Electronic structure with rovibrational and dipole moment calculations of the LaS molecule

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The potential energy and the dipole moment curves have been investigated for the 23 lowest electronic states in the $^{2s+1}\Lambda^{(\pm)}$ representation of the molecule LaS via CASSCF. Multireference CI calculations (single and double excitations with Davidson corrections) were performed by using Gaussian basis sets for the two considered atoms. The harmonic frequency ω_e, the internuclear distance r_e and the electronic energy with respect to the ground state T_e have been calculated for 23 electronic states along with the rovibrational data E_v and B_v. Nineteen electronic states have been studied here for the first time. The comparison of the investigated values with the theoretical and experimental results available in the literature shows a very good agreement

Keywords: ab initio calculation, spectroscopic constants, potential energy curves, dipole moment, rovibrational calculation)

1. INTRODUCTION

Diatomic transition metal sulfides molecules are of astrophysical interest. They have also potential applications in chalcogenide based pigments and optical fibers [1-3]. Despite its importance and its various applications [4], the diatomic transition metal sulfides could still be ranked among the least studied diatomic transition metal system [5]. Hinkle *et al.* [6] called for laboratory search for the LaS molecule because of its presence in stellar spectra and S stars [7]. Macrano and Barrow [8] recorded five bands of the $B^2\Sigma^+$-$X^2\Sigma^+$ transition of LaS. They produced the spectrum by using a high-temperature carbon tube furnace and observed it with a diffraction grating spectrograph. The spectrum showed five four-headed bands degraded to the red in the region 700-850 nm. From their data analysis, they predicted that the origin of the $A^2\Pi_r$-$X^2\Sigma^+$ system of LaS should be at approximately 1100 nm. By using the Los Alamos Fourier transform spectrometer Winkel *et al.* [9] recorded the spectrum of diatomic lanthanum sulfide. The region 7500-16000 cm^{-1} is rich in complex bands that were identified as the A-X and B-X transitions. A rotational analysis of both the $A^2\Pi$ -$X^2\Sigma^+$, $B^2\Sigma^+$-$X^2\Sigma^+$ and a new $A^2\Pi$ -$A'^2\Delta$ transitions has been performed by Anderson *et al.* [10] where the vibrational and rotational constants have been calculated for the states $X^2\Sigma^+$, $B^2\Sigma^+$, $A^2\Pi$, and $A'^2\Delta$. The (0,0) band of the $B^2\Sigma^+$-$X^2\Sigma^+$ transition of LaS near 726 nm has been studied by He *et al.* [11] at high resolution using laser vaporization/reaction supersonic free jet expansion and laser induced fluorescence spectroscopy. A total of 1850 rotational-hyperfine transition

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lines have been assigned and measured. Accurate rotational, spin and hyperfine parameters for the $X^2\Sigma^+$, $B^2\Sigma^+$ states have been obtained.

The advances in new methods to cool and manipulate neutral molecules offer new possibilities for precision tests of fundamental physics theories. In general relativity the equivalence principle postulates that the outcome of any non-gravitational experiment is independent of position and time. In theories that attempt to unify gravity with other fundamental forces, on the other hand, violation of the equivalence principle may occur and can be consistently described [12]. Precision molecular spectroscopy is a new and promising direction of search for variation of fundamental constants. Molecular spectra are sensitive to both $\mu = m_p/m_e$ and $\alpha = \frac{e^2}{\hbar c}$, and by measuring close lying levels great enhancement of relative variation may be observed [13, 14, 15]. In particular, diatomic molecules that have a near cancellation between hyperfine structure and rotational intervals or between fine structure and vibrational intervals are of interest in the context of such an enhancement. A number of such molecules have been proposed, e.g. Cs_2 [16], CaH, MgH, CaH^+ [17, 18], Cl^{+2}, IrC, HfF^+, SiBr, LaS, LuO, and others [19].

Quantum computers based upon the principles of quantum superposition and entanglement are expected to provide more powerful computation ability than classical ones [20]. To realize quantum information processing, many schemes of quantum circuits have been proposed. Two of these schemes are i) The vibrational and rotational modes of diatomic molecule can be used to construct elementary quantum gates and to encode two qubits [21], and ii) the electric dipole moments of diatomic molecules, oriented along or against an external electric field consists of the qubits [22].

The important connection between energy relations of solids and molecules [23] and the absence of electronic structure with rovibrational study and dipole moment calculation of higher excited states of the molecule LaS stimulated us, in the present work, to investigate more extensive *ab initio* calculation of this molecule. Based on our previous theoretical calculation [24-34], the potential energy curves and the spectroscopic constants of the low lying 23 electronic states have been calculated where 19 new electronic states have been studied here for the first time. The transition energy with respect to the minimum energy for the ground state T_e, the equilibrium internuclear distance r_e, the harmonic frequency ω_e, the rotational constant B_e, and the permanent dipole moment curves have been obtained for the considered electronic states of this molecule. Taking advantage of the electronic structure of the investigated electronic states of the LaS molecule and by using the canonical functions approach [34-36], the eigenvalue E_v, the rotational constant B_v, and the abscissas of the turning points r_{min} and r_{max} have been calculated for several vibrational levels of the considered electronic states. These investigated results are expected to be useful for further investigations of the LaS spectra and for the astronomers to search the presence of more transition metal sulfides in the atmosphere of cool stars, the possibilities for precision tests of fundamental physics theories, and the quantum information processing.

2. Computational approach

2.1 Ab initio calculations

The potential energy curves of the lowest-lying electronic states of the LaS molecule have been investigated via CASSCF method. Multireference CI calculations (single and double excitations with Davidson corrections) were performed. The sulfur atom is treated in all electron schemes where the 16 electrons of sulfur atom are considered using for s, p, d, and f functions of the ROOS basis set [38]. For the Lanthanum species the basis set ECP46MHF

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[39] has been used for the s, p, and d functions with effective core potential of 46 inner electrons and 11 valance electrons. The potential energy calculations for the states ${}^{2s+1}\Lambda^{(+-)}$ of the molecule LaS have been carried using CAS-SCF method. Among the 27 electrons 22 electrons were frozen in subsequent calculations so that 5 electrons were explicitly treated as valence electrons. The active space contains 2σ(La: $5d_0$; S: $3p_0$), 2π(La: $5d_{\pm1}$; S: $3p_{\pm1}$), 1δ(La: $5d_{\pm2}$) orbitals in the C_{2v} symmetry; this corresponds to 8 active molecular orbitals distributed into irreducible representation a_1, b_1, a_2, b_2 in the following way: $3a_1$, $2b_1$, $2b_2$, $1a_2$, noted [3,2,2,1]. This calculation has been performed via the computational chemistry program MOLPRO [40] taking advantage of the graphical user interface GABEDIT [41].

2.2 The vibration-rotation calculation

A promising approach for realizing a quantum computer is based on using the vibrational states of molecules to represent qubits and tailored femtosecond laser pulses to implement quantum gate operations [47-48]. This vibrational state approach has several advantages: i) the number of qubits is proportional to the number of vibrational degrees of freedom, ii) more qubits can be realized using a N-atom molecule, iii) the vibrational states of molecules are stable over the time scales of interest, iv) the number of qubits is not limited to ten and, v) by using more vibrational states, it may be possible to represent quantum information units having more than two states |0>, |1>, |2>, |3>…. [49].

Another interest of the rovibrational states of the LaS diatomic molecule is the possibilities of precision tests of fundamental physics theories. Degeneracy between levels of different symmetry happens frequently in diatomic molecules with unpaired electrons, such as LaS, LaO, LuS, LuO, YbF and similar ions that have a cancellation between their hyperfine and rotational interval [16].

Within the Born-Oppenheimer approximation, the vibration rotation motion of a diatomic molecule in a given electronic state is governed by the radial Schrödinger equation

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

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

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

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

with $e_0 = E_v$, $e_1 = B_v$, $e_2 = - D_v$ ………, ϕ_0 is the pure vibrational wave function and ϕ_n its rotational corrections. By replacing Eqs.(2) and (3) into Eq.(1) and since this equation is satisfied for any value of λ, one can write [34-36]

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

$$\phi_1''(r)+[e_0-U(r)]\phi_1(r)=-[e_1-R(r)]\phi_0(r) \qquad (5\text{-}1)$$

$$\phi_2''(r)+[e_0-U(r)]\phi_2(r)=-[e_1-R(r)]\phi_1(r)-e_2\,\phi_0(r) \qquad (5\text{-}2)$$

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$$\phi''_n(r) + [e_0 - U(r)]\phi_n(r) = R(r)\,\phi_{n-1} - \sum_{m=1}^{n} e_m\,\phi_{n-m}(r) \qquad (5\text{-}n)$$

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

$$<\phi_0 \,|\, \phi_0> e_1 = <\phi_0 \,|\, \frac{1}{r^2} \,|\, \phi_0> \qquad (6\text{-}1)$$

$$<\phi_0 \,|\, \phi_0> e_2 = <\phi_0 \,|\, \frac{1}{r^2} \,|\, \phi_1> - e_1 <\phi_0 \,|\, \phi_1> \qquad (6\text{-}2)$$

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$$<\phi_0 \,|\, \phi_0> e_n = <\phi_0 \,|\, \frac{1}{r^2} \,|\, \phi_{n-1}> - \sum_{m=1}^{n-1} e_m <\phi_{n-m} \,|\, \phi_0> \qquad (6\text{-}n)$$

Once e_0 is calculated from Eq.(4), e_1, e_2, e_3 … can be obtained by using alternatively Eqs.(5) and (6).

3. RESULTS AND DISCUSSION

The potential energy curves for 23 states in the representation $^{2s+1}\Lambda^{(-+)}$ have been calculated for 47 internuclear distances in the range 2.00Å≤r≤3.44 Å. These PECs for the doublet and quartet states in the different symmetries are drawn respectively in Figs. (1-4).

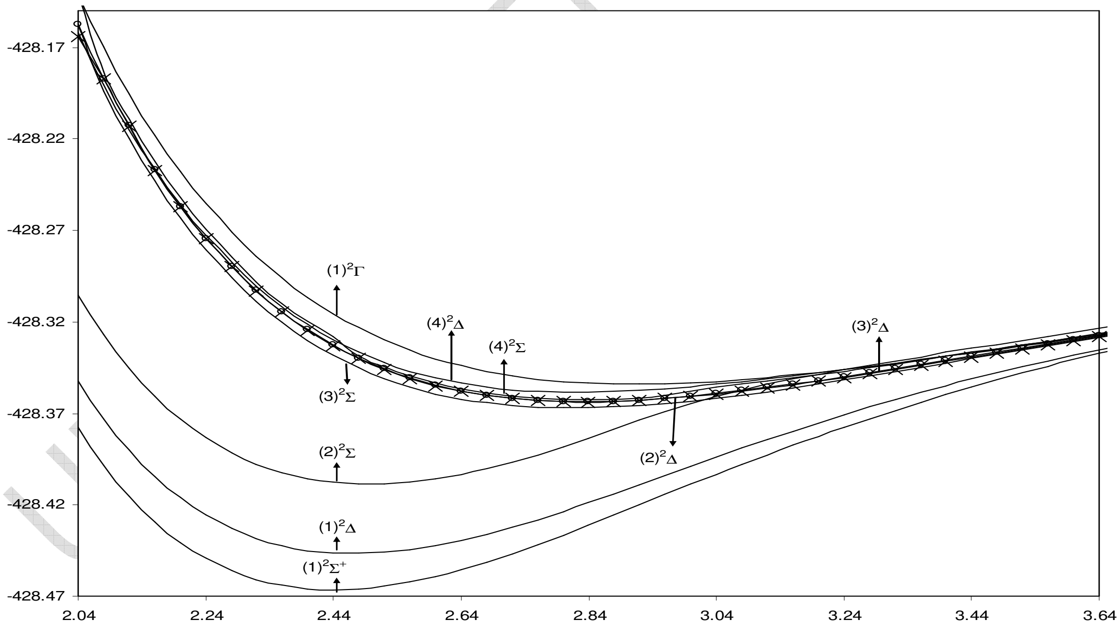

Fig. 1. Potential energy curves for the doublet states $^2\Sigma$, $^2\Delta$ and $^2\Gamma$ of the molecule LaS

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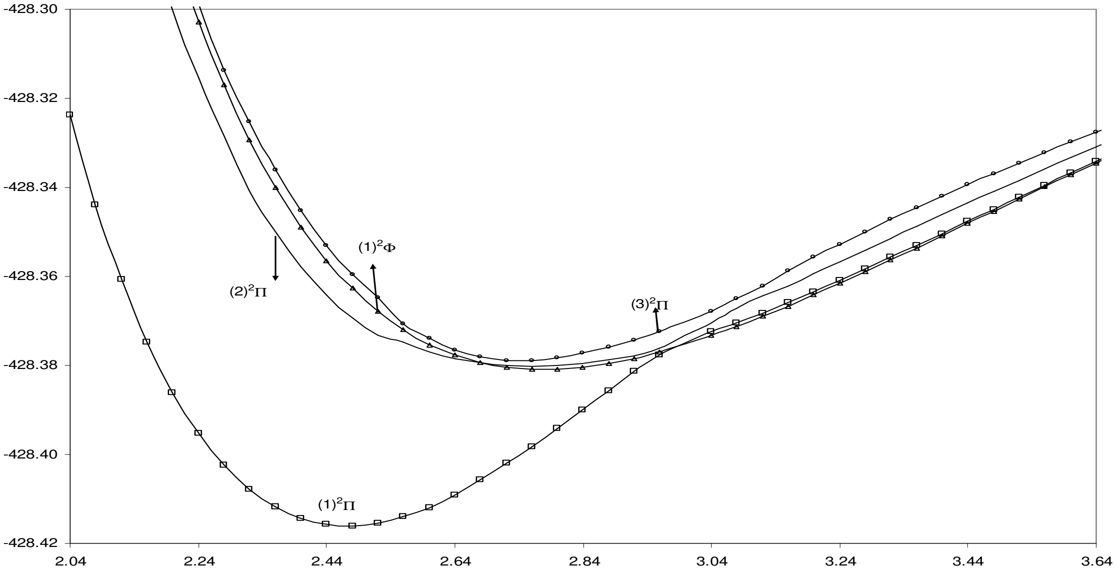

Fig. 2. Potential energy curves for the doublet states $^2\Pi$ and $^2\Phi$ of the molecule LaS

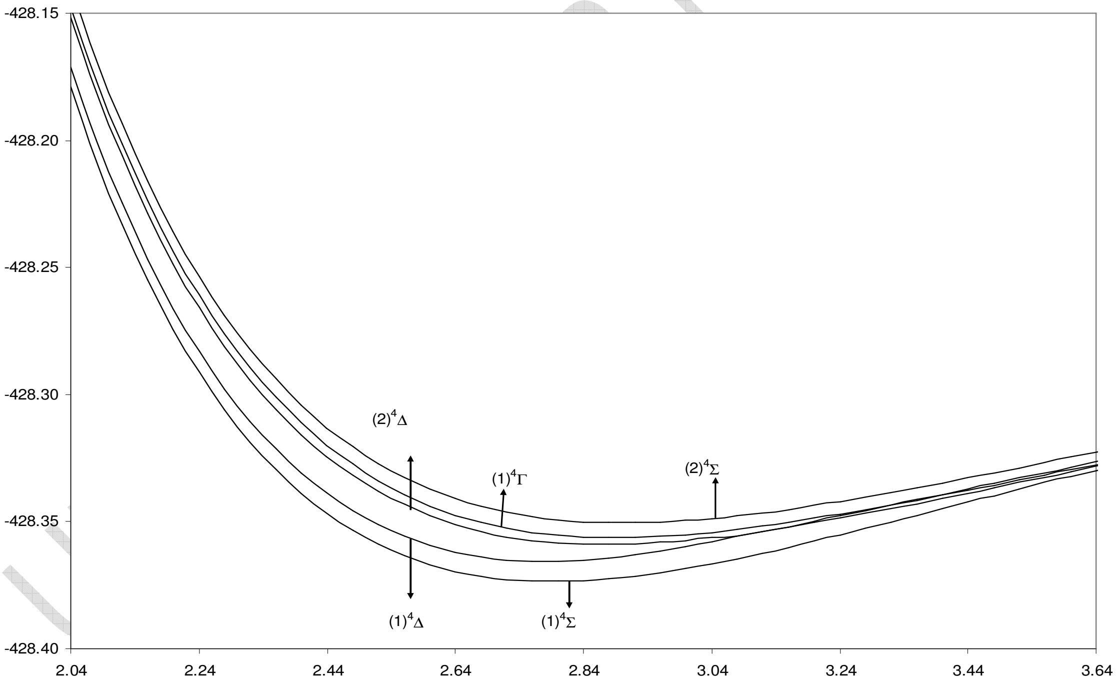

Fig. 3. Potential energy curves for the quartet states $^4\Sigma$, $^4\Delta$ and $^4\Gamma$ of the molecule LaS

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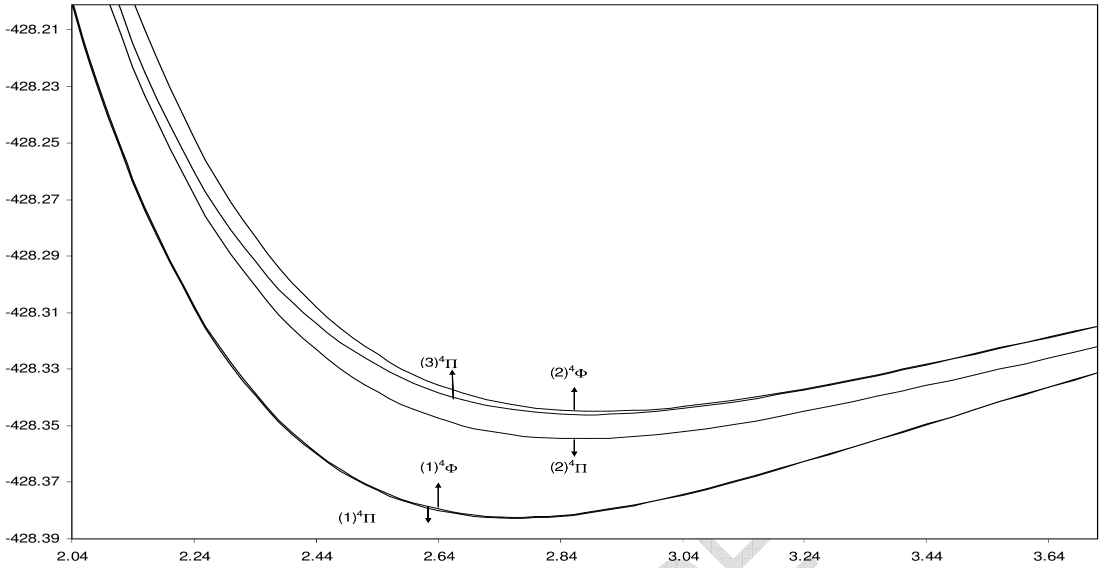

Fig. 4. Potential energy curves for the quartet states $^4\Pi$ and $^4\Phi$ of the molecule LaS

It is quite common to study a crossing or an avoided crossing, known as conical intersections, between ground and excited state potential energy curves of molecules which are important points in photochemistry. Such crossings or avoided crossings can dramatically alter the stability of molecules. In fact, the avoided crossing regions are likely to be a leakage channels along which the molecules flow from the higher down to the lower potential energy curves. If these crossings are overlooked then low barrier transitions can be missed and an incorrect chemical picture will arise [42]. In the range of r considered, several crossings have been detected in the potential energy curves for the excited electronic states at short and large values of internuclear distance and for the highest and lowest states, the positions of these crossings r_c are given in Table 1.

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Table1. Positions of the crossings between the different electronic states of the molecule LaS

state1	state2	Crossing between (n_1)state1/(n_2)state2	r_c(Å)
$X^2\Sigma+$	$^2\Delta$	1/1	3.84
	$^2\Delta$	2/3	3.05
		2/4	3.24
		3/2	2.60
		3/4	2.06
	$^2\Sigma$	2/3	3.02
		2/4	3.20
		3/4	2.46
$^2\Sigma$	$^2\Pi$	3/3	3.33
	$^4\Delta$	3/2	2.57
		3/1	3.66
		4/2	3.16
		4/1	3.01
	$^4\Gamma$	3/1	3.64
		4/1	3.22
	$^2\Sigma$	1/2	3.25
		1/3	3.79
		1/4	3.41
	$^2\Delta$	1/2	3.72
		1/3	3.67
		1/4	3.30
$^2\Gamma$	$^2\Pi$	1/3	3.70
	$^4\Delta$	1/2	3.45
	$^4\Pi$	1/2	2.82
		1/3	2.35
	$^2\Pi$	2/3	3.43
		3/3	3.57
	$^4\Delta$	2/2	2.93
		2/1	3.56
$^2\Delta$		4/1	2.76
		3/2	2.95
		3/1	3.64
	$^4\Gamma$	2/1	3.67
		4/1	3.04
	$^2\Phi$	1/1	2.99
		2/1	2.69
	$^4\Sigma$	3/1	3.11
	$^4\Gamma$	3/1	3.65
$^2\Pi$	$^4\Delta$	3/1	3.51
	$^4\Phi$	1/1	2.97
		2/1	2.63
	$^4\Pi$	1/1	2.97
		2/1	2.60
$^4\Delta$	$^4\Gamma$	2/1	3.34
	$^4\Delta$	2/1	3.08
	$^4\Sigma$	3/2	2.43
$^4\Pi$	$^4\Delta$	2/1	2.31
	$^4\Gamma$	2/1	2.57
		3/1	2.16

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The spectroscopic constants such as the vibrational harmonic constant ω_e, the internuclear distance at equilibrium r_e, the rotation constant B_e, and the electronic transition energy with respect to the ground state T_e have been calculated by fitting the energy values around the equilibrium position to a polynomial in terms of the internuclear distance, these values are displayed in Table 2 together with the available values in the literature either theoretical or experimental.

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Table 2. Calculated spectroscopic constants for the lowest 23 electronic states of the LaS molecule.

State	T_e (cm^{-1})	$\Delta T_e/T_e$ %	ω_e (cm^{-1})	$\Delta\omega_e/\omega_e$ %	B_e (cm^{-1})	$\Delta B_e/B_e$ %	r_e (Å)	$\Delta r_e/r_e$ %
X $^2\Sigma^+$	0.00[a]				0.10875		2.4395	
	0.00[b]		434.48	4.67				
	0.00[c]			4.67				
	0.00[d]		456.70	1.04			2.37[d]	2.83
	0.00[e1]		456.7				2.38[e1]	2.42
			439[d]	12.78			2.23[e2]	8.57
	0.00[f]		490[e1]		0.117155[f]	7.72		
	0.00[g]				0.116976[g]	7.03		
(1)$^2\Delta$	4329.46				0.10568		2.4745	
			424.82					
(1)$^2\Pi$	11043.47[a]		421.41		0.10547		2.4771	
	10487.17[b]	5.03	412.79	2.04				
(2)$^2\Sigma$	12696.59[a]		416.55		0.10546		2.4983	
	13793.21[b]	7.90	410.12	1.54				
	13790.17[c]	7.93	410.07	1.54				
	13766.79[f]	8.43			0.11107	5.3		
	13766.79[g]	8.43			0.11103	5.3		
(1)$^4\Pi$	18587.35		286.03		0.08449		2.7677	
(1)$^4\Phi$	18666.11		285.94		0.08437		2.7697	
(1)$^2\Phi$	18762.72		285.12		0.08376		2.7797	
(2)$^2\Pi$	18932.00		251.61		0.08428		2.7706	
(3)$^2\Pi$	19184.48[a]		352.23		0.08642		2.7366	
	22694[b]	15.46	344	2.34				
(1)$^4\Sigma$	20388.91		288.54		0.08295		2.7931	
(3)$^2\Sigma$	21791.09		272.97		0.08160		2.8145	
(1)$^4\Delta$	22116.21		296.97		0.08363		2.7819	
(2)$^2\Delta$	22509.87		265.13		0.08043		2.8364	
(3)$^2\Delta$	22564.00		271.96		0.08060		2.8336	
(4)$^2\Sigma$	22726.51		321.94		0.08056		2.8342	
(2)$^4\Delta$	23588.60		248.21		0.07956		2.8530	
(4)$^2\Delta$	23713.00		250.50		0.08114		2.824	
(1)$^4\Gamma$	24128.83		280.75		0.07746		2.8901	
(1)$^2\Gamma$	24633.02		246.57		0.07652		2.9081	
(2)$^4\Pi$	24747.86		261.71		0.07830		2.8747	
(2)$^4\Sigma$	25408.26		277.44		0.07701		2.8986	
(3)$^4\Pi$	26591.66		268.99		0.07762		2.8873	
(2)$^4\Phi$	26865.56		237.65		0.07688		2.9016	

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a)Present work, b)Ref.[9], c)Ref.[8], d)Ref.[4], e_1)Ref.[43 empirical method 1], e_2)Ref.[43 empirical method 2], f)Ref.[11], g)Ref.[10]

The comparison of our calculated values with the few fragmented results in the literature shows a good agreement for T_e with relative difference 5.03% Ref.[9]$<\Delta T_e/T_e<8.43\%$ Ref.[10] for the states□$(1)^2\Pi$□ and □$(2)^2\Sigma^+$. This agreement becomes less for the state □$(3)^2\Pi$ □with $\Delta T_e/T_e = 15.46\%$. For the vibrational harmonic constant □ω_e, our calculated values are in good agreement for the published values for the studied states in literature with relative difference 1.04%Ref.[4]$<\Delta\omega_e/\omega_e<$4.67%Ref.[9] except the value given in Ref.[44] where the relative difference is 12.78%. The three published values in literature for each of B_e (for the states $X^2\Sigma^+$ and $(2)^2\Sigma$□ and r_e (for the state $X^2\Sigma^+$) showed a good agreement with our calculated values with relative differences 5.3%Refs.[10,11]$<\Delta B_e/B_e<$7.72%Ref.[11] and 2.42%Refs.[43(method1)]$<\Delta r_e/r_e<$8.57%Ref.[43(method2)] respectively. The comparison for the other calculated values is not possible since they are given here for the first time.

The permanent dipole moment operator is among the most reliably predicted physical properties. DeMille [22] described the molecular qubits as permanent electric dipoles oriented along |0> or against |1> in an external electric field. Bits are coupled by the electric dipole-dipole interaction. Loading with ultracold molecules makes it possible to use a weak trapping potential, which should allow long decoherence times for the system. The expectation value of the permanent dipole moment is sensitive to the nature of the least energetic and most chemically relevant valence electrons [44-46]. Since the Hartree-Fock dipole moment is usually large, and in order to obtain the best accuracy, multireference configuration interaction (MRCI) wave functions were constructed using multi configuration Self-consistent field (MCSCF) active space. By taking the La atom as an origin in our calculation, the permanent dipole moments of the investigated electronic states have been analyzed for the 23 lowest electronic states of the molecule LaS. The calculated values of the dipole moments (in Debye) for these electronic states in terms of the internuclear distance r are plotted in figures (5-9). All these calculations were performed by using the MOLPRO [40] program.

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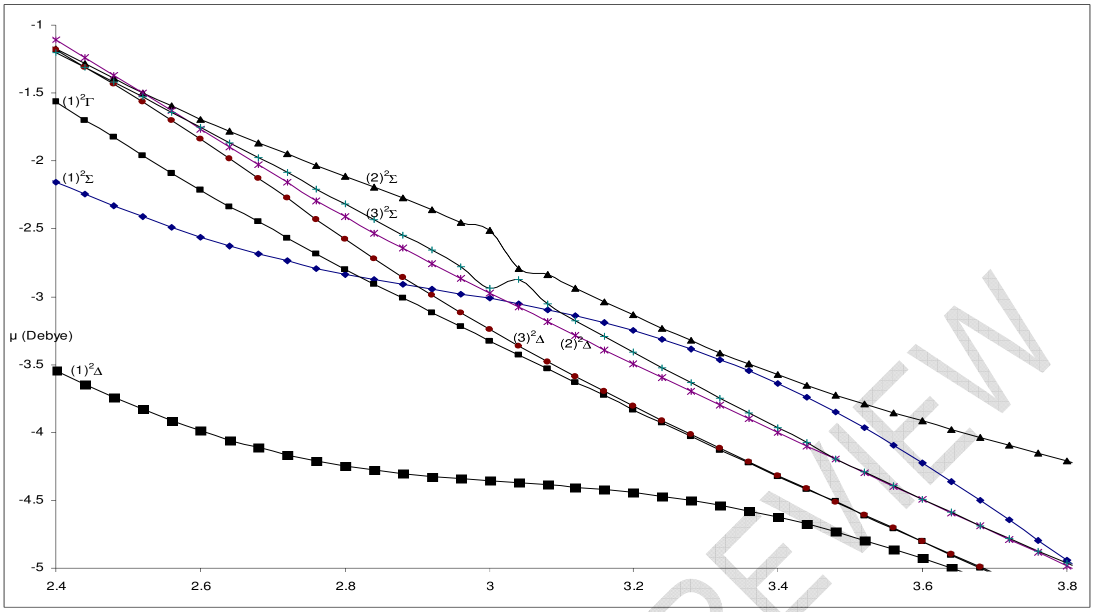

Fig.5. Dipole moments curves for the doublet states (1-3)$^2\Sigma$, (1-3)$^2\Delta$ and (1)$^2\Gamma$ of the molecule LaS

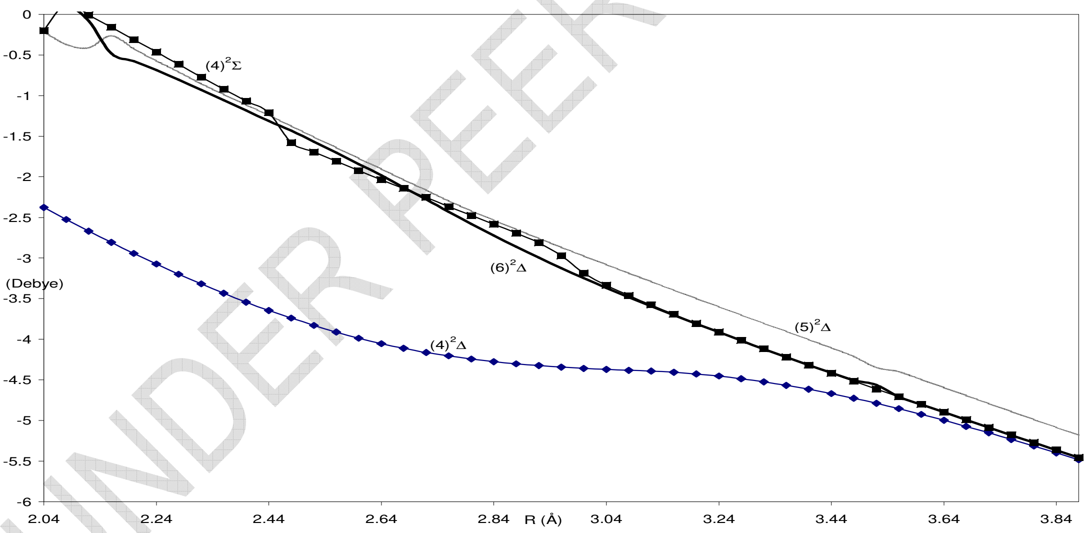

Fig. 6. Dipole moments curves for the doublet states (4)$^2\Sigma$ and (4-6)$^2\Delta$ of the molecule LaS

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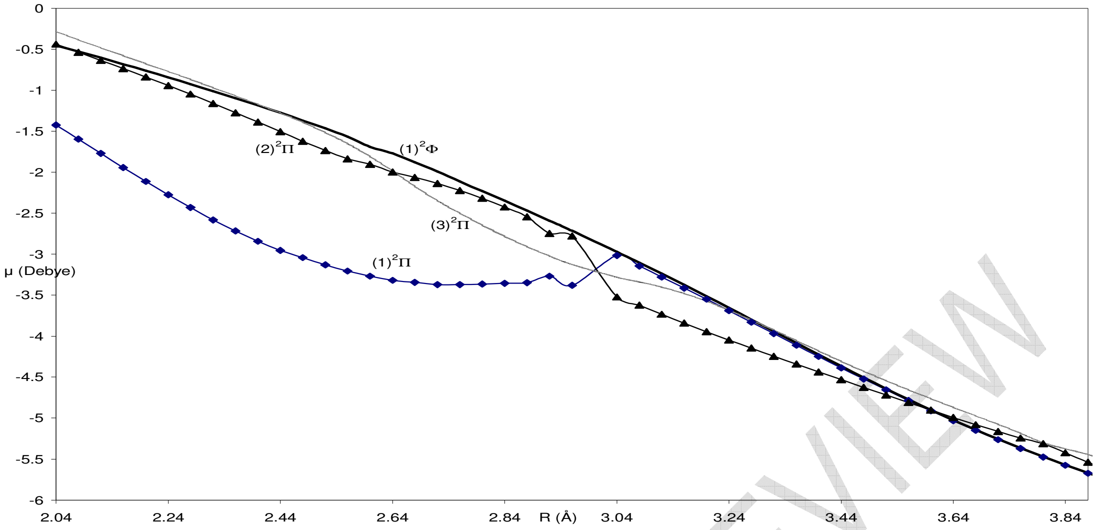

Fig. 7. Dipole moments curves for the doublet states $^2\Pi$ and $^2\Phi$ of the molecule LaS.

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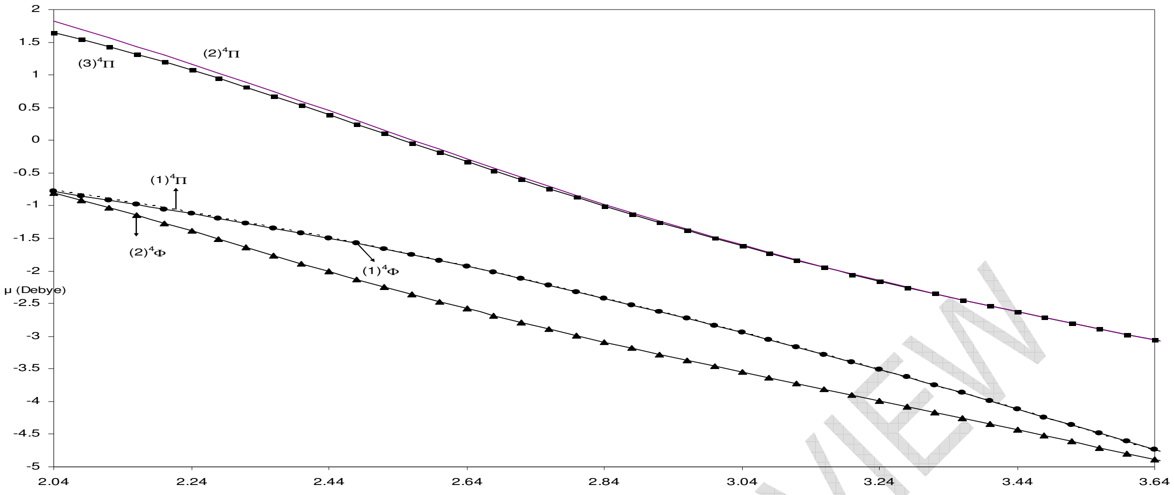

Fig. 8. Dipole moments curves for the quartet states $^4\Pi$ and $^4\Phi$ of the molecule LaS.

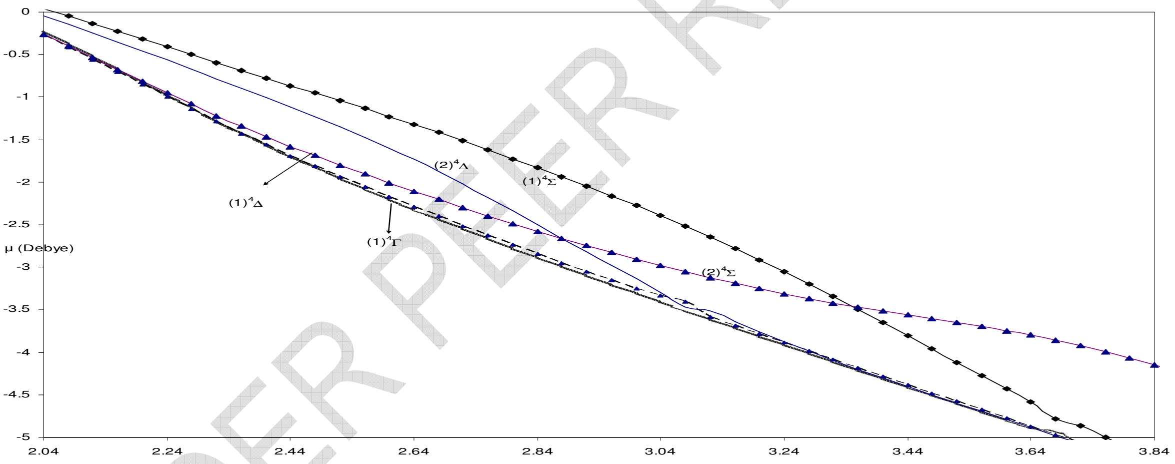

Fig. 9. Dipole moments graphs for the quartet states $^4\Sigma$, $^4\Gamma$, and $^4\Delta$ of the molecule LaS

By using the canonical functions approach and the cubic spline interpolation between each two consecutive points of the potential energy curves obtained from the *ab initio* calculation of the LaS 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 up to the vibrational levels v=20 for the considered electronic states. These values for the states $(1)^2\Delta$, $(1)^2\Pi$, $(1)^4\Pi$, $(2)^2\Sigma$ (as illustration) are given in Table 3. No comparison of these values with those in literature since they are given here for the first time.

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Table 3. Values of the eigenvalues E_v, the abscissas of the turning points r_{min}, r_{max}, and the rotational constant B_v for the different vibrational levels of the $(1)^2\Delta$, $(1)^2\Pi$, $(1)^4\Pi$, $(2)^2\Sigma$ of the LaS molecule.

	$(1)^2\Delta$				$(1)^2\Pi$			
V	**E_v (cm^{-1})**	**r_{min} (Å)**	**r_{max} (Å)**	**B_v×10 (cm-1)**	**E_v (cm-1)**	**r_{min} (Å)**	**r_{max} (Å)**	**B_v ×10 (cm-1)**
0	215.35	2.417	2.529	1.0583	210.89	2.419	2.531	1.0567
1	625.60	2.379	2.574	1.0549	620.12	2.391	2.575	1.0537
2	1036.24	2.354	2.606	1.0525	1029.19	2.356	2.607	1.0517
3	1445.29	2.335	2.632	1.0493	1436.73	2.336	2.634	1.0483
4	1853.59	2.318	2.656	1.0470	1842.22	2.319	2.657	1.0464
5	2261.01	2.304	2.677	1.0443	2246.44	2.304	2.679	1.0435
6	2667.70	2.290	2.697	1.0414	2647.88	2.290	2.699	1.0412
7	3072.03	2.279	2.716	1.0382	3046.32	2.278	2.719	1.0375
8	3474.14	2.268	2.735	1.0350	3441.73	2.267	2.738	1.0339
9	3874.15	2.258	2.752	1.0321	3833.24	2.257	2.756	1.0296
10	4272.53	2.248	2.764	1.0291	4222.04	2.248	2.774	1.0257
11	4669.38	2.239	2.785	1.0263	4607.97	2.239	2.791	1.0223
12	5064.72	2.230	2.801	1.0234	4992.02	2.231	2.808	1.0187
13	5458.56	2.223	2.816	1.0204	5373.49	2.223	2.824	1.0151
14	5850.64	2.215	2.832	1.0174	5751.86	2.215	2.841	1.0111
15	6240.93	2.208	2.846	1.0142	6127.25	2.208	2.857	1.0070
16	6629.41	2.201	2.861	1.0112	6499.81	2.873	2.873	1.0031
17					6868.81	2.195	2.888	0.9935

	$(1)^4\Pi$				$(2)^2\Sigma$			
v	**E_v (cm^{-1})**	**r_{min} (Å)**	**r_{max} (Å)**	**B_v×10^2 (cm^{-1})**	**E_v (cm^{-1})**	**r_{min} (Å)**	**r_{max} (Å)**	**B_v×10 (cm^{-1})**
0	142.50	2.702	2.836	8.4375	206.46	2.440	2.554	1.03768
1	429.32	2.657	2.890	8.4085	607.34	2.402	2.599	1.0351
2	715.48	2.628	2.930	8.3781	1008.10	2.377	2.631	1.0321
3	999.44	2.606	2.962	8.3489	1412.61	2.357	2.657	1.0302
4	1282.48	2.586	2.992	8.3151	1814.77	2.340	2.680	1.0288
5	1564.12	2.570	3.019	8.2849	2219.00	2.325	2.701	1.0259
6	1843.83	2.554	3.044	8.2545	2620.21	2.312	2.721	1.0233
7	2121.77	2.541	3.068	8.2234	3019.67	2.300	2.740	1.0205
8	2398.05	2.528	3.091	8.1923	3148.47	2.289	2.758	1.0185
9	2672.69	2.517	3.113	8.1612	3816.56	2.278	2.775	1.0160
10	2945.67	2.506	3.135	8.1302	4213.97	2.268	2.791	1.0137
11	3216.99	2.496	3.155	8.0993	4610.15	2.259	2.807	1.0113
12	3486.67	2.486	3.175	8.0685	5005.45	2.251	2.822	1.0088
13	3754.70	2.476	3.195	8.0380	5399.43	2.244	2.834	1.0062
14	4021.08	2.468	3.215	8.0075	5792.01	2.235	2.851	1.0035
15	4285.79	2.460	3.234	7.9770	6183.02	2.227	2.866	1.0007
16	4548.85	2.452	3.252	7.9436	6572.09	2.220	2.880	9.9773
17	4810.28	2.444	3.271	7.9155	6959.08	2.213	2.894	9.9451
18	5070.12	2.437	3.289	7.8846	7343.55	2.207	2.908	9.9112
19	5328.40	2.430	3.307	7.8534	7725.20	2.200	2.923	9.8740
20	5585.17	2.423	3.325	7.8223	8103.68	2.194	2.937	9.8341

4. Conclusion

In the present work, the *ab initio* investigation for 23 low-lying electronic states of LaS molecule has been performed via CAS-SCF/MRCI method. The potential energy and permanent dipole moments curves have been determined along with the spectroscopic constants T_e, r_e, ω_e and the rotational constant B_e for the lowest-lying electronic states. Based on the canonical function approach a rovibrational calculation has been performed for

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the investigated electronic states. The comparison of our results with those available in the literature has demonstrated the good accuracy except the value of T_e for the state $(3)^2\Pi$. Nineteen electronic states have been investigated in the present work for the first time. As these results are expected to be useful for further investigations of the LaS spectra, quantum computation and the fundamental physics theories, extensive energy values versus internuclear distance r and the rovibrational energy levels of the ground and excited electronic states are available upon request.

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