Functions of dynamic polarizability of LiH and Li_2 molecules

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An analytical approach to description of the dynamic electronic polarizability tensor $\alpha_{ii}(R,\omega)$ for LiH and Li_2 molecules as functions of their internuclear distance R and external electromagnetic field frequency ω are proposed. The description is based on estimating the upper and lower bounds of $\alpha_{ii}(R,\omega)$, which are calculated using the known static polarizability function $\alpha_{ii}(R,0)$ and a limited number of energies of excited electronic states of $E_m(R)$ and electric dipole transition moments $(d_i)_{0m}(R)$.

Introduction

Electronic polarizability of a diatomic molecule is a second-rank tensor with two independent components $\alpha_{zz}(R,\omega)$ and $\alpha_{xx}(R,\omega) = \alpha_{yy}(R,\omega)$; each defining the surface as a function of internuclear distance R and external electromagnetic field frequency ω (z-axis of the Cartesian coordinates coincides with the molecule axis). At present, polarizability surfaces are most completely calculated for hydrogen molecules.[1,2]

Polarizability of H_2 molecule was calculated in Ref. 1 within the internuclear distance range $0.6 \le R \le 10.0$ a.u. for the frequencies $\omega = 0.07200$; 0.15351; 0.19785; 0.23538; 0.25000; 0.30000 a.u. on the base of a specially purposed *ab initio* method,[3] using the James–Coolidge functions.

A method for analytical description of polarizability surfaces of a diatomic molecule was suggested in Ref. 2, where $\alpha_{ii}(R,\omega)$ of hydrogen molecule were accurately calculated within the measurement range $R \in [0, \infty)$ and at the frequencies $\omega \le 0.6$ a.u.

Among other works, presenting polarizabilities $\alpha_{ii}(R,\omega)$ within a wide range of R and ω variations, note Refs. 4 and 5, where polarizability surfaces of LiH and N_2 molecules, respectively, were calculated. Polarizability functions of LiH molecule[4] were *ab initio* calculated within the range $2.0 \le R \le 12.0$ a.u. for a static field and two frequencies $\omega = 0.0147$ and 0.0294 a.u. However, the calculation accuracy was noticeably lower than for hydrogen molecule.

An analytical description of polarizability surfaces of N_2 molecule is given in Ref. 5, but approximations, used here, give noticeably overvalued functions $\alpha_{ii}(R,\omega)$ and the frequency domain of the function is limited to the frequency of first allowed electric dipole electronic transition. Along with the above-mentioned works, there is a series of *ab initio* calculations (see, e.g., Refs. 6–14), presenting only small areas of polarizability surfaces of different diatomic molecules in vicinities of their equilibrium states R_e and sufficiently wide frequency range.

The aim of this work is to obtain polarizability surfaces $\alpha_{zz}(R,\omega)$ and $\alpha_{xx}(R,\omega) = \alpha_{yy}(R,\omega)$ for LiH and Li_2 molecules in the electronic ground state. For calculations, we use our method suggested in Ref. 2, which allows the functions to be represented analytically.

1. Analytical representation of dynamic polarization functions

The quantum-mechanical expression for dynamic electronic polarizability of a diatomic molecule in electronic ground state can be presented as (a.u.)

$$\alpha_{ii}(R,\omega) = 2\sum_{m\neq 0} \frac{\left[E_m(R) - E_0(R)\right]\left|(d_i)_{0m}(R)\right|^2}{\left[E_m(R) - E_0(R)\right]^2 - \omega^2}, \quad (1)$$

where $|(d_i)_{0m}(R)|$ is the ith component of transition dipole moment between ground and excited electronic states with the energies $E_0(R)$ and $E_m(R)$; the summation is carried out over an infinite number of excited states, including the continuous spectrum states (hereinafter, the energies $E_0(R)$ and $E_m(R)$ are considered as pure electronic energies without the potential energy of molecule nuclei repulsion). Though equation (1) is formally correct for any frequency ω (far from resonance), it is of little use for calculating the molecule dynamic polarizability because of infinite number of summands. Nevertheless, the equation can be used for calculating the upper and lower bounds of dynamic polarizability functions $\alpha_{ii}(R,\omega)$ of a diatomic molecule, when only the function of its static polarizability $\alpha_{ii}(R,0)$, as well as a limited number of electronic energies $E_m(R)$ and transition moments $(d_i)_{0m}(R)$ are known.[2]

Let the functions $\alpha_{ii}(R,0)$ and $E_0(R)$ are known for the electronic ground state and the functions $E_m(R)$ and $(d_i)_{0m}(R)$ – for k lower excited electronic states of a molecule. Then equation (1) is written as

$$\alpha_{ii}(R,\omega)=2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\,\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}+$$

$$+2\sum_{m=k+1}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\,\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}. \qquad (2)$$

To preset the upper and lower bounds $\alpha_{ii}^{\max}(R,\omega)$ and $\alpha_{ii}^{\min}(R,\omega)$, use the fact that the multiplier $[E_m(R)-E_0(R)]^2/\{[E_m(R)-E_0(R)]^2-\omega^2\}$ in the second item of Eq. (2) steadily decreases in absolute magnitude with an increase of m for $\omega < E_{k+1}(R)-E_0(R)$. On the base of this equation, one can write[2]

$$\alpha_{ii}^{\max}(R,\omega)=2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}+$$

$$+\frac{\left[E_{k+1}(R)-E_0(R)\right]^2}{\left[E_{k+1}(R)-E_0(R)\right]^2-\omega^2}\,2\sum_{m=k+1}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)} \qquad (3)$$

and

$$\alpha_{ii}^{\min}(R,\omega)=2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}+$$

$$+\frac{\left[E_0(R)\right]^2}{\left[E_0(R)\right]^2-\omega^2}\,2\sum_{m=k+1}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}. \qquad (4)$$

It is possible to avoid summing over an infinite number of excited states (including continuous spectrum states) in the second items of Eqs. (3) and (4) using the equation for static polarizability of a molecule (see Eq. (1)):

$$\alpha_{ii}(R,0)=2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}+$$

$$+2\sum_{m=k+1}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}. \qquad (5)$$

Taking into account Eq. (5), equations (3) and (4) can be rewritten as

$$\alpha_{ii}^{\max}(R,\omega)=\alpha_{ii}(R,0)\frac{\left[E_{k+1}(R)-E_0(R)\right]^2}{\left[E_{k+1}(R)-E_0(R)\right]^2-\omega^2}+$$

$$+2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\left\{\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}-\right.$$

$$\left.-\frac{\left[E_{k+1}(R)-E_0(R)\right]^2}{\left[E_{k+1}(R)-E_0(R)\right]^2-\omega^2}\right\} \qquad (6)$$

and

$$\alpha_{ii}^{\min}(R,\omega)=\alpha_{ii}(R,0)\frac{\left[E_0(R)\right]^2}{\left[E_0(R)\right]^2-\omega^2}+2\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\times$$

$$\times\left\{\frac{\left[E_m(R)-E_0(R)\right]^2}{\left[E_m(R)-E_0(R)\right]^2-\omega^2}-\frac{\left[E_0(R)\right]^2}{\left[E_0(R)\right]^2-\omega^2}\right\}, \qquad (7)$$

where sums with infinite upper limit are eliminated. The dynamic polarizability function of a diatomic molecule can be presented as

$$\alpha_{ii}(R,\omega)=\frac{\alpha_{ii}^{\max}(R,\omega)+\alpha_{ii}^{\min}(R,\omega)}{2}\pm$$

$$\pm\frac{\alpha_{ii}^{\max}(R,\omega)-\alpha_{ii}^{\min}(R,\omega)}{2}=\bar{\alpha}_{ii}(R,\omega)\pm\Delta\alpha_{ii}(R,\omega), \qquad (8)$$

where $\bar{\alpha}_{ii}(R,\omega)$ is the estimating function of dynamic polarizability $\alpha_{ii}(R,\omega)$; $\Delta\alpha_{ii}(R,\omega)$ is the error in determining $\alpha_{ii}(R,\omega)$, intrinsic to the considered method. Equations (6)–(8) correctly describe $\alpha_{ii}(R,\omega)$ within the frequency range up to $\omega_{k+1}=E_{k+1}(R)-E_0(R)$. The functions $\bar{\alpha}_{ii}(R,\omega)$ evidently tend to $\alpha_{ii}(R,\omega)$ at $k\to\infty$ while the error $\Delta\alpha_{ii}(R,\omega)$ tends to zero. Note also, that $\Delta\alpha_{ii}(R,\omega)=0$ at $\omega=0$, since $\alpha_{ii}^{\max}(R,\omega)=$ $=\alpha_{ii}^{\min}(R,0)=\alpha_{ii}(R,0)$, and monotonically increases with increasing ω ($\omega<\omega_{k+1}$).

The dynamic polarizability $\alpha_{ii}(R,\omega)$ is also presented in the form of Cauchy variance expansion, which correctly describes the frequency dependence of polarizability in the long-wave spectral region. In this case, $\bar{\alpha}_{ii}(R,\omega)$ and $\Delta\alpha_{ii}(R,\omega)$ can be written as

$$\bar{\alpha}_{ii}(R,\omega)=\sum_{n=0}^{\infty}\bar{S}_i^{(-2n-2)}(R)\,\omega^{2n}, \qquad (9)$$

$$\Delta\alpha_{ii}(R,\omega)=\sum_{n=0}^{\infty}\Delta S_i^{(-2n-2)}(R)\,\omega^{2n}, \qquad (10)$$

where $\bar{S}_i^{(-2n-2)}(R)$ and $\Delta S_i^{(-2n-2)}(R)$ are the estimation and error of nth Cauchy coefficient determination and depend on the molecule internuclear distance. These functions have the following forms:

$$\bar{S}_i^{(-2n-2)}(R)=\frac{\alpha_{ii}(R,0)}{2}\times$$

$$\times\left\{\frac{1}{\left[E_{k+1}(R)-E_0(R)\right]^{2n}}+\frac{1}{\left[E_0(R)\right]^{2n}}\right\}+$$

$$+\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\left\{\frac{2}{\left[E_m(R)-E_0(R)\right]^{2n}}-\right.$$

$$\left.-\frac{1}{\left[E_{k+1}(R)-E_0(R)\right]^{2n}}-\frac{1}{\left[E_0(R)\right]^{2n}}\right\}, \qquad (11)$$

$$\Delta S_i^{(-2n-2)}(R)=\left[\frac{\alpha_{ii}(R,0)}{2}-\sum_{m=1}^{k}\frac{|(d_i)_{0m}(R)|^2}{E_m(R)-E_0(R)}\right]\times$$

$$\times\left\{\frac{1}{\left[E_{k+1}(R)-E_0(R)\right]^{2n}}-\frac{1}{\left[E_0(R)\right]^{2n}}\right\}. \qquad (12)$$

The error of Cauchy coefficients estimation $\Delta S_i^{(-2n-2)}(R)$ evidently tends to zero at $k\to\infty$ while the estimation itself $\bar{S}_i^{(-2n-2)}(R)$ tends to the well-known equation for Cauchy coefficients:

$$S_i^{(-2n-2)}(R) = 2\sum_m \frac{\left|(d_i)_{0m}(R)\right|^2}{\left[E_m(R) - E_0(R)\right]^{2n+1}} \qquad (13)$$

at an arbitrary internuclear distance R.

2. Calculation results

The above method has been used to construct the dynamic polarizability functions for LiH and Li_2 molecules in the electronic ground states $^1\Sigma^+$ and $^1\Sigma_g^+$. The dipole moment matrix elements for the polarizability tensor components $\alpha_{zz}(R,\omega)$ and $\alpha_{xx}(R,\omega) \equiv \alpha_{yy}(R,\omega)$ define different Λ-selection rules, where Λ is the characteristic value of the projection of electron orbital moments on the molecule axis. Thus, for the polarizability tensor $\alpha_{zz}(R,\omega)$, the excited electronic state $E_m(R)$, where transitions are allowed, is defined by the selection rule $\Delta\Lambda = 0$ ($^1\Sigma^+ \to {}^1\Sigma^+$, $g \to u$) and for the components $\alpha_{xx}(R,\omega) \equiv \alpha_{yy}(R,\omega)$ – by the selection rule $|\Delta\Lambda| = 1$ ($^1\Sigma^+ \to {}^1\Pi$, $g \to u$).

LiH molecule

The components of polarizability tensor $\alpha_{ii}(R,\omega)$ for LiH molecule were calculated with the use of numerical values of excited electronic energy levels $E_m(R)$ (in two lower symmetry levels $^1\Sigma^+$ and $^1\Pi$) from Ref. 15 (minus electrostatic nuclei repulsion energy Z_1Z_2/R). Missing values of electronic energy levels within the region of small internuclear distances ($R < 1.8$ a.u. for the excited states $^1\Pi$ and $R < 2$ a.u. for the excited states $^1\Sigma^+$) were extended by cubic-spline interpolation to corresponding states of the united atom Be.[16] The dipole moment values of transitions to the above states $(d_i)_{0m}(R)$ were calculated in Ref. 17 and similarly extended to the values of transition dipole moments between corresponding states of Be atom.

The functions $E_m(R)$ and $(d_i)_{0m}(R)$, as well as static polarizability ones $\alpha_{ii}(R,0)$ [Ref. 18] were used later to calculate the upper and lower bounds of the dynamic polarizability function $\alpha_{ii}(R,\omega)$ and its estimating function $\bar{\alpha}_{ii}(R,\omega)$ of the LiH molecule ground state (see Eqs. (6)–(8) with $k = 2$). Figure 1 shows $\bar{\alpha}_{ii}(R,\omega)$, calculated in this work, as well as *ab initio* calculated[4] polarizability functions $\alpha_{ii}(R,\omega)$ at different frequencies ω.

Evidently, these functions are in good agreement with each other, except for the region of $\alpha_{zz}(R,\omega)$ function maximum. Besides, the calculated functions $\alpha_{ii}^{\max}(R_e,\omega)$ and $\alpha_{ii}^{\min}(R_e,\omega)$ differ insignificantly (< 3%) for frequencies $\omega < 0.12$ a.u. and are close to $\alpha_{ii}(R_e,\omega)$ from Ref. 19.

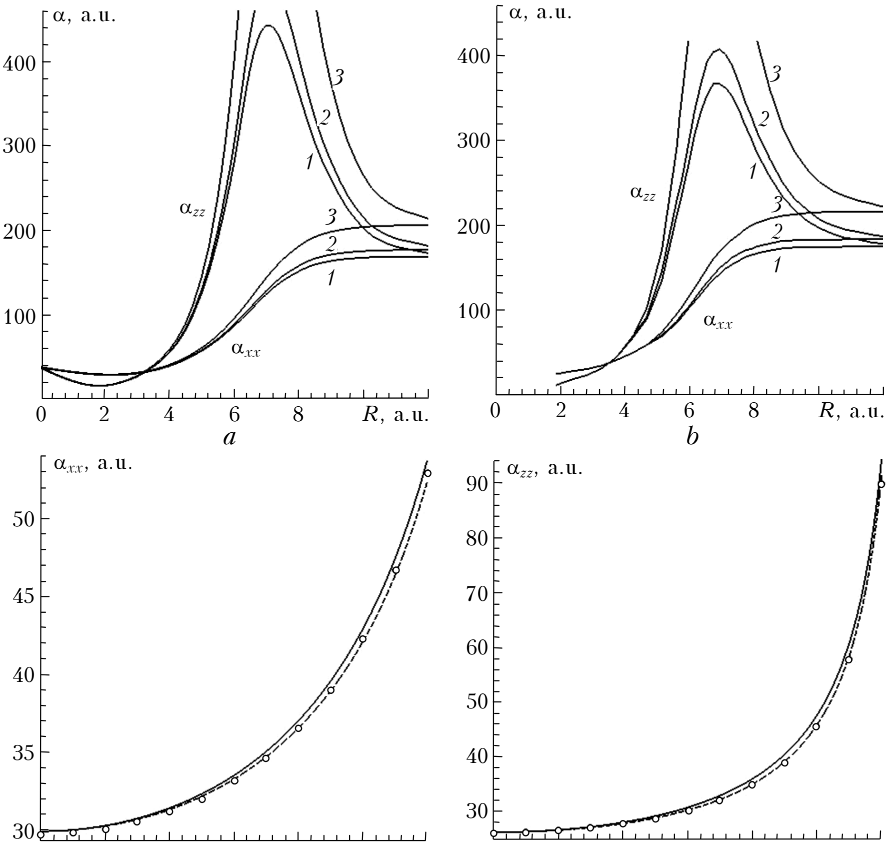
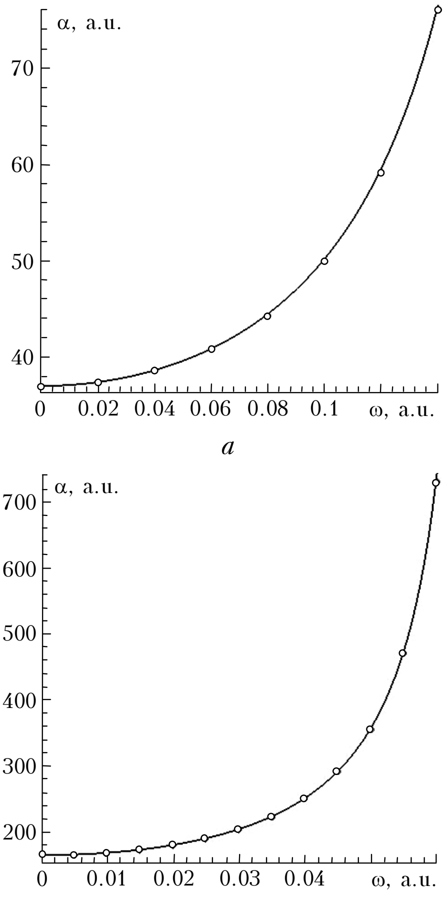


Fig. 1. Polarizability functions $\alpha_{xx}(R,\omega)$ and $\alpha_{zz}(R,\omega)$, upper and lower bounds $\alpha_{ii}^{\max}(R_e,\omega)$ and $\alpha_{ii}^{\min}(R_e,\omega)$ of LiH molecule: this work (*a*); *ab initio* calculation[4] ($\omega = 0$ (*1*), 0.0147 (*2*), and 0.0294 a.u. (*3*)) (*b*); this work (solid lines correspond to $\alpha_{ii}^{\max}(R_e,\omega)$, dashed – to $\alpha_{ii}^{\min}(R_e,\omega)$, circles – to *ab initio* calculation[19]) (*c* and *d*).

Comparison of the frequency dependence of polarizability $\bar{\alpha}_{ii}(R,\omega)$ with available literature data is also of interest for $R \to 0$ and $R \to \infty$, i.e., when conversing LiH molecule to the "united" atom Be and decomposing to Li and H atoms. The calculation results of dynamic polarizability $\bar{\alpha}_{ii}(0,\omega)$ and $\bar{\alpha}_{zz}(\infty,\omega) = \bar{\alpha}_{xx}(\infty,\omega)$ for LiH molecule, shown in Fig. 2, are in good agreement with the results of *ab initio* calculations.[20–22]



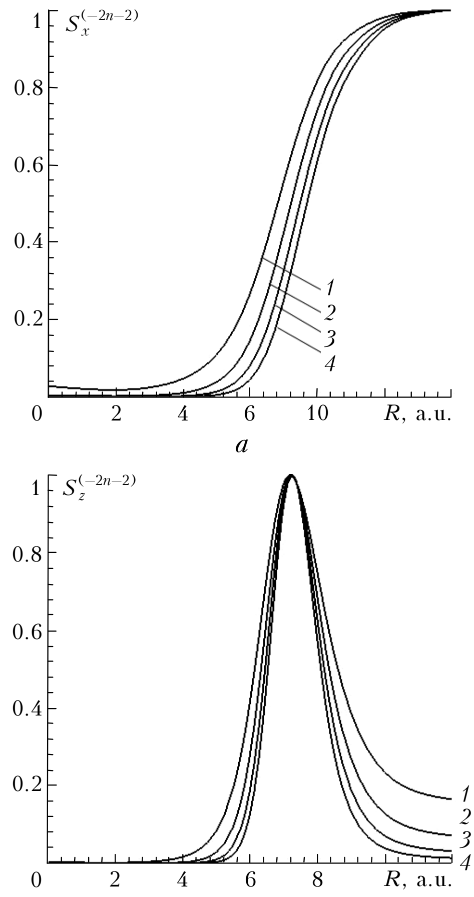
a

b

Fig. 2. Components of the LiH molecule dynamic polarizability tensor: polarizability function $\alpha_{ii}(0,\omega)$ (solid line) and *ab initio* calculated polarizability of the ground state of Be atom[20] (circles) (*a*); $\alpha_{ii}(\infty,\omega)$ (solid line) and sum of polarizabilities of the ground states of Li [Ref. 21] and H [Ref. 22] atoms (circles) (*b*).

Thus, the calculated functions $\bar{\alpha}_{ii}(R,\omega)$ are a good approximation to the real polarizability functions $\alpha_{ii}(R,\omega)$ in the whole range R and for frequencies $\omega < \omega_{1i}$, where ω_{1i} are the frequencies of the first resonance transitions.

Within the considered approach, the Cauchy coefficients are functions of R; this allows us to trace their behavior at different internuclear distances of the molecule. Figure 3 shows the functions $\bar{S}_x^{(-2n-2)}(R)$ and $\bar{S}_z^{(-2n-2)}(R)$ calculated for the ground state of LiH molecule.



a

b

Fig. 3. Normalized Cauchy coefficients $S_i^{(-2n-2)}(R)$ of LiH molecule: $n = 1$ (curve *1*), 2 (*2*), 3 (*3*), 4 (*4*). The normalization factors for $S_x^{(-2n-2)}(R)$ equal to $0.3492 \cdot 10^5$, $0.7495 \cdot 10^7$, $0.1618 \cdot 10^{10}$, and $0.3497 \cdot 10^{12}$, while for $S_z^{(-2n-2)}(R)$ – $0.2315 \cdot 10^6$, $0.1201 \cdot 10^9$, $0.6217 \cdot 10^{11}$, and $0.3228 \cdot 10^{14}$ for n = 1, 2, 3, and 4, respectively.

Different types of these functions are of interest. Thus, the functions $\bar{S}_x^{(-2n-2)}(R)$ smoothly increase with increasing R, reaching the maximum at $R \to \infty$, while the functions $\bar{S}_z^{(-2n-2)}(R)$ have sharply expressed maxima, with the smoothly displacing peaks from ≈ 7.2 to ≈ 7.25 a.u. when n varies from 1 to 4. The presented type of functions $\bar{S}_x^{(-2n-2)}(R)$ witnesses for stronger frequency dependence of Li atom polarizability in comparison with those of LiH molecule at small and mean R (the contribution of H atom in total polarizability of H and Li atom is negligible).

Similar behavior is typical for the Cauchy coefficients $\bar{S}_x^{(-2n-2)}(R)$ and $\bar{S}_z^{(-2n-2)}(R)$ with larger n. The dependence of Cauchy coefficients on molecule internuclear distance was considered in scientific literature only for hydrogen molecule[2]; therefore, the obtained Cauchy coefficients for LiH (and Li_2) molecule can be compared with results of other authors only fore some fixed R. Table 1 presents the calculated Cauchy coefficients $S_i^{(-2n-2)}$

for Be atom and LiH molecule for its equilibrium state R_e. In this case, the obtained coefficients ($\bar{S}_z^{(-2n-2)}(0) = \bar{S}_x^{(-2n-2)}(0)$) are comparable with the Cauchy coefficients $S^{(-2n-2)}$, *ab initio* calculated for the ground state of Be atom.

Table 1. Cauchy coefficients $S_i^{(-2n-2)}$ for Be atom and LiH molecule at $R = R_e$, a.u.

n	Be	LiH	
		$i = x$	$i = z$
0	0.3703E + 02 0.4207E + 02* 0.4524E + 02**	0.2996E + 02	0.2608E + 02
1	0.9708E + 03 0.9697E + 03* 0.1422E + 04**	0.8496E + 03	0.9769E + 03
2	0.2567E + 05 0.23357E + 05* 0.4512E + 05**	0.2686E + 05	0.4778E + 05
3	0.6807E + 06 0.57614E + 06* 0.1434E + 07**	0.8952E + 06	0.2594E + 07
4	0.1808E + 08 0.14415E + 08* 0.4559E + 08**	0.3056E + 08	0.1459E + 09
5	0.4804E + 09 0.36375E + 09* 0.1498E + 10**	0.1055E + 10	0.8300E + 10
6	0.1277E + 11 0.92267E + 10* 0.4611E + 11**	0.3659E + 11	0.4740E + 12
7	0.3395E + 12 0.234783E + 12* 0.1466E + 13**	0.1272E + 13	0.2711E + 14
8	0.9025E + 13 0.598578E + 13* 0.4663E + 14**	0.4427 + 14	0.1551E + 16

* From Ref. 23. ** From Ref. 24. ($E + n$ is equivalent to multiplication by 10^n).

As is evident from Table 1, the calculated Cauchy coefficients better agree with data from Ref. 23 than from Ref. 24. Taking into account the fact that energy levels and transition moments, used in this work, have been calculated more accurate,[15–18] we consider our Cauchy coefficients as more realistic, than in Refs. 23 and 24.

Li_2 molecule

The components of Li_2 molecule polarizability tensor $\alpha_{ii}(R,\omega)$ were calculated with the use of numerical values of electronic energy levels $E_m(R)$ from Refs. 25 and 26, i.e., two lower excited electronic energy levels ${}^1\Sigma_u^+$ and ${}^1\Pi_u$ were used for the polarizability tensor components $\alpha_{zz}(R,\omega)$ and $\alpha_{xx}(R,\omega) = \alpha_{yy}(R,\omega)$, respectively.

Note, that these numerical energy values are available only for $R \geq 3.5$ a.u., therefore, the polarizability functions of Li_2 molecule have been calculated only in this range. The static polarizability functions $\alpha_{ii}(R,0)$ were taken from Ref. 27 and the values of transition dipole moments – from Ref. 28.

The functions $E_m(R)$, $(d_i)_{0m}(R)$, and $\alpha_{ii}(R,0)$ were used for calculating the upper and lower bounds of dynamic polarizability functions of the Li_2 molecule ground state.

According to the calculations, the functions $\alpha_{ii}^{\max}(R,\omega)$ and $\alpha_{ii}^{\min}(R,\omega)$ are virtually equal. The calculated functions of Li_2 molecule dynamic polarizability are shown in Fig. 4.

The calculated functions $\alpha_{ii}(R_e,\omega)$ are evidently in good agreement with *ab initio* calculations from Ref. 29. Note also, that the functions $\bar{\alpha}_{ii}(R = \infty,\omega)/2$ of Li_2 molecule are in good agreement with *ab initio* calculated Li atom dynamic polarizability[21] and LiH molecule polarizability functions $\bar{\alpha}_{ii}(R = \infty,\omega)$ (see Fig. 2*b*).

The Cauchy coefficients $\bar{S}_x^{(-2n-2)}(R)$ and $\bar{S}_z^{(-2n-2)}(R)$, calculated as functions of Li_2 molecule internuclear distance, are shown in Fig. 5.

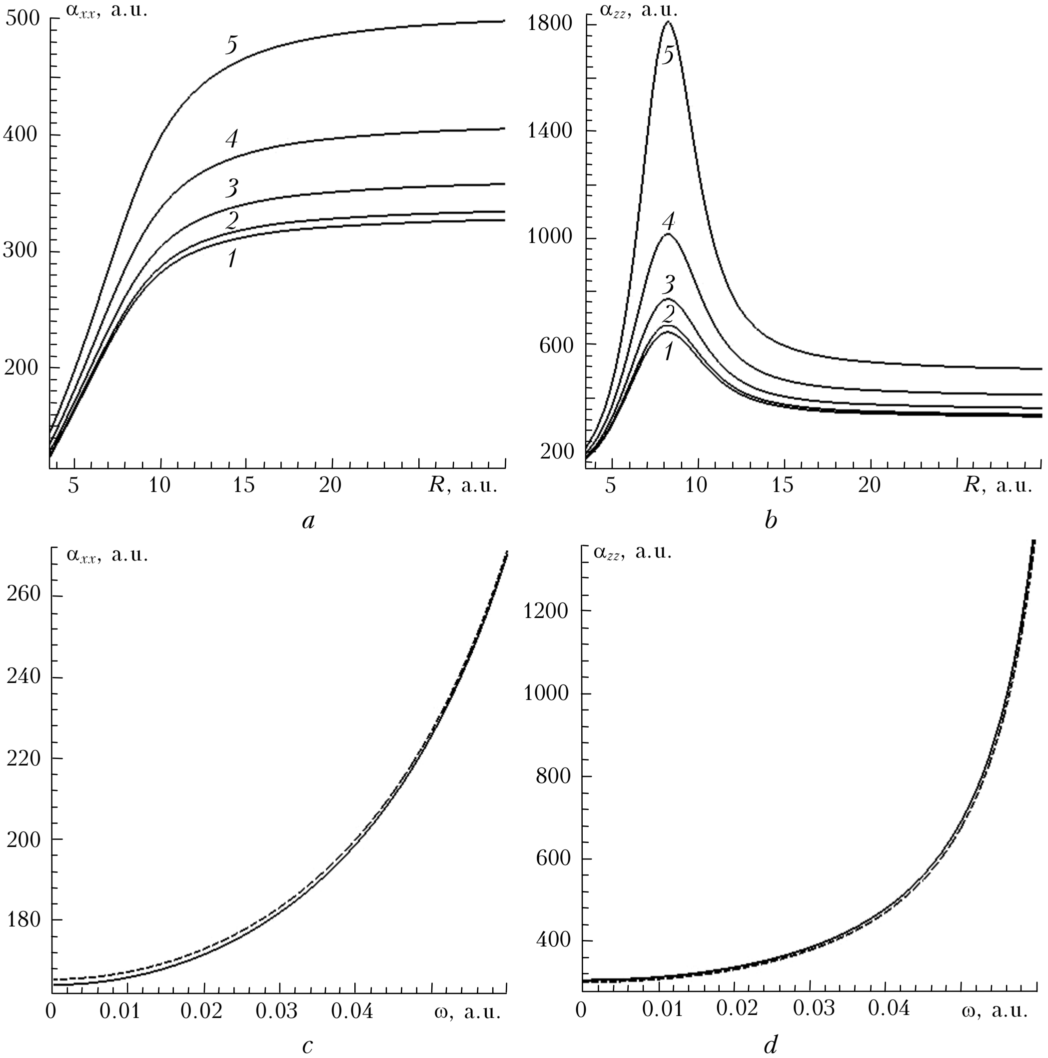
A main distinction from LiH molecule is in the fact, that the Cauchy coefficients $\bar{S}_z^{(-2n-2)}(R)$ of Li_2 molecule reach their maxima at a larger internuclear distance ($R = 8.3$ a.u.) and are virtually independent of n.

The Cauchy coefficients $S_i^{(-2n-2)}$ calculated for Li atom and Li_2 molecule at its equilibrium state R_e are in good agreement with *ab initio* calculations from Ref. 29 (Table 2).

Table 2. Cauchy coefficients $S_i^{(-2n-2)}$ for Li atom and Li_2 molecule at $R = R_e$, a.u.

n	Li	Li_2	
		$i = x$	$i = z$
0	0.1644E + 03 0.1639E + 03*	0.1638E + 03 0.1653E + 03*	0.3012E + 03 0.2977E + 03*
1	0.3585E + 05 0.3507E + 05*	0.1784E + 05 0.1784E + 05*	0.6449E + 05 0.6313E + 05*
2	0.7804E + 07 0.7578E + 07*	0.1968E + 07 0.1965E + 07*	0.1393E + 08 0.1363E + 08*
3	0.1698E + 10 0.1639E + 10*	0.2177E + 09 0.2178E + 09*	0.3013E + 10 0.2947E + 10*
4	0.3697E + 12 0.3544E + 12*	0.2412E + 11 0.2417E + 11*	0.6520E + 12 0.6373E + 12*
5	0.8049E + 14 0.7664E + 14*	0.2672E + 13 0.2683E + 13*	0.1411E + 15 0.1378E + 15*
6	0.1753E + 17 0.1657E + 17*	0.2961E + 15 0.2979E + 15*	0.3053E + 17 0.2981E + 17*
7	0.3820E + 19 0.3584E + 19*	0.3281E + 17 0.3308E + 17*	0.6608E + 19 0.6446E + 19*
8	0.8328E + 21 0.7751E + 21*	0.3636E + 19 0.3673E + 19*	0.1430E + 22 0.1394E + 22*

* Calculated with the use of data from Ref. 29.



a *b*

c *d*

Fig. 4. Polarizability functions of Li_2 molecule: $\alpha_{xx}(R,\omega)$ (*a*); $\alpha_{zz}(R,\omega)$ (*b*) ($\omega = 0$ (*1*), 0.01 (*2*), 0.02 (*3*), 0.03 (*4*), and 0.04 a.u. (*5*)); $\alpha_{xx}(R_e,\omega)$ (*c*); and $\alpha_{zz}(R_e,\omega)$ (*d*) (solid lines – this work, dashed lines – *ab initio* calculations[29]).

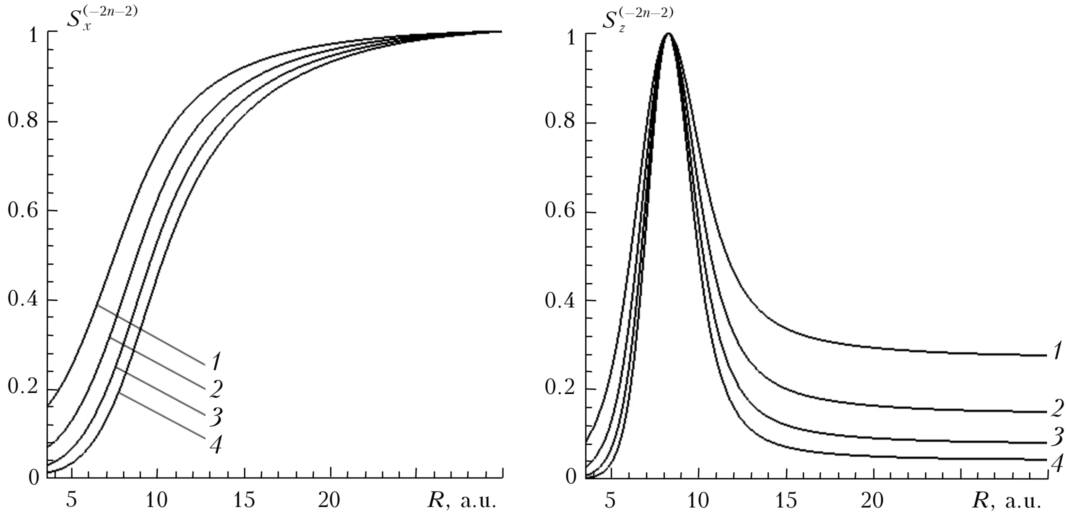


Fig. 5. Normalized Cauchy coefficients $S_i^{(-2n-2)}(R)$ of Li_2 molecules (numbers in figures correspond to n values). Normalization factors for $S_x^{(-2n-2)}(R)$ are equal to $0.6995 \cdot 10^5$; $0.1500 \cdot 10^8$; $0.3219 \cdot 10^{10}$; $0.6906 \cdot 10^{12}$, and for $S_z^{(-2n-2)}(R)$ are $0.2606 \cdot 10^6$; $0.1045 \cdot 10^9$; $0.4186 \cdot 10^{11}$; $0.1678 \cdot 10^{14}$ for $n = 1$ (curve *1*), 2 (*2*), 3 (*3*), 4 (*4*) , respectively.

Conclusion

The analytical expressions obtained in this work for polarizability surface of diatomic LiH and Li_2 molecules in a wide range of variation of their internuclear distances and frequency of external electromagnetic field are highly competitive in accuracy with *ab initio* calculations of dynamic polarizability of these molecules and are presented in more convenient form for further analysis. The dependence of Cauchy coefficients of LiH and Li_2 molecules on internuclear distance has been obtained for the first time.

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