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

M. Korek\* and H. Hammour

Faculty of Science, Beirut Arab University, P.O.Box 11-5020 Riad El Solh, Beirut 1107 2809, Lebanon

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  $\omega_e$ , 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

13

1

2

3 4 5

6 7

8

10 11 12

14 15

16 17 Keywords: ab initio calculation, spectroscopic constants, potential energy curves, dipole moment, rovibrational calculation)

# 18 1. INTRODUCTION

19

20 Diatomic transition metal sulfides molecules are of astrophysical interest. They have also 21 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 22 ranked among the least studied diatomic transition metal system [5]. Hinkle et al. [6] called 23 24 for laboratory search for the LaS molecule because of its presence in stellar spectra and S 25 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 26 27 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 28 the origin of the  $A^2\Pi_r X^2\Sigma^+$  system of LaS should be at approximately 1100 nm. By using the 29 30 Los Alamos Fourier transform spectrometer Winkel et al. [9] recorded the spectrum of diatomic lanthanum sulfide. The region 7500-16000 cm<sup>-1</sup> is rich in complex bands that were 31 identified as the A-X and B-X transitions. A rotational analysis of both the  $A^2\Pi$  - $X^2\Sigma^+$ ,  $B^2\Sigma^+$ -32  $X^{2}\Sigma^{+}$  and a new  $A^{2}\Pi - A'^{2}\Delta$  transitions has been performed by Anderson *et al.* [10] where the 33 vibrational and rotational constants have been calculated for the states  $X^{2}\Sigma^{+}$ ,  $B^{2}\Sigma^{+}$ ,  $A^{2}\Pi$ , and 34 A'<sup>2</sup> $\Delta$ . The (0,0) band of the B<sup>2</sup> $\Sigma$ <sup>+</sup>-X<sup>2</sup> $\Sigma$ <sup>+</sup> transition of LaS near 726 nm has been studied by He 35 et al. [11] at high resolution using laser vaporization/reaction supersonic free jet expansion 36 37 and laser induced fluorescence spectroscopy. A total of 1850 rotational-hyperfine transition

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402: E-mail address:

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

47 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 (the transition frequency between two quasi-degenerated states are sensitive to the variation in fundamental constants; the enhancement is result of cancellation between the hyperfine and rotational intervals). A number of such molecules have been proposed, e.g. Cs<sub>2</sub> [16], CaH, MgH, CaH<sup>+</sup> [17, 18], Cl<sup>+2</sup>, IrC, HfF<sup>+</sup>, SiBr, LaS, LuO, and others [19].

55 A promising approach for realizing a quantum computer is based on using the vibrational 56 states of molecules to represent qubits and tailored femtosecond laser pulses to implement 57 quantum gate operations [20-21]. This vibrational state approach has several advantages: i) 58 the number of gubits is proportional to the number of vibrational degrees of freedom, ii) more 59 qubits can be realized using a N-atom molecule, iii) the vibrational states of molecules are 60 stable over the time scales of interest, iv) the number of qubits is not limited to ten and, v) by 61 using more vibrational states, it may be possible to represent quantum information units 62 having more than two states |0>, |1>, |2>, |3>.... [22].

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].

Quantum computers based upon the principles of quantum superposition and entanglement are expected to provide more powerful computation ability than classical ones [23]. 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 [24], and ii) the electric dipole moments of diatomic molecules, oriented along or against an

74 external electric field consists of the qubits [25].

75 The important connection between energy relations of solids and molecules [26] and the 76 absence of electronic structure with rovibrational study and dipole moment calculation of 77 higher excited states of the molecule LaS stimulated us, in the present work, to investigate 78 more extensive ab initio calculation of this molecule. Based on our previous theoretical 79 calculation [26-36], the potential energy curves and the spectroscopic constants of the low 80 lying 23 electronic states have been calculated where 19 new electronic states have been 81 studied here for the first time. The transition energy with respect to the minimum energy for 82 the ground state  $T_e$ , the equilibrium internuclear distance  $r_e$ , the harmonic frequency  $\omega_{e}$ , the rotational constant Be, and the permanent dipole moment curves have been obtained for the 83 considered electronic states of this molecule. Taking advantage of the electronic structure of 84

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

the investigated electronic states of the LaS molecule and by using the canonical functions approach [37-40], 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.

92

109

# 93 2. Computational approach

## 94 **2.1 Electronic state calculation**

95 The potential energy curves of the lowest-lying electronic states of the LaS molecule have 96 been investigated via CASSCF method. Multireference CI calculations (single and double excitations with Davidson corrections) were performed. The sulfur atom is treated in all 97 98 electron schemes where the 16 electrons of sulfur atom are considered using for s, p, d, and f functions of the ROOS basis set [41]. For the Lanthanum species the basis set ECP46MHF 99 [42] has been used for the s, p, and d functions with effective core potential of 46 inner 100 electrons and 11 valance electrons. The potential energy calculations for the states  $^{2s+1}\Lambda^{(+-)}$ 101 102 of the molecule LaS have been carried using CAS-SCF method. Among the 27 electrons 22 103 electrons were frozen in subsequent calculations so that 5 electrons were explicitly treated as valence electrons. The active space contains  $2\sigma(\text{La: 5d}_0; \text{S: 3p}_0), 2\pi(\text{La: 5d}_{+1}; \text{S: 3p}_{+1}),$ 104 105  $1\delta$ (La: 5d<sub>±2</sub>) orbitals in the C<sub>2v</sub> symmetry; this corresponds to 8 active molecular orbitals 106 distributed into irreducible representation a<sub>1</sub>, b<sub>1</sub>, a<sub>2</sub>, b<sub>2</sub> in the following way: 3a<sub>1</sub>, 2b<sub>1</sub>, 2b<sub>2</sub>, 1a<sub>2</sub>, noted [3,2,2,1]. This calculation has been performed via the computational chemistry 107 108 program MOLPRO [43] taking advantage of the graphical user interface GABEDIT [44].

# 110 2.2 The vibration-rotation calculation

111 Within the Born-Oppenheimer approximation, the vibration rotation motion of a diatomic 112 molecule in a given electronic state is governed by the radial Schrödinger equation

113 
$$\left[\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2}(E_{\nu J} - U(r)) - \frac{\lambda}{r^2}\right] \Psi_{\nu J}(r) = 0$$
(1)

114 where r is the internuclear distance, v and J are respectively the vibrational and rotational 115 quantum numbers,  $\lambda = J(J+1) \square E_{vJ}$  and  $\Psi_{vJ}$  are respectively the eigenvalue and the 116 eigenfunction of this equation. In the perturbation theory these functions can be expanded as

117 
$$E_{vJ} = \sum_{n=0}^{\infty} e_n \lambda^n$$
(2)

118 
$$\Psi_{vJ}(r) = \sum_{n=0} \phi_n(r)\lambda^n$$
(3)

119 with  $e_0 = E_v$ ,  $e_1 = B_v$ ,  $e_2 = D_v$  .....,  $\phi_0$  is the pure vibrational wave function and  $\phi_n$  its 120 rotational corrections. By replacing Eqs.(2) and (3) into Eq.(1) and since this equation is 121 satisfied for any value of  $\lambda$ , one can write [37-39]

122 
$$\phi_0^{"}(r) + [e_0 - U(r)]\phi_0(r) = 0$$
 (4)  
123  $\phi_1^{"}(r) + [e_0 - U(r)]\phi_1(r) = -[e_1 - R(r)]\phi_0(r)$  (5-1)  
124  $\phi_2^{"}(r) + [e_0 - U(r)]\phi_2(r) = -[e_1 - R(r)]\phi_1(r) - e_2\phi_0(r)$  (5-2)

126 
$$\phi_n^{"}(r) + [e_0 - U(r)]\phi_n(r) = R(r)\phi_{n-1} - \sum_{m=1}^n e_m \phi_{n-m}(r)$$
 (5-n)

where  $R(r)=1/r^2$ , the first equation is the pure vibrational Schrödinger equation and the 127 128 remaining equations are called the rotational Schrödinger equations. One may project 129 Eqs.(7) onto  $\phi_0$  and find

130 
$$<\phi_0 \mid \phi_0 > e_1 = <\phi_0 \mid \frac{1}{r^2} \mid \phi_0 >$$
 (6-1)

131 
$$<\phi_0 | \phi_0 > e_2$$

$$<\phi_0 \mid \phi_0 > e_2 = <\phi_0 \mid \frac{1}{r^2} \mid \phi_1 > -e_1 < \phi_0 \mid \phi_1 >$$

133 
$$<\phi_0 | \phi_0 > e_n = <\phi_0 | \frac{1}{r^2} | \phi_{n-1} > -\sum_{m=1}^{n-1} e_m <\phi_{n-m} | \phi_0 >$$
 (6-n)

134 Once  $e_0$  is calculated from Eq.(4),  $e_1$ ,  $e_2$ ,  $e_3$  ... can be obtained by using alternatively Eqs.(5) 135 and (6). 136

(6-2)

#### **3. RESULTS AND DISCUSSION** 137

138

132

125

The potential energy curves for 23 states in the representation  ${}^{2s+1}\Lambda^{(-+)}$  have been calculated 139 for 47 internuclear distances in the range 2.00Å≤r≤3.44 Å. These PECs for the doublet and 140 quartet states in the different symmetries are drawn respectively in Figs. (1-4). 141







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

Corresponding author, Tel : +961 3 747617; Fax : +961 1 818 402 : E-mail address: fkorek@yahoo.com

146

144 145



148

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

150 It is quite common to study a crossing or an avoided crossing, known as conical 151 intersections, between ground and excited state potential energy curves of molecules which 152 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 153 be a leakage channels along which the molecules flow from the higher down to the lower 154 potential energy curves. If these crossings are overlooked then low barrier transitions can be 155 missed and an incorrect chemical picture will arise [45]. In the range of r considered, several 156 crossings have been detected in the potential energy curves for the excited electronic states 157 at short and large values of internuclear distance and for the highest and lowest states, the 158 159 positions of these crossings  $r_c$  are given in Table 1.

160

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

state1	state2	Crossing between (n <sub>1</sub> )state1/(n <sub>2</sub> )state2	r <sub>c</sub> (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
$2\Sigma$		3/4	2.46
	<sup>2</sup> П	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
$^{2}\Gamma$		1/4	3.30
-	$^{2}\Pi$	1/3	3.70
	$^{4}\Delta$	1/2	3.45
	$^{4}\Pi$	1/2	2.82
		1/3	2.35
	<sup>2</sup> П	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
	0	4/1	3.04
	$^{2}\Phi$	1/1	2.99
		2/1	2.69
	$^{4}\Sigma$	3/1	3.11
2	${}^{4}\Gamma$	3/1	3.65
ŕΠ	$^{4}\Delta$	3/1	3.51
	$^{4}\Phi$	1/1	2.97
		2/1	2.63
	<sup>4</sup> П	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

164 The spectroscopic constants such as the vibrational harmonic constant  $\omega_e$ , the internuclear 165 distance at equilibrium  $r_e$ , the rotation constant  $B_e$ , and the electronic transition energy with 166 respect to the ground state  $T_e$  have been calculated by fitting the energy values around the 167 equilibrium position to a polynomial in terms of the internuclear distance, these values are 168 displayed in Table 2 together with the available values in the literature either theoretical or 169 experimental.

170

 171
 Table 2. Calculated spectroscopic constants for the lowest 23 electronic states of the

 172
 LaS molecule.

State	T <sub>e</sub>	$\Delta T_e/T_e$	ω <sub>e</sub>	$\Delta \omega_e / \omega_e$	B <sub>e</sub>	$\Delta B_e/B_e$	r <sub>e</sub> (Å)	∆r <sub>e</sub> /r <sub>e</sub>
	(cm <sup>-</sup> )	%	(cm ')	%	(cm )	%		%
$X^{2}\Sigma^{+}$	0.00 <sup>a</sup>				0.10875		2.4395	
	0.00 <sup>b</sup>		434.48	4.67				
	0.00 <sup>c</sup>			4.67				
	0.00 <sup>d</sup>		456.70	1.04			2.37 <sup>d</sup>	2.83

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

	0.00 <sup>e1</sup>		456.7	10 70			2.38 <sup>e1</sup>	2.42
	0.00 <sup>f</sup> 0.00 <sup>g</sup>		439° 490 <sup>e1</sup>	12.78	0.117155 <sup>f</sup> 0.116976 <sup>g</sup>	7.72 7.03	2.23**	8.57
$(1)^2 \Delta$	4329.46		40.4.00		0.10568		2.4745	
(1) <sup>2</sup> Π	11043.47 <sup>a</sup> 10487.17 <sup>b</sup>	5.03	424.82 421.41 412.79	2.04	0.10547		2.4771	
(2) <sup>2</sup> Σ	12696.59 <sup>a</sup> 13793.21 <sup>b</sup> 13790.17 <sup>c</sup> 13766 79 <sup>f</sup>	7.90 7.93 8.43	416.55 410.12 410.07	1.54 1.54	0.10546	53	2.4983	
(1) <sup>4</sup> ∏	13766.79 <sup>9</sup> 18587.35	8.43	286.03		0.11103 0.08449	5.3	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) <sup>2</sup> Π	18932.00		251.61		0.08428		2.7706	
(3) <sup>2</sup> Π	19184.48 <sup>a</sup> 22694 <sup>b</sup>	15.46	352.23 344	2.34	0.08642		2.7366	
(1) <sup>4</sup> Σ	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) <sup>4</sup> П	24747.86		261.71		0.07830		2.8747	
(2) <sup>4</sup> Σ	25408.26		277.44		0.07701		2.8986	
(3) <sup>4</sup> П	26591.66		268.99		0.07762		2.8873	
$(2)^{4}\Phi$	26865.56		237.65		0.07688		2.9016	

a)Present work, b)Ref.[9], c)Ref.[8], d)Ref.[4], e1)Ref.[47 empirical method 1], e2)Ref.[47 empirical method 2], f)Ref.[11], g)Ref.[10]

175

176 The comparison of our calculated values with the few fragmented results in the literature with 177 shows good agreement for  $T_{e}$ relative difference а 5.03% Ref.[9]< $\Delta T_e/T_e$ <8.43% Ref.[10] for the states  $\Box(1)^2\Pi \Box$  and  $\Box(2)^2\Sigma^+$ . This agreement 178 becomes less for the state  $\Box(3)^2\Pi$   $\Box$  with  $\Delta T_e/T_e = 15.46\%$ . For the vibrational harmonic 179 constant  $\Box \omega_{e}$ , our calculated values are in good agreement for the published values for the 180 181 studied states in literature with relative difference 1.04%Ref.[4]< $\Delta \omega_e / \omega_e < 4.67\%$ Ref.[9] except

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

186 2.42%Refs.[ $\frac{47}{(\text{method 1})} < \Delta r_e/r_e < 8.57\% \text{Ref}.[\frac{47}{(\text{method 2})}]$  respectively. The comparison for 187 the other calculated values is not possible since they are given here for the first time.

188 The permanent dipole moment operator is among the most reliably predicted physical 189 properties. DeMille [25] described the molecular qubits as permanent electric dipoles 190 oriented along |0> or against |1> in an external electric field. Bits are coupled by the electric 191 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 192 193 expectation value of the permanent dipole moment is sensitive to the nature of the least energetic and most chemically relevant valence electrons [47-49]. Since the Hartree-Fock 194 195 dipole moment is usually large, and in order to obtain the best accuracy, multireference 196 configuration interaction (MRCI) wave functions were constructed using multi configuration 197 Self-consistent field (MCSCF) active space. The permanent dipole moments of the investigated electronic states have been analyzed for the 23 lowest electronic states of the 198 molecule LaS. The calculated values of the dipole moments (in Debye) for these electronic 199 200 states in terms of the internuclear distance r are plotted in figures (5-9). All these calculations 201 were performed by using the MOLPRO [40] program. 202









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 215 By using the canonical functions approach and the cubic spline interpolation between each two 216 consecutive points of the potential energy curves obtained from the ab initio calculation of the 217 LaS molecule, the eigenvalue E<sub>v</sub>, the rotational constant B<sub>v</sub>, and the abscissas of the turning 218 point r<sub>min</sub> and r<sub>max</sub> have been calculated up to the vibrational levels v=20 for the considered 219 electronic states. These values for the states  $(1)^2 \Delta$ ,  $(1)^2 \Pi$ ,  $(1)^4 \Pi$ ,  $(2)^2 \Sigma$  (as illustration) are given 220 in Table 3. No comparison of these values with those in literature since they are given here for 221 222 the first time.

# 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.

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

		(1) <sup>2</sup> Δ					(1) <sup>2</sup> ∏	
V	Ev	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)	B <sub>v</sub> ×10	Ev	r <sub>min</sub>	r <sub>max</sub>	B <sub>v</sub> ×10
	(cm⁻¹)			(cm-1)	(cm-1)	(Å)	(Å)	(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) <sup>4</sup> Π					(2) <sup>2</sup> Σ	
v	E <sub>v</sub>	r <sub>min</sub> (Å)	r <sub>max</sub> (Å)	B <sub>v</sub> × <mark>10</mark>	Ev	r <sub>min</sub>	r <sub>max</sub>	B <sub>v</sub> ×10
	/'\							
	(cm )			(cm <sup>-</sup> ')	(cm <sup>-</sup> ')	(A)	(A)	(cm <sup>-</sup> )
0	(cm ) 	2.702	2.836	(cm <sup>-</sup> ') 8.4375	(cm <sup>-</sup> ) 206.46	( <b>A</b> ) 2.440	( <b>A</b> ) 2.554	(cm <sup>-</sup> ) 1.03768
0	(cm ) 142.50 429.32	2.702 2.657	2.836 2.890	(cm <sup>-</sup> ') 8.4375 8.4085	(cm <sup>-</sup> ) 206.46 607.34	( <b>A</b> ) 2.440 2.402	( <b>A</b> ) 2.554 2.599	(cm <sup>-</sup> ') 1.03768 1.0351
0 1 2	(cm ) 142.50 429.32 715.48	2.702 2.657 2.628	2.836 2.890 2.930	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781	(cm <sup>-1</sup> ) 206.46 607.34 1008.10	(A) 2.440 2.402 2.377	(A) 2.554 2.599 2.631	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321
0 1 2 3	(cm ) 142.50 429.32 715.48 999.44	2.702 2.657 2.628 2.606	2.836 2.890 2.930 2.962	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489	(cm <sup>-1</sup> ) 206.46 607.34 1008.10 1412.61	(A) 2.440 2.402 2.377 2.357	(A) 2.554 2.599 2.631 2.657	(cm <sup>-1</sup> ) 1.03768 1.0351 1.0321 1.0302
0 1 2 3 4	142.50 429.32 715.48 999.44 1282.48	2.702 2.657 2.628 2.606 2.586	2.836 2.890 2.930 2.962 2.992	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77	(A) 2.440 2.402 2.377 2.357 2.340	(A) 2.554 2.599 2.631 2.657 2.680	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288
0 1 2 3 4 5	(cm) 142.50 429.32 715.48 999.44 1282.48 1564.12	2.702 2.657 2.628 2.606 2.586 2.570	2.836 2.890 2.930 2.962 2.992 3.019	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00	(A) 2.440 2.402 2.377 2.357 2.340 2.325	(A) 2.554 2.599 2.631 2.657 2.680 2.701	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259
0 1 2 3 4 5 6	(cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83	2.702 2.657 2.628 2.606 2.586 2.570 2.554	2.836 2.890 2.930 2.962 2.992 3.019 3.044	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21	(A) 2.440 2.377 2.357 2.340 2.325 2.312	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233
0 1 2 3 4 5 6 7	(cm ) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.554	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.721 2.740	(cm <sup>-</sup> ) 1.03768 1.0351 1.0302 1.0288 1.0259 1.0233 1.0205
0 1 2 3 4 5 6 7 8	(cm ) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.554 2.541 2.528	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300 2.289	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.721 2.740 2.758	(cm <sup>-</sup> ) 1.03768 1.0351 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185
0 1 2 3 4 5 6 7 8 9	(cm ) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.554 2.541 2.528 2.517	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300 2.289 2.278	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.721 2.740 2.758 2.775	(cm <sup>-1</sup> ) 1.03768 1.0351 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160
0 1 2 3 4 5 6 7 8 9 10	(cm ) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.554 2.541 2.528 2.517 2.506	2.836 2.890 2.930 2.962 3.019 3.044 3.068 3.091 3.113 3.135	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300 2.289 2.278 2.268	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791	(cm <sup>-1</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137
0 1 2 3 4 5 6 7 8 9 10 11	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.541 2.528 2.541 2.528 2.517 2.506 2.496	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300 2.289 2.278 2.268 2.259	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807	(cm <sup>-</sup> ) 1.03768 1.0351 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113
0 1 2 3 4 5 6 7 8 9 10 11 12	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.486	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45	(A) 2.440 2.377 2.357 2.340 2.325 2.312 2.300 2.289 2.278 2.268 2.259 2.251	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807 2.822	(cm <sup>-</sup> ) 1.03768 1.0351 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088
0 1 2 3 4 5 6 7 8 9 10 11 12 13	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.486 2.476	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.135 3.155 3.175 3.195	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> </ul>	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807 2.822 2.834	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14	(cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.486 2.476 2.468	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.155 3.175 3.195 3.215	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.235</li> </ul>	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807 2.822 2.834 2.851	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79	2.702 2.657 2.628 2.606 2.586 2.570 2.554 2.554 2.528 2.517 2.526 2.496 2.486 2.476 2.468 2.460	2.836 2.890 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175 3.195 3.215 3.234	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02	(A) 2.440 2.377 2.377 2.357 2.340 2.325 2.312 2.300 2.289 2.278 2.268 2.259 2.251 2.244 2.235 2.227	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807 2.822 2.834 2.851 2.866	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035 1.0007
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79 4548.85	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.496 2.496 2.476 2.468 2.460 2.452	2.836 2.890 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.155 3.175 3.195 3.215 3.215 3.234 3.252	(cm <sup>-1</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770 7.9436	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02 6572.09	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.235</li> <li>2.227</li> <li>2.220</li> </ul>	<ul> <li>(A)</li> <li>2.554</li> <li>2.599</li> <li>2.631</li> <li>2.657</li> <li>2.680</li> <li>2.701</li> <li>2.721</li> <li>2.740</li> <li>2.758</li> <li>2.775</li> <li>2.791</li> <li>2.807</li> <li>2.822</li> <li>2.834</li> <li>2.851</li> <li>2.866</li> <li>2.880</li> </ul>	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035 1.0007 0.9977
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79 4548.85 4810.28	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.496 2.496 2.476 2.468 2.460 2.452 2.444	2.836 2.890 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175 3.195 3.215 3.215 3.234 3.252 3.271	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770 7.9436 7.9155	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02 6572.09 6959.08	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.235</li> <li>2.227</li> <li>2.220</li> <li>2.213</li> </ul>	(A) 2.554 2.599 2.631 2.657 2.680 2.701 2.721 2.740 2.758 2.775 2.791 2.807 2.822 2.834 2.851 2.866 2.880 2.894	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035 1.0007 0.9977 0.9945
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79 4548.85 4810.28 5070.12	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.496 2.486 2.460 2.468 2.460 2.452 2.444 2.437	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175 3.155 3.175 3.215 3.215 3.234 3.252 3.234 3.252 3.271 3.289	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770 7.9436 7.9155 7.8846	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02 6572.09 6959.08 7343.55	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.235</li> <li>2.227</li> <li>2.220</li> <li>2.213</li> <li>2.207</li> </ul>	<ul> <li>(A)</li> <li>2.554</li> <li>2.599</li> <li>2.631</li> <li>2.657</li> <li>2.680</li> <li>2.701</li> <li>2.721</li> <li>2.740</li> <li>2.758</li> <li>2.775</li> <li>2.791</li> <li>2.807</li> <li>2.822</li> <li>2.834</li> <li>2.851</li> <li>2.866</li> <li>2.880</li> <li>2.894</li> <li>2.908</li> </ul>	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035 1.0007 0.9977 0.9945 0.9911
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19	(cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79 4548.85 4810.28 5070.12 5328.40	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.486 2.496 2.486 2.468 2.460 2.452 2.444 2.437 2.430	2.836 2.890 2.930 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175 3.195 3.215 3.215 3.234 3.252 3.271 3.289 3.307	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770 7.9436 7.9155 7.8846 7.8534	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02 6572.09 6959.08 7343.55 7725.20	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.255</li> <li>2.227</li> <li>2.220</li> <li>2.213</li> <li>2.207</li> <li>2.200</li> </ul>	<ul> <li>(A)</li> <li>2.554</li> <li>2.599</li> <li>2.631</li> <li>2.657</li> <li>2.680</li> <li>2.701</li> <li>2.721</li> <li>2.740</li> <li>2.758</li> <li>2.775</li> <li>2.791</li> <li>2.807</li> <li>2.822</li> <li>2.834</li> <li>2.851</li> <li>2.866</li> <li>2.880</li> <li>2.894</li> <li>2.908</li> <li>2.923</li> </ul>	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0062 1.0035 1.0007 0.9945 0.9911 0.9874
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20	(Cm) 142.50 429.32 715.48 999.44 1282.48 1564.12 1843.83 2121.77 2398.05 2672.69 2945.67 3216.99 3486.67 3754.70 4021.08 4285.79 4548.85 4810.28 5070.12 5328.40 5585.17	2.702 2.657 2.628 2.506 2.586 2.570 2.554 2.541 2.528 2.517 2.506 2.496 2.496 2.486 2.496 2.486 2.460 2.452 2.444 2.437 2.430 2.423	2.836 2.890 2.930 2.962 2.992 3.019 3.044 3.068 3.091 3.113 3.135 3.155 3.175 3.175 3.215 3.215 3.215 3.234 3.252 3.271 3.289 3.307 3.325	(cm <sup>-</sup> ) 8.4375 8.4085 8.3781 8.3489 8.3151 8.2849 8.2545 8.2234 8.1923 8.1612 8.1302 8.0993 8.0685 8.0380 8.0075 7.9770 7.9436 7.9155 7.8846 7.8534 7.8223	(cm <sup>-</sup> ) 206.46 607.34 1008.10 1412.61 1814.77 2219.00 2620.21 3019.67 3148.47 3816.56 4213.97 4610.15 5005.45 5399.43 5792.01 6183.02 6572.09 6959.08 7343.55 7725.20 8103.68	<ul> <li>(A)</li> <li>2.440</li> <li>2.402</li> <li>2.377</li> <li>2.357</li> <li>2.340</li> <li>2.325</li> <li>2.312</li> <li>2.300</li> <li>2.289</li> <li>2.278</li> <li>2.268</li> <li>2.259</li> <li>2.251</li> <li>2.244</li> <li>2.235</li> <li>2.227</li> <li>2.220</li> <li>2.213</li> <li>2.207</li> <li>2.200</li> <li>2.194</li> </ul>	<ul> <li>(A)</li> <li>2.554</li> <li>2.599</li> <li>2.631</li> <li>2.657</li> <li>2.680</li> <li>2.701</li> <li>2.721</li> <li>2.740</li> <li>2.758</li> <li>2.775</li> <li>2.791</li> <li>2.807</li> <li>2.822</li> <li>2.834</li> <li>2.851</li> <li>2.866</li> <li>2.880</li> <li>2.894</li> <li>2.908</li> <li>2.923</li> <li>2.937</li> </ul>	(cm <sup>-</sup> ) 1.03768 1.0351 1.0321 1.0302 1.0288 1.0259 1.0233 1.0205 1.0185 1.0160 1.0137 1.0113 1.0088 1.0062 1.0035 1.0007 0.9977 0.9945 0.9911 0.9874 0.9834

# 228

# 229 **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  $T_e$ ,  $r_e$ ,  $\omega_e$  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 the investigated electronic states. The comparison of our results with those available in the

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

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.

### 242 243 **REFERENCES**

244 1. Freedmann H, Emge TJ, Brennan JG.  $(THF)_8Ln_8E_6(EPh)_{12}$  Cluster Reactivity: 245 Systematic Control of Ln, E, EPh, and Neutral Donor Ligands, Inorg. Chem. 1999; 38: 246 4400-4404.

247 2. Freedman D, Sayan S, Emge TJ, Croft M, Brennan JG, Heterovalent Clusters: 248  $Ln_4Se(SePh)_8$  ( $Ln_4 = Sm_4$ , Yb<sub>4</sub>,  $Sm_2Yb_2$ , Nd<sub>2</sub>Yb<sub>2</sub>), J. Am. Chem. Soc. 1999; 121: 11713-249 11719.

3. Melman JH, Fitzgerald M, Freedman D, Emge TJ, Brennan JG, Chalcogen-Rich
Lanthanide Clusters from Lanthanide Halide Starting Materials: A New Approach to the
Low-Temperature Synthesis of LnS<sub>x</sub> Solids from Molecular Precursors, J. Am. Chem.
Soc. 1999; 121: 10247-10248.

[4] Luo Yi, Xiaohong Wan, Yuki Ito, Seiichi Takami, Momoji Kubo, Akira Miyamoto, A
density functional theory calculation on lanthanide monosulfides, Chem. Phys. 2002;
282: 197206.

5. Harrison JF, Electronic Structure of Diatomic Molecules Composed of a First-Row Transition Metal and Main-Group Element (H–F), Chem. Review 2000; 100: 679-716.

259 6. Hinkel KH, Lambert DL, and Wing RF, Mon. Not. R. Astron. Soc. 1989; 238: 1365.

260 7. Lambert DL and Celgg RES, Mon. Not. R. Astron. Soc. 1980; 191: 367.

8. Macrano M and Barrow RF, Analysis of the transition B<sup>2</sup>  $\Sigma$  <sup>+</sup>-X<sup>2</sup>  $\Sigma$  <sup>+</sup> in gaseous LaS, J. phys. B 1970; 3: L121-L122.

263 9. Winkel RJ Jr., Davis SP, and Abrams MC, Fourier transform spectroscopy of LaS in the 264 infrared, Appl. Opt. 1996; 35: 2874-2878.

10. Anderson N, Davis SP, Edvinsson G, and Winkel RJ Jr., Rotational Analysis of the LaS Spectrum in the Region 5000–15000 cm<sup>-1</sup>, phys. Scr. 2001; 64: 134-139.

267 11. He SG, Tam WS, Leung JW-H, and Cheung AS-C, Laser spectroscopy of LaS:

268 Hyperfine structure in the  $B^2 \Sigma^+ - X^2 \Sigma^+$  (0,0) band, J. Chem. Phys. 2002; 117: 5764-5769.

- 269 12. Hendrick L, Bethlem L, and Ubachs W, Testing the time-invariance of fundamental
- constants using microwave spectroscopy on cold diatomic radicals, The Royal Soc. of Chem.
   Farad. Discuss 2009; 142: 25-36.

13. Flambaum VV, Berengut JC, Space-time variation of coupling constants and

273 fundamental masses, International journal of modern physics A 2009; 24: 3342 .

14. Chin C, Flambaum VV, and Kozlov MG, Ultracold molecules: new probes on the variation of fundamental constants, New J. Phys. 2009; 11: 055048.

- 15. Murphy MT, Flambaum VV, Muller S, and Henkel C, Strong limit on a variable proton-
- to-electron mass ratio from molecules in the distant universe, Science 2008; 320: 1611-1613.
- 16. DeMille D, Sainis S, Sage J, Bergeman T, Kotochigova S, and Tiesinga E, Enhanced Sensitivity to Variation of  $m_e/m_o$  in Molecular Spectra, Phys. Rev. Lett. 2008; 100: 043202-
- 280 043206.
- 281 17. Kajita M, Prospects of detecting  $m_e/m_p$  variance using vibrational transition frequencies 282 of <sup>2</sup>Σ-state molecules, Phys. Rev. A 2008; 77:012511-012522.
- 18. Kajita M and Moriwaki Y, Proposed detection of variation in  $m_p/m_e$  using a vibrational transition frequency of a CaH<sup>+</sup> ion, J. Phys. B 2009; 42: 154022.

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402: E-mail address:

- 19. Flambaum VV and Kozlov MG, Enhanced Sensitivity to the Time Variation of the Fine-
- Structure Constant and  $m_p/m_e$  in Diatomic Molecules, Phys. Rev. Lett. 2007; 99: 150801-150805.
- 288 20. Tesch CM, Kurtz L, and de Vivie-Riedle R, Applying optimal control theory for 289 elements of quantum computation in molecular systems, Chem. Phys. Lett. 2001; 343:
- 290 633-641.
- 291 21. K. Mishima K, Tokumo K, and Yamashita K, Quantum computing using molecular
- electronic and vibrational states, Chem. Phys. 2008; 343: 61-75.
- 293 22. Zhao M and Babikov D, Phase control in the vibrational qubit, J. Chem. Phys. 2006;125:
  294 024105-024111.
- 295 23. Lee C. and Ostrovskaya EA, Quantum Computation with Diatomic Bits in Optical
   296 Lattices, arXiv:guant-ph/0502154v4 4 Nov 2005.
- 297 24. Babikov D, Accuracy of gates in a quantum computer based on vibrational eigenstates, J.
  298 Chem. Phys. 2004; 121: 7577-7586.
- 299 25. DeMille D, Quantum computation with trapped polar molecules, arXiv:quant-
- 300 ph/0109083v2 27 Oct 2001
- 26. Smith JR, Schlosser H, Leaf W, Ferrante J, Rose JH, Connection between energy
- relations of solids and molecules, Phys. Rev. A. 1989; 39: 514-517.
- 303 27. Abdul Al SN, Korek M, Allouche AR. Theoretical electronic structure of the lowest-lying
   304 states of the YI molecule. Chem. Phys. 2005; 308: 1-6.
- 305 28. Korek M, Moghrabi YA, A. R. Allouche AR. Theoretical calculation of the excited states of
  306 the KCs molecule including the spin-orbit interaction. J. Chem. Phys. 2006; 124: 094309307 094310.
- 308 29. Korek M, Bleik S, Allouche AR. Theoretical calculation of the low laying electronic states of the molecule NaCs with spin-orbit effect. J. Chem. Phys. 2007; 126: 124313-124322
- 30. Taher-Mansour F, Allouche AR, Korek M. Theoretical electronic structure of the lowest-
- lying states of ScCl molecule below 22 500 cm<sup>-1</sup>. J. Mol. Spectrosc. 2008; 248: 61-65.
   Korek M, Kontar S, Taher-Mansour F, Allouche AR, Theoretical electronic structure of the
- 31. Korek M, Kontar S, Taher-Mansour F, Allouche AR. Theoretical electronic structure of the
   molecule Scl. Int. J. Quant. Chem. 2009; 109: 236-242.
- 314 32. Korek M, Al-Shawa S, Younes GA. Theoretical calculation of the electronic structure of
- the molecule LiRb including the spin–orbit interaction. J. Mol. Struct. THEOCHEM 2009; 899:
  25-31.
- 317 33. Korek M and Abdul-Al SN. Rovibrational study and dipole moment calculation of the 318 molecule YF with spin–orbit interaction. Chem. Phys. 2009; 355: 130-134.
- 319 34. Hamdan A and Korek M. Theoretical calculation of the low-lying sextet electronic states320 of CrF molecule. Chem. Phys. 2010; 369: 13-18.
- 321 35. Hamdan A and Korek M. Theoretical calculation of the low-lying quartet states of the CrF 322 molecule. Can. J. Chem. 2011; 89: 1304-13011.
- 323 36. Hamdan A and Korek M. Theoretical study with vibration–rotation and dipole moment 324 calculations of quartet states of the CrCl molecule. Int. J. Quant. Chem. 2011; 111: 2960-325 2965.
- 326 37. Kobeissi H, Korek M, and Dagher M. On the computation of diatomic centrifugal 327 distortion constants: Exact solutions for initial value problems. J. Mol. Spectrosc. 1989; 138:
- 328 1-12.
- 329 38. Korek M and Kobeissi H. Highly accurate diatomic centrifugal distortion constants for 330 high orders and high levels. J. Comput. Chem. 1992; 13: 1103-1108.
- 331 39. Korek M, A one directional shooting method for the computation of diatomic centrifugal 332 distortion constants. Comput. Phys. commun. 1999; 119: 169-178.
- 40. Tohme SN and korek M, Electronic Structure and Rovibrational Calculation
- 334 of the molecule RbYb, 2012, (*in Press*)

Corresponding author, Tel: +961 3 747617; Fax: +961 1 818 402 : E-mail address:

- 335 41. MOLPRO Roos Basis set.
- 336 42. MOLPRO Basis Query, Pseudopotentials of the Stuttgart/Cologne group 337 (Revision: July 09, 2009).
- 338 43. MOLPRO is a package of *ab initio* programs written by H.-J. Werner,
- 339 P.J.Knowles, R. Lindh, F. R. Manby, M. Schütz, P. Celani, T. Korona, G. Rauhut. 340 R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J.
- Dobbyn, F. Eckert, C. Hampel, G. Hetzer, A. W. Lloyd, S. J. McNicholas, W. 341
- Meyer, M. E. Mura, A. Nicklaß, P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A. J. 342
- 343 Stone, R. Tarroni, and T. Thorsteinsson.
- 44. Allouche AR, "Gabedit, A graphical user interface for computational chemistry 344 345 softwares", J. Comput. Chem., 2011; 32:174-182.
- 45. Fedorov DG, Koseki S, Schmidt MW, Gordon MS, Spin-orbit coupling in molecules: 346
- Chemistry beyond the adiabatic approximation, Int. Rev. Phys. Chem. 2003; 22: 551-347 348 592.
- 349 46. Czack G, Hein H, Hinz I, Bergmann H, Kuhun P, Gmelin Handbook of Inorganic
- Chemistry, C7, eighth edition, Spinger, New York, 1983. 350
- 351 47. Barenco A, Deutsch D, Ekert A, and Jozsa R, Conditional Quantum Dynamics and
- 352 Logic Gates, Phys. Rev. Lett. 1995; 74: 4083-4086.
- 48. Brennen GK, Caves CM, Jessen PS, and Deutsch IH, Quantum Logic Gates in Optical 353 354 Lattices, Phys. Rev. Lett. 1999; 82: 1060 -1063.
- 355 49. Platzman P and Dykman M, Quantum computing with electrons floating on liquid helium,
- Science 1999; 284:1967-1969. 356