3.5518         | 2.4774          | 1.4088           |
| 10 | 9245.719        | 1.6685         | 3.6765         | 2.3885          | 1.3371           |
| 11 | 9872.822        | 1.6556         | 3.7986         | 2.3070          | 1.2809           |
| 12 | 10 474.801      | 1.6438         | 3.9205         | 2.2258          | 1.2826           |
| 13 | 11 050.489      | 1.6329         | 4.0455         | 2.1408          | 1.3704           |

(2)^II

|    |  \( E_v \) (cm\(^{-1}\)) |  \( r_{min} \) (Å) |  \( r_{max} \) (Å) |  \( B_v \) (cm\(^{-1}\)) |  \( D_o \times 10^{-4} \) (cm\(^{-1}\)) |
|----|-----------------|----------------|----------------|-----------------|------------------|
| 0  | 239.037         | 2.5770         | 3.1102         | 2.0966          | 1.6747           |
| 1  | 696.889         | 2.5524         | 3.1489         | 2.0098          | 1.8259           |
| 2  | 1114.222        | 2.3502         | 3.6320         | 1.8856          | 2.1990           |
| 3  | 1472.634        | 2.2938         | 3.9213         | 1.7113          | 2.8908           |

(3)^II
Table 8. (Continued.)

| $\nu$ | $E_v$ (cm$^{-1}$) | $r_{\text{min}}$ (Å) | $r_{\text{max}}$ (Å) | $B_v$ (cm$^{-1}$) | $D_v \times 10^{-4}$ (cm$^{-1}$) |
|------|------------------|----------------------|----------------------|-----------------|----------------------------------|
| 0    | 561.031          | 2.0587               | 2.4087               | 3.4005          | 1.2693                           |
| 1    | 1658.912         | 1.9932               | 2.5693               | 3.3207          | 1.2595                           |
| 2    | 2723.452         | 1.8978               | 2.6969               | 3.2369          | 1.2751                           |
| 3    | 3750.665         | 1.8520               | 2.8104               | 3.1556          | 1.2432                           |
| 4    | 4745.994         | 1.8152               | 2.9170               | 3.0742          | 1.2657                           |
| 5    | 5706.832         | 1.7835               | 3.0195               | 2.9945          | 1.2315                           |
| 6    | 6635.611         | 1.7573               | 3.1199               | 2.9125          | 1.2390                           |
| 7    | 7531.733         | 1.7338               | 3.2192               | 2.8331          | 1.2396                           |
| 8    | 8395.057         | 1.7130               | 3.3186               | 2.7508          | 1.2139                           |
| 9    | 9226.113         | 1.6943               | 3.4190               | 2.6674          | 1.2467                           |
| 10   | 10 023.400       | 1.6776               | 3.5212               | 2.5843          | 1.2673                           |
| 11   | 10 785.934       | 1.6624               | 3.6262               | 2.4976          | 1.2748                           |
| 12   | 11 512.805       | 1.6486               | 3.7353               | 2.4069          | 1.3304                           |
| 13   | 12 201.718       | 1.6361               | 3.8502               | 2.3125          | 1.4129                           |
| 14   | 12 849.574       | 1.6248               | 3.9730               | 2.2106          | 1.4956                           |
| 15   | 13 452.722       | 1.6147               | 4.1072               | 2.0970          | 1.6062                           |
| 16   | 14 005.865       | 1.6057               | 4.2592               | 1.9671          | 1.8190                           |
Once \( e_0 \) is obtained, \( e_1, e_2, \ldots, e_n \) can be got sequentially from equation (4). The eigenvalue \( E_v \), the rotational constant \( B_v \), the centrifugal distortion constant \( D_v \), and the abscissas of the turning point \( R_{\text{min}} \) and \( R_{\text{max}} \) have been calculated for the investigated electronic states of the considered 3 molecules. These values are given in tables 6–8. These constants are calculated for the electronic states \( X^2\Sigma^+ \), \( C^2\Sigma^+ \), \( A^2\Pi \), \( 5^2\Pi \), \( 3^2\Pi \), \( 1^2\Sigma^+ \) of the molecule BeH. The comparison of calculated values of these constants with the available data for the ground state \( \Pi \) states shows an overall acceptable agreement for \( B_v \) with the relative difference 0.74% \( \leq \delta B_v/B_v \leq 2.3\% \) and less agreement for \( E_v \) with 5.15% \( \leq \delta E_v/E_v \leq 33\% \). It should be noted that, the absence of the spin–orbit effect must affect the values of the vibrational energies \( E(v) \) reported in different tables. These values might be affected by the lack of the proper treatment, especially for the \( \Pi \) states in the case of closely lying \( \Pi \) states. Moreover, we repeated the calculation of the vibrational energy levels \( E_v \) for the two electronic states \( X^2\Sigma^+ \) and \( (1)^2\Pi \) of the molecule BeH by using the LEVEL program of LeRoy [37] table 6. The comparison between these values, calculated by the two techniques, shows a relative difference 0.00% \( \leq \delta E_v/E_v \leq 0.272\% \) for 12 vibrational levels of the ground state. While the values of the 14 vibrational energy levels of the \( (1)^2\Pi \) state calculated by the canonical function [38, 45–47] approach are shifted up by an average \( \approx 9 \) cm\(^{-1}\) with a relative difference 0.23% \( \leq \delta E_v/E_v \leq 0.909\% \). For the molecules MgH and SrH the rovibrational constants have been calculated for the electronic states \( X^2\Sigma^+ \), \( (1)^2\Pi \), \( (5)^2\Pi \), \( (1)^2\Delta \), \( (1)^2\Sigma^+ \) and \( X^2\Sigma^+ \), \( (1)^2\Pi \), \( (2)^2\Pi \), \( (3)^2\Pi \), \( (3)^2\Delta \) respectively. No comparison of the constants for these states with other results since they are calculated here for the first time.

5. Summary and conclusion

In the present work, and for the three molecules BeH, MgH, and SrH an \textit{ab initio} calculation for high-lying electronic states has been performed via CAS-SCF/MRCI method. The potential energy curves and the static dipole moment have been determined for 78 electronic states for these molecules. The comparison of our calculated values of the spectroscopic constants \( T_E, R_e \), \( \omega_0 \), and \( B_e \) for the three molecules with those available in literature shows an overall a very good agreement.

We plotted in each one of figures 1–12 the potential energy curves with the corresponding static dipole moment curves. In all these figures we noticed the agreement between the positions of the avoided crossing of the potential energy curves and the crossing of the corresponding dipole moment curves. Moreover, one can notice the agreement between our calculated values of \( \omega_0 \) and those obtained from the rovibrational calculation by using the relation \( E_v \sim \omega_0 (v + 1/2) \). From these agreements we do believe this is the best answer we could current obtain, with the existing methods, for the calculated data of the new investigated electronic states.

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