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Electronic Structure of LiH$^+$ Revisited by a Model Potential-Type Method

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A theoretical study of the electronic structure of LiH$^+$ is reported. Potential energy curves and dipole moments for the ground and numerous electronic excited states have been computed in the framework of a model potential type method. Spectroscopic constants have been determined for the lowest bound states, and they are compared with available theoretical values. Static dipole polarizabilities are presented for the two lowest states.

I. Introduction

With the achievement of Bose−Einstein condensation in alkali atomic samples[1,2] leading to the study of ultracold collisions[3,4] and possible formation of molecular species as neutral and ionic molecules,[5−6] accurate calculations on the electronic structure of alkali ionic diatomic compounds are presently required to interpret and/or suggest such experiments.

Being involved in the theoretical determination of the electronic structure of alkali molecules (neutral and ionic) by specific methods (pseudopotential and model potential type methods), we have recently demonstrated that potential energy curves of the ground and numerous excited states of these alkali molecular systems, could be computed accurately with a model potential-type method[7−11] at short and large internuclear distances. As an application of our previous developments, we present here a complete description of the LiH$^+$ electronic structure, including a determination of molecular static dipole polarizabilities for the first electronic states X$^2\Sigma^+$ (Li$^+$ + H(1s)) and 2$^2\Sigma^+$ (Li(2s) + H$^+$) as a function of internuclear distances.

II. Method

We used the procedure developped previously for alkali molecular ions.[7−10] In such approach, alkali hydride cation LiH$^+$ is treated as a one-active electron system in which the outermost electron is moving in the field of an ionic core Li$^+$ and a proton separated by a distance R. Calling r_a and r_b positions of the valence electron relative to Li$^+$ and the proton, respectively, model one-electron Schrödinger equation is written as

$$[T + V(r_a) + V(r_b) + V_{pol}(r_a,R) + V_{core}(R)]\Psi^{2\Lambda^{(+)}}(r_a,r_b,R) = E^{2\Lambda^{(+)}}\Psi^{2\Lambda^{(+)}}(r_a,r_b,R) \quad (1)$$

where T is the valence electron kinetic energy operator.

Interaction between Li$^+$ and the valence electron is represented by a model potential $V(r_a)$:[12]

$$V(r_a) = -\frac{1}{r_a} - \frac{2e^{-7.90875r_a}}{r_a} - \frac{10.321r_a e^{-3.90006r_a}}{r_a} \quad (2)$$

whereas that with the proton corresponds to the Coulomb potential:

$$V(r_b) = \frac{-1}{r_b} \quad (3)$$

Core polarization effects are described by an effective potential $V_{pol}(r_a,R)$:[13,14]

$$V_{pol}(r_a R) = -\frac{\alpha_d^a \vec{r}_a\cdot\vec{R}}{{r_a}^3 R^3}\sqrt{1 - e^{-(r_a/\rho)^6}} + ... \quad (4)$$

where the parameter ρ is defined to avoid divergence at short r_a and is determined from a variational calculation of the molecular ground-state energy.

Repulsion between the alkali ionic core and the proton is described by a model limited to Coulombic and polarization interactions, overlap and exchange effects being neglected:

$$V_{core}(R) = \frac{1}{R} - \frac{\alpha_d^a}{2R^4} \quad (5)$$

For the static dipole polarizability of Li$^+$ (α_d^a) involved in eqs 4 and 5, we used the value $\alpha_d(\mathrm{Li}^+(1s^2)) = 0.1915{a_0}^3$.[15]

The one-electron model Schrödinger equation (eq 1) is solved in prolate spheroidal coordinates ($\lambda = r_a + r_b/R$, $\mu = r_a - r_b/R$, $0 \le \varphi \le 2\pi$), well suited for monoelectronic molecular ions. The wave function $\Psi^{2\Lambda^{(+)}}(r_a,r_b,R)$ of a given molecular state $^2\Lambda^{(+)}$, is expanded on a set of generalized Slater-type orbitals:

$$\Psi^{2\Lambda^{(+)}}(r_a,r_b,R) = \sum_{n=1}^{2}\sum_{k=1}^{N_{couple}}\sum_{j=1}^{N_k} c_{ij}[(\lambda^2 - 1)(1 - \mu^2)]^{|\Lambda|/2}\lambda^{p_j}\mu^{q_j}e^{(-R\beta_k/2)(\lambda+\epsilon_n\mu)}e^{i\Lambda\varphi} \quad (6)$$

where $\epsilon_1 = 1$ and $\epsilon_2 = -1$. Integer exponents p_j and q_j vary from 0 to $N_k = n_k - |\Lambda| + 1$, where n_k is the atomic principal quantum number. The exponential parameter β_k is defined by $\sqrt{-E_{nk}l_k}$, E_{nklk} being the experimental energy of an atomic state n_kl_k.[16]

N_{couple} corresponds to the number of couples (n_k,β_k) and indicates the size of the basis set. For each atom Li and H, the

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TABLE 1: Comparison between Molecular Energies Computed at $R = 500a_0$ and Relevant Experimental Data Averaged on J Values[15] in cm^{-1}

dissociation limit	E_{exp} (cm^{-1})	E_{computed} (cm^{-1})	ΔE (cm^{-1})
Li$^+$ + H(1s)	109 737.31	109 737.30	0.01
Li(2s) + H$^+$	43 487.19	43 481.35	5.84
Li(2p) + H$^+$	28 583.30	28 575.75	7.55
Li$^+$ + H(2s)	27 434.33	27 436.96	2.63
Li$^+$ + H(2p)	27 434.33	27 431.69	2.64
Li(3s) + H$^+$	16 281.07	16 307.24	26.17
Li(3p) + H$^+$	12 561.81	12 576.85	15.04
Li(3d) + H$^+$	12 204.01	12 200.17	3.84
Li$^+$ + H(3s)	12 193.03	12 187.99	5.04
Li$^+$ + H(3p)	12 193.03	12 179.74	13.29
Li+ + H(3d)	12 193.03	12 173.93	19.10
Li(4s) + H$^+$	8 475.13	8 487.84	12.71
Li(4p) + H+	7 017.64	7 026.99	9.35
Li(4d) + H$^+$	6 863.79	6 871.71	7.92
Li$^+$ + H(4s)	6 858.58	6 849.34	9.24
Li$^+$ + H(4p)	6 858.58	6 845.80	12.78
Li$^+$ + H(4d)	6 858.58	6 833.51	25.01

basis set is determined by solving the model one-electron Schrödinger equation (eq 1) in which only the electron−core interaction $V(r_{a/b})$ is considered (i.e., $V_{\mathrm{pol}}(r_a,R)$ and $V_{\mathrm{core}}(R)$ are excluded). An averaged discrepancy of 5×10^{-5} au ($\approx$11 cm^{-1}) is obtained for the twenty lowest states of each atom. Accuracy of such energies and wave functions is checked by computing static dipole polarizability of the atomic ground state. We found $\alpha_d(\mathrm{Li(2s)}) = 164.18a_0^3$ and $\alpha_d(\mathrm{H(1s)}) = 4.50a_0^3$ in good agreement with the experimental value $\alpha_d(\mathrm{Li(2s)}) = 164 \pm 3a_0^3$ [17] and with the exact data $\alpha_d(\mathrm{H(1s)}) = 4.5a_0^3$.[18]

The atomic basis sets being defined, the equilibrium distance R_e^{computed} for the ground state of LiH$^+$ are then searched without including core polarization effects. The parameter ρ is afterward determined by minimizing the calculated ground-state energy of LiH$^+$at $R = R_e^{\mathrm{computed}}$. We obtained $R_e^{\mathrm{computed}} = 4.15a_0$ and $\rho = 3.00a_0$. As a check of our overall procedure (length of basis sets, value of ρ), molecular energies have been computed at large R ($R = 500a_0$). A comparison to experimental energies of separated species[16] is presented in Table 1 for the seventeen lowest asymptotes i.e. up to Li$^+$ + H(4d). The averaged discrepancy is found to be equal to $\approx$10 cm^{-1} with the largest one $\approx$26 cm^{-1}.

III. Potential Energy Curves, Spectroscopic Constants, and Static Dipole Polarizabilities

During the two past decades, various collisionnal experiments and relevant cross section calculations probing potential energy curves[19−31] have been achieved whereas no spectoscopy experiments were performed up to our knowledge. Nevertheless, various methods[32−38] have been applied to compute potential energy curves of the lowest states of LiH$^+$ over a domain of internuclear distances usually restricted to $25a_0$. Relevant spectroscopic constants have been deduced and large discrepancies have been observed between these calculations.[31−38] Recently, potential energy curves of highly excited states adiabatically correlated up to the Li(3d) + H$^+$ asymptote have been computed in the framework of a pseudopotential method.[36] Those of the two lowest states and relevant dipole moments have been also determined through CI calculations based on the use of Slater-type orbitals.[37] These results have lead to a better knowledge of the LiH$^+$ electronic structure and they have been used in investigations on the lithium chemistry in the early universe.[37−40]

Present energy and dipole moment calculations have been performed over a large range of internuclear distances from $2.5a_0$ up to $60a_0$. Potential energy curves of electronic states dissociating below Li$^+$ + H(4d) are displayed in Figures1−3, for $^2\Sigma^+$, $^2\Pi$, and $^2\Delta$ symmetries, respectively. Although most potential energy curves are purely repulsive, some of them display a potential well located at short ($R < 12a_0$) or at large internuclear distances. Relevant spectroscopic constants have been determined through the use of the Hutson's code.[41] They are presented in Table 2 in which available theoretical calculations[31−38] are reported. Permanent dipole moment moment μ at R_e, is also given for the lowest bound states (X$^2\Sigma^+$ (Li$^+$ + H(1s)), 2$^2\Sigma^+$ (Li(2s) + H$^+$), 3$^2\Sigma^+$ (Li(2p) + H$^+$), and 1$^2\Pi$ (Li(2p) + H$^+$)) and recent determinations[37,38] are reported.

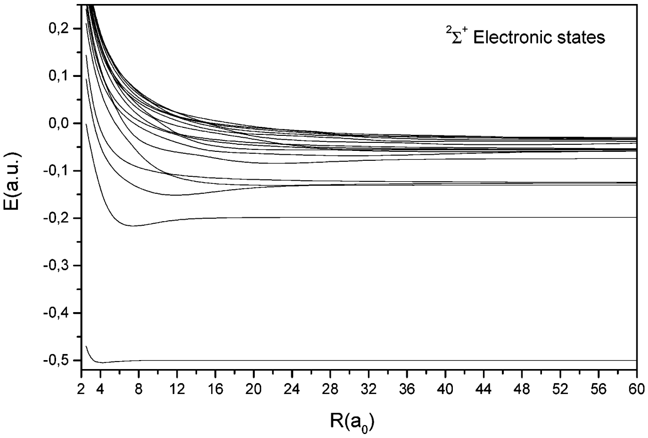

Figure 1. Potential energy curves (in atomic units) for $^2\Sigma^+$ electronic states adiabatically correlated below Li(4d) + H$^+$ asymptote.

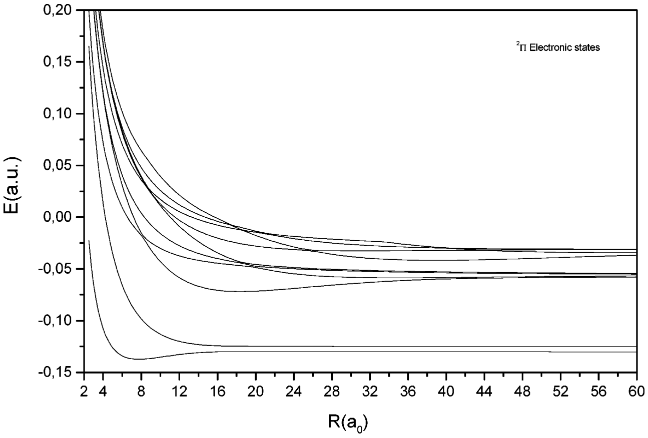

Figure 2. Potential energy curves (in atomic units) for $^2\Pi$ electronic states adiabatically correlated below Li(4d) + H$^+$ asymptote.

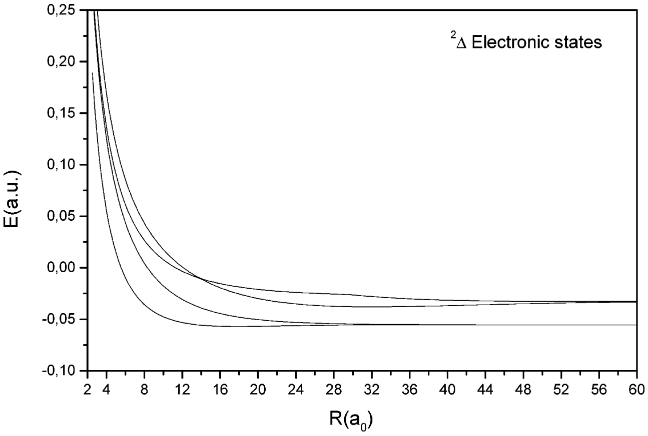

Figure 3. Potential energy curves (in atomic units) for $^2\Delta$ electronic states adiabatically correlated below Li(4d) + H$^+$ asymptote.

TABLE 2: Spectroscopic Constants for the LiH$^+$ Bound States (R_e in a_0; ω_e,T_e, D_e in cm^{-1}; and $\mu(R_e)$ in Debye)

molecular state	R_e	ω_e	T_e	D_e	$\mu(R_e)$
		$X^2\Sigma^+$ (Li$^+$ + H(1s))			
theory (a)	4.12			1 129	
theory (b)	4.12			1 048	
theory (c)	4.08			1 048	
theory (d)	4.15			1 129	
theory (e)	4.11			1 137	
theory (f)	4.13	422.10		1 132	
theory (g)	4.15			1 048	−0.702
present work	4.15	417.03		1 048	−0.703
		$2^2\Sigma^+$ (Li(2s) + H$^+$)			
theory (c)	7.35			4 033	
theory (d)	7.27			3 307	
theory (h)	7.47			3 952	
theory (e)	7.45			4 008	
theory (f)	7.39		63 540	3 871	
present work	7.46	384.98	63 311	3 993	−3.516
		$3^2\Sigma^+$ (Li(2p) + H$^+$)			
theory (c)	7.10			4 275	
theory (d)	10.50				
theory (e)	11.76			4 509	
present work	11.87	221.42	77 568	4 642	
		$4^2\Sigma^+$ (Li$^+$ + H(2s))			
theory (e)	22.03			1 202	
present work	22.50	59.95	82 118	1 231	
		$6^2\Sigma^+$ (Li(3s) + H$^+$)			
theory (e)	22.82			2 153	
present work	22.37	105.46	92 307	2 171	
		$7^2\Sigma^+$ (Li(3p) + H$^+$)			
theory (e)	25.87			1 782	
present work	30.37	59.91	95 794	2 415	
		$1^2\Pi$ (Li(2p) + H$^+$)			
theory (e)	7.58			1 428	
present work	7.74	206.54	80 647	1 562	−6.041
		$3^2\Pi$ (Li(3p) + H$^+$)			
theory (e)	18.21			2307	
present work	18.33	99.31	95 015	3 194	
		$4^2\Pi$ (Li(3d) + H$^+$)			
theory (e)	dissociative state				
present work	35.10		97 907	680	
		$7^2\Pi$ (Li(4p) + H$^+$)			
present work	38.87		10 162	2 932	
		$1^2\Delta$ (Li(3d) + H$^+$)			
theory (e)	dissociative state				
present work	17.97	54.77	98 255	322	
		$3^2\Delta$ (Li(4d) + H$^+$)			
present work	31.89	40.59	102 467	1 455	

[a] Available theoretical data are considered: (a) = ref 32, (b) = ref 33, (c) = ref 34, (d) = ref 35, (e) = ref 36, (f) = ref 37, (g) = ref 38, (h) = ref 31. Dipole moment values are relative to the center of mass.

For the ground state, present results and calculations of ref 38 are in excellent agreement, because they are seen to be identical. Comparison with other theoretical data[32−37] is also satisfying for vibrational constant ω_e and equilibrium position R_e. In case of R_e, the discrepancy does not exceed $0.04a_0$ except for model potential calculations ref 34 which is predicted shorter than $4.10a_0$. We obtained the same dissociation energy value than that of Refs.[33−34,38] although a difference of 81, 89, and 84 cm^{-1} is found with data of refs 32 and 35, ref 36, and ref 37, respectively. Comparison with calculations of refs 31 and 34−37 is very satisfying for the $2^2\Sigma^+$ (Li(2s) + H$^+$)state despite a discrepancy of 686 cm^{-1} with MRSD-CI calculations[35] and 122 cm^{-1} with CI calculations.[37]

TABLE 3: Avoided Crossing Positions (in a_0) Observed in Both Potential Energy Curves

molecular states	$R_{\text{avoided crossing}}$ (a_0)
$3^2\Sigma^+$ (Li(2p) + H$^+$) − $4^2\Sigma^+$ (Li$^+$ + H(2s))	25.00
$4^2\Sigma^+$ (Li$^+$ + H(2s)) − $5^2\Sigma^+$ (Li$^+$ + H(2p))	10.90
$8^2\Sigma^+$ (Li(3d) + H$^+$) − $9^2\Sigma^+$ (Li$^+$ + H(3s))	11.50 and 29.00
$9^2\Sigma^+$ (Li$^+$ + H(3s)) − $10^2\Sigma^+$ (Li$^+$ + H(3p))	12.25
$10^2\Sigma^+$ (Li$^+$ + H(3p)) − $11^2\Sigma^+$ (Li$^+$ + H(3d))	9.50 and 23.00
$12^2\Sigma^+$ (Li(4s) + H$^+$) − $13^2\Sigma^+$ (Li(4p) + H$^+$)	18.50 and 36.00
$14^2\Sigma^+$ (Li(4d) + H$^+$) − $15^2\Sigma^+$ (Li$^+$ + H(4s))	15.00 and 30.00
$15^2\Sigma^+$ (Li$^+$ + H(4s)) − $16^2\Sigma^+$ (Li$^+$ + H(4p))	14.75
$16^2\Sigma^+$ (Li$^+$ + H(4p)) − $17^2\Sigma^+$ (Li$^+$ + H(4d))	11.50 and 22.00
$3^2\Pi$ (Li(3p) + H$^+$) − $4^2\Pi$ (Li(3d) + H$^+$)	8.20
$4^2\Pi$ (Li(3d) + H$^+$) − $5^2\Pi$ (Li$^+$ + H(3p))	20.00
$5^2\Pi$ (Li(3p) + H$^+$) − $6^2\Pi$ (Li$^+$ + H(3d))	18.50
$6^2\Pi$ (Li$^+$ + H(3d)) − $7^2\Pi$ (Li(4p) + H$^+$)	8.70
$7^2\Pi$ (Li(4p) + H$^+$) − $8^2\Pi$ (Li(4d) + H$^+$)	8.70
$7^2\Pi$ (Li(4p) + H) − $8^2\Pi$ (Li(4d) + H$^+$)	26.00
$8^2\Pi$ (Li(4d) + H$^+$) − $9^2\Pi$ (Li$^+$ + H(4p))	18.5 and 43.50
$9^2\Pi$ (Li$^+$ + H(4p)) − $10^2\Pi$ (Li$^+$ + H(4d))	17.40 and 20.6
$3^2\Delta$ (Li(4d) + H$^+$) − $4^2\Delta$ (Li$^+$ + H(4d))	13.90

For higher excited states ($3^2\Sigma^+$ (Li(2p) + H$^+$), $4^2\Sigma^+$ (Li$^+$ + H(2s)), $6^2\Sigma^+$ (Li(3s) + H$^+$), and $1^2\Pi$ (Li(2p) + H$^+$)) pseudopotential predictions[36] and present results are in excellent agreement in particular for potential wells located at $R > 20a_0$. However, large discrepancies between two calculations are found for the $7^2\Sigma^+$ (Li(3p) + H$^+$), $3^2\Pi$ (Li(3p) + H$^+$), $4^2\Pi$ (Li(3d) + H$^+$), and $1^2\Delta$ (Li(3d) + H$^+$) electronic states. For instance, we obtained $\Delta R_e = 4.5a_0$ and $\Delta D_e = 633$ cm $^{-1}$ for the $7^2\Sigma^+$ (Li(3p) + H$^+$) state. Although they are predicted purely dissociative in ref 36, present model potential energy curves of $1^2\Delta$ and $4^2\Pi$ electronic states, each adiabatically correleted to Li(3d) + H$^+$, display a potential well located at $R_e = 17.97a_0$ and $R_e = 35.10a_0$ with a depth of 322 and 680 cm^{-1}, respectively. These differences can partly be explained by the use of a limited number of diffuse Gaussian-type orbitals in pseudopotential calculations.[36] Only long range extrapolations could confirm or invalidate these predictions at such interatomic separation, as previously done on various alkali cations.[7−10]

Structures rich in avoided crossings are found mainly in potential energy curves of highly excited states at $R > 8a_0$. Their position is given in Table 3. Some of them should play an important role in subsequent dynamical investigations as the interpretation of multiphoton dissociation processes,[43] for which potential energy curves and dipole moments are required. For instance, the avoided crossing between $4^2\Sigma^+$ (Li$^+$ + H(2s)) and $5^2\Sigma^+$ (Li$^+$ + H(2p)) potential energy curves corresponds to a crossing between relevant dipole moments as displayed in Figure 4 and strong variations of dipole moments with internuclear distances are observed. For the two lowest states, a comparison with recent CI calculations[37] is displayed in Figure 5 for the ground-state permanent dipole moment and in Figure 6 for the transition dipole moment between $X^2\Sigma^+$ (Li$^+$ + H(1s)) and $2^2\Sigma^+$ (Li(2s) + H$^+$). A satisfying agreement is found between the two calculations, in particular for transition dipole moment. In case of the ground state permanent dipole moment, we obtained pratically the same value as that of ref 38 computed at the equilibrium position, our origin corresponding to the center of mass. The present estimation is also seen to be in agreement with values −0.747 and −0.784 D of refs 37 and 42, respectively, calculated at $R = 4.25a_0$.

As an application, we have determined in a sum over states approach, the molecular static dipole polarizabilities as a function of internuclear distances. Variations with R for the components α_{zz} ($=\alpha_{\|}$) and α_{xx} ($=\alpha_{\perp}$) are displayed for the two first electronic states $X^2\Sigma^+$ (Li$^+$ + H(1s)) and $2^2\Sigma^+$ (Li(2s) +

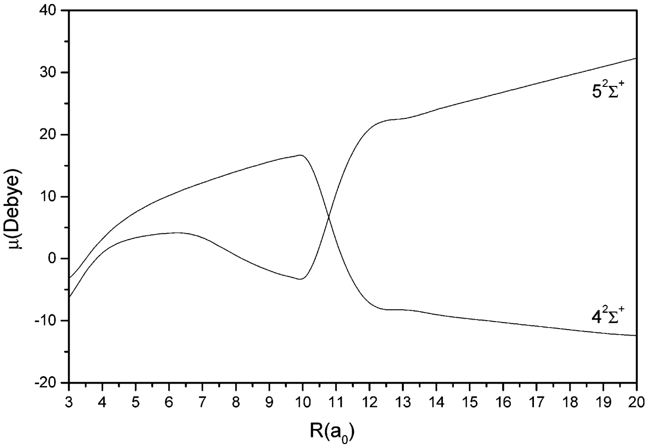

Figure 4. Variation with *R* (in a_0) of permanent dipole moments for $4^2\Sigma^+$ and $5^2\Sigma^+$ states adiabatically correlated to $Li^+ + H(2s)$ and $Li^+ + H(2p)$, respectively.

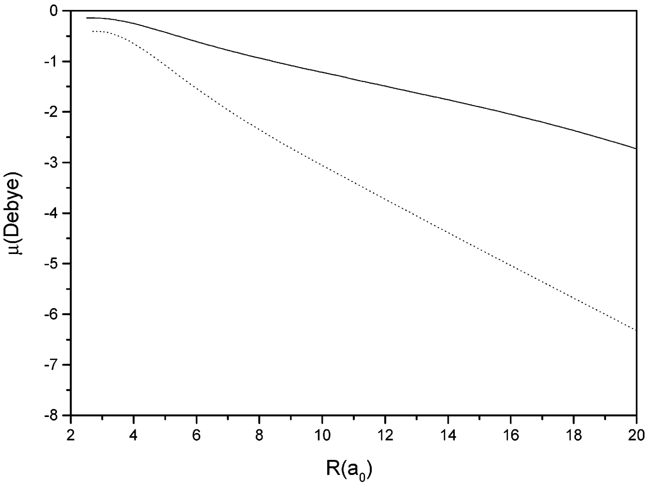

Figure 5. Comparison between CI calculations[37] (dotted line) and present data (solid line) for the ground-state permanent dipole moment. *R* is given in a_0 and μ in Debye.

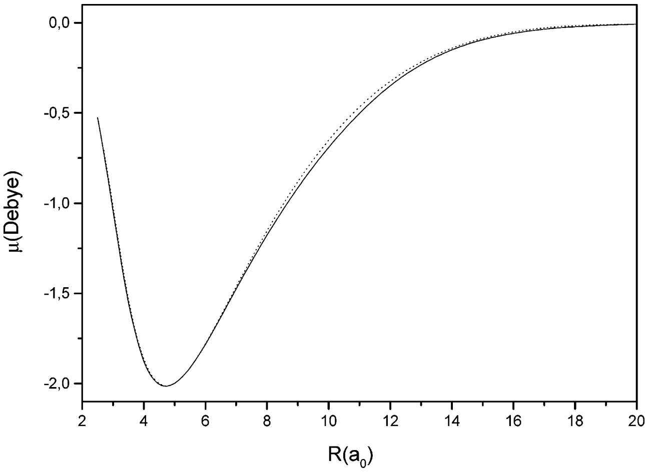

Figure 6. Comparison between CI calculations[37] (dotted line) and present data (solid line) for the transition dipole moment between $X^2\Sigma^+$ ($Li^+ + H(1s)$) and $2^2\Sigma^+$ ($Li(2s) + H^+$). *R* is given in a_0 and μ in Debye.

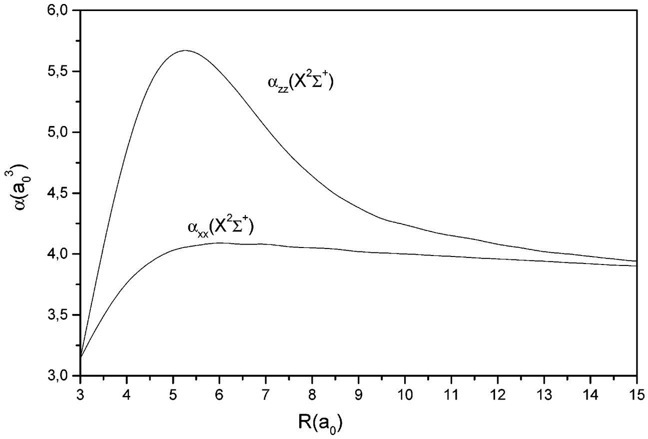

Figure 7. Variation with *R* (in a_0) of static dipole polarizability components $\alpha_{\parallel}$ and $\alpha_{\perp}$ for the LiH^+ ground state $X^2\Sigma^+$ ($Li^+ + H(1s)$). Data are given in a_0^3.

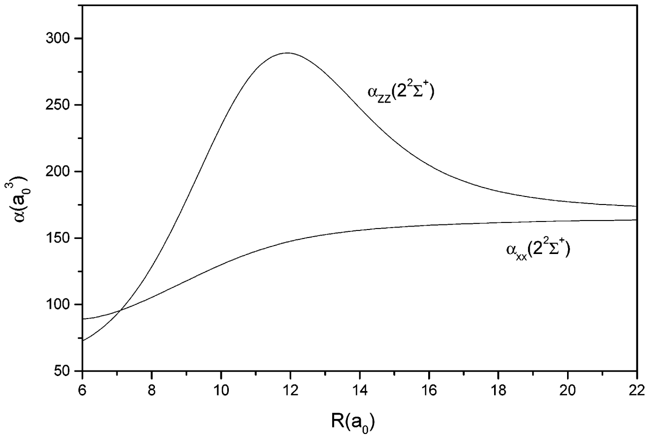

Figure 8. Same as Figure 7 but for the first excited state $2^2\Sigma^+$ ($Li(2s) + H^+$).

H^+), in Figures 7 and 8, respectively. Component α_{xx} ($=\alpha_{\perp}$) varies slowly with *R* and is seen to tend to the sum of $\alpha(Li^+(1s^2)) = 0.1915a_0^3$ [15] and $\alpha(H(1s)) = 4.50a_0^3$ [18] for the ground state and to $\alpha_d(Li(2s)) = 164 \pm 3a_0^3$ [17] in the case of the first excited one. The opposite is found for component α_{zz} ($=\alpha_{\parallel}$) wich is seen to increase and decrease very rapidly with *R* for the two states. Part of this pattern has been previously observed at short internuclear distances for the ground state of H_2^+ [44] and Li_2^+ [45] and more recently in the case of the first electronic states of LiNa.[46]

IV. Conclusion

Model potential type calculations including potential energies and dipole moments have been performed for the 17 lowest $^2\Sigma^+$, the 10 lowest $^2\Pi$ and the 4 lowest $^2\Delta$ electronic states of LiH^+. As the large amount of numerical data cannot be reported here, potential energy curves of all considered electronic states, relevant dipole moments, and static dipole polarizabilities have been listed in a database available on request.

Both potential energy curves display structures rich in crossings and avoided crossings. Despite the lack of experiments, long-range calculations are necessary to check part of the present and pseudopotential predictions.[36] The present results will be used in the determination of the LiH electronic structure through a model potential type method applied previously with success on Na_2.[11]

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