

# EVALUATION OF ROTATIONAL $g$ -FACTOR OF ${}^6\text{Li}^1\text{H}$ AND ${}^6\text{Li}^2\text{H}$ FROM PURE ROTATIONAL AND VIBRATION-ROTATIONAL SPECTRA OF $\text{LiH } X^1\Sigma^{+*}$

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A deformationally self-consistent procedure and dependent local parameters  $t_0^{\text{Li}}$ ,  $t_0^{\text{H}}$  are applied to estimate the values of the rotational  $g$ -factor of  ${}^6\text{Li}^2\text{H}$   $g_{J=1} = -0.279032(88)$  and  ${}^6\text{Li}^1\text{H}$   $g_{J=1} = -0.661020(32)$  in the rotational state  $J = 1$ , from pure rotational and vibration-rotational spectra of  $\text{LiHX}^1\Sigma^+$ .

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## 1. Introduction

Investigations of electric and magnetic properties of isotopic variants of LiH in the electronic state  $X^1\Sigma^+$  by Rothstein [1] and Freeman et al. [2] provided the values of the rotational  $g$ -factor  $g_J$  and dipole moment  $\mu_J$  measurable in the  $J = 1$  rotational state

$$g_{J=1}^{71} = -0.65842(17), \quad g_{J=1}^{72} = -0.27674(11), \quad (1)$$

$$\mu_{J=1}^{71} = 1.96224(20), \quad \mu_{J=1}^{72} = 1.95747(17), \quad (2)$$

$$\mu_{J=1}^{61} = 1.96277(40), \quad \mu_{J=1}^{62} = 1.95803(33). \quad (3)$$

Neither experimental nor theoretical value of the rotational  $g$ -factor of  ${}^6\text{Li}^1\text{H}$  and  ${}^6\text{Li}^2\text{H}$  is known as yet.

As there exist simple relations [3]

$$g_J(R) = m_p \sum_{i=0} \sum_{\mu=a,b} t_i^\mu m_\mu^{-1} z^i, \quad (4)$$

$$\mu_J(R) = (eR/2) \sum_{i=0} (t_i^a - t_i^b) z^i, \quad (5)$$

linking  $g_J$ ,  $\mu_J$  and coefficients  $t_i^{a(b)}$  of the radial function [4]

$$\alpha(R) = m_e \sum_{i=0} \sum_{\mu=a,b} t_i^\mu m_\mu^{-1} z^i, \quad (6)$$

describing nonadiabatic rotational effects, one may estimate [5-7] the values of the rotational  $g$ -factor and dipolar moment directly from frequency data in vibration-

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-rotational spectra. In Eqs. (4)–(6)  $z = 2(R - R_0)/(R + R_0)$  denotes Ogilvie's variable [8] for reduced displacement from equilibrium<sup>†</sup>  $R_0$ ,  $m_e$ ,  $m_p$ ,  $m_a$ ,  $m_b$  are masses of electron, proton and nuclei, respectively;  $R_0$  is the equilibrium internuclear distance according to the Born–Oppenheimer (BO) procedure and  $e$  is the magnitude of an electronic charge.

To accomplish this we solve the Herman–Asgharian wave equation [9]

$$\left\{ -\frac{\hbar^2}{2m} \frac{d}{dR} [1 + \beta(R)] \frac{d}{dR} + U_J(R) - E_{vJ} \right\} \psi_{vJ}(R) = 0, \quad (7)$$

$$U_J(R) = \frac{\hbar^2 J(J+1)[1 + \alpha(R)]}{2mR^2} + V(R) + V'(R) \quad (8)$$

$$V(R) = c_0 z^2 \left( 1 + \sum_{i=1} c_i z^i \right), \quad (9)$$

$$V'(R) = m_e \sum_{i=1} \sum_{\mu=a,b} u_i^\mu m_\mu^{-1} z^i, \quad (10)$$

in which  $V(R)$  describes a potential energy independent of mass,  $V'(R)$  is an adiabatic term reflecting the dependence of internuclear potential energy on not only the distance between nuclei but also their relative momenta, whereas  $\alpha(R)$ , defined in (4), takes into account nonadiabatic rotational effects, reflecting the fact that electrons fail to follow perfectly the nuclei rotating about the centre of molecular mass. In the case of LiH we neglect a function  $\beta(R)$  describing nonadiabatic vibrational effects appearing due to vibrational inertia of electrons, as the available spectral data are insufficient for their separate evaluation [10, 11].

Having solved Eq. (7), for example by making use of the semi-classical Wentzel–Kramers–Brillouin (WKB) approach [12], one may employ the discrete molecular energies  $E_{vJ}$  to determine the parameters of the radial functions  $\alpha(R)$ ,  $V(R)$  and  $V'(R)$  by fitting the spectral data. The calculations carried out for LiH have shown that  $t_i^{a(b)}$  evaluated in this way fail to reproduce satisfactorily the experimental values of  $g_J$  and  $\mu_J$ . Hence, Tiemann and Ogilvie [10], and Ogilvie [11], have proposed the inverted procedure that consists in fitting the observed transitions in LiH using  $t_0^{\text{Li}}$  and  $t_0^{\text{H}}$  constrained to values consistent with their relations

$$t_0^{\text{Li}} = m[g_0/m_p + 2\mu_0/(eR_0m_{\text{H}})], \quad (11)$$

$$t_0^{\text{H}} = m[g_0/m_p - 2\mu_0/(eR_0m_{\text{Li}})], \quad (12)$$

to know experimental values of electric dipolar moment and rotational  $g$ -factor. To substitute in the above equations we can use

$$g_0^{71} \approx g_{J=1}^{71}, \quad g_0^{72} \approx g_{J=1}^{72}, \quad (13)$$

for the vibrational ground state whereas [13]  $\mu_0 = 1.94407(22)$  is a weighted average of the extrapolated values  $\mu_{J=1}$ , specified by Eqs. (2) and (4), for the vibrationless state [14].

<sup>†</sup>In this work we use the notation  $R_0$ ,  $\mu_0$  instead of the standard one  $R_e$ ,  $\mu_e$ , referring to quantities in the rotationless state  $J = 0$ .

The calculations performed have shown that values of  $t_0^{a(b)}$  determined for two isotopic variants  ${}^7\text{Li}^1\text{H}$  and  ${}^7\text{Li}^2\text{H}$  differ from each other; hence these parameters appear to have a slight dependence on mass, although according to conventional theory [9] they are not expected to possess such a property.

Hence, Tiemann and Ogilvie [10], and Ogilvie [11], calculated  $t_0^{a(b)}$  by arithmetic averaging of values from Eqs. (11) and (12)

$$t_0^{\text{Li}} = \{m^{7,1}[g_0^{7,1}/m_p + 2\mu_0/(eR_0m_1)] + m^{7,2}[g_0^{7,2}/m_p + 2\mu_0/(eR_0m_2)]\}/2, \quad (14)$$

$$t_0^{\text{H}} = \{m^{7,1}[g_0^{7,1}/m_p - 2\mu_0/(eR_0m_7)] + m^{7,2}[g_0^{7,2}/m_p - 2\mu_0/(eR_0m_7)]\}/2 \quad (15)$$

to obtain

$$t_0^{\text{Li}} = 0.75335, \quad t_0^{\text{H}} = -0.76823. \quad (16)$$

In the above equations  $m^{k,l}$  denotes reduced atomic mass,  $m_k$  is a mass of a separate atom, whereas  $g_J^{k,l}$  is a rotational  $g$ -factor, for a given isotopic variant  ${}^k\text{Li}^l\text{H}$ .

In this paper we present a hypothesis that in the case of  $\text{LiH}$   $t_0^{a(b)}$  parameters depend on mass. Consequently we include in calculations the *local constraints*, i.e. values of  $t_0^{\text{Li}}$  and  $t_0^{\text{H}}$  calculated for  $\text{LiH}$  in its two isotopic variants for which values of  $g_J$  are available. Because we lack experimental values of the rotational  $g$ -factor of  ${}^6\text{Li}^1\text{H}$  and  ${}^6\text{Li}^2\text{H}$  we propose to work in the scheme with dependent [3], and not constrained parameters  $t_0^{a(b)}$ , in which  $g_{J=1}^{61}$  and  $g_{J=1}^{62}$  are treated as fitted *local* parameters. This approach not only permits a successful analysis of infrared and microwave spectra of  $\text{LiH}$  but also enables us to evaluate unknown values of  $g_{J=1}^{61}$  and  $g_{J=1}^{62}$ .

## 2. The method

To implement the above objective we adopt a procedure [3] employed in the previous work for quantitative analysis of adiabatic and nonadiabatic effects in  $\text{GaH } X^1\Sigma^+$ . The starting point is a wave equation (7) in which we expand  $U_J(R)$

$$U_J(\eta) = \sum_{n=0} b_n^J \eta^n, \quad (17)$$

into a series of a Dunham variable dependent on  $J$ ,

$$\eta = (R - R_J^{\text{ad}})/R_J^{\text{ad}}, \quad (18)$$

recognizing that vibrational displacements of nuclei in a vibration-rotational diatomic system take place in the vicinity of a dynamic equilibrium conformation  $R_J^{\text{ad}}$ , dependent [15, 16] on  $J$ , and not the BO conformation  $R_0$ . The  $R_J^{\text{ad}}$  appearing in (18) are defined according to a criterion for a minimum of the effective potential energy

$$\left( \frac{dU_J(R)}{dR} \right)_{R_J^{\text{ad}}} = 0 \quad (19)$$

enabling calculation of a modified reference conformation for each rotational state  $J$ , and to remove the linear term  $b_1^J \eta$  in the expansion (17). Accordingly, we achieve an effective wave equation

$$\left[ -B_J \frac{d^2}{d\eta^2} + a_0^J \eta^2 \left( 1 + \sum_{s=1} a_s^J \eta^s \right) - (E_{vJ} - b_0^J) \right] \psi_{vJ}(\eta) = 0, \quad (20)$$

in which

$$a_0^J = b_2^J, \quad a_{s>0}^J = b_{s+2}^J / a_0^J, \quad B_J = \hbar^2 / [2m(R_J^{\text{ad}})^2], \quad (21)$$

which is amenable to straightforward solution according to Dunham's quasi-classical scheme [12] generating eigenvalues

$$E_{vJ} = b_0^J + \sum_{k=0} \mathcal{Y}_{k0}(v + 1/2)^k. \quad (22)$$

The coefficients  $\mathcal{Y}_{k0}$  appearing in (22) are purely vibrational coefficients [12] in which substitutions  $\{R_0, a_n\} \rightarrow \{R_J^{\text{ad}}, a_n^J\}$  can be made. As eigenvalues (22) contain unknown parameters  $R_J^{\text{ad}}$  defined according to the general condition for equilibrium (19) we can effect a quantitative analysis of spectral data working in an iterative scheme, called the deformational self-consistent (DSC) procedure, described in detail elsewhere [3, 15, 16].

### 3. Dependent local parameters

A detailed analysis of the constraints (16) indicates that they are obtained with an approximation (13). Such estimation is charged with an error [3] due to the rotational dependence of  $g_J$  in the *vibrationless* state  $v = 0$ ,  $J > 0$

$$g_J = m_p \sum_{i=0} \sum_{\mu=a,b} t_i^\mu m_\mu^{-1} z_J^i, \quad (23)$$

$z_J = 2(R_J^{\text{ad}} - R_0)/(R_J^{\text{ad}} + R_0)$  is Ogilvie's variable  $z$  in rotational state  $J$ . Consequently, constant terms (11) and (12) take the form [17]

$$t_0^a = m[G_J/m_p + 2\mu_0/(eR_0m_b)], \quad (24)$$

$$t_0^b = m[G_J/m_p - 2\mu_0/(eR_0m_a)], \quad (25)$$

in which

$$G_J = g_J - m_p \sum_{i=1} \sum_{\mu=a,b} t_i^\mu m_\mu^{-1} z_J^i. \quad (26)$$

Having introduced the above correction we define a set of dependent local parameters as follows:

$$t_0^{7\text{Li}} = m[G_J^{71}/m_p + 2\mu_0/(eR_0m_1)], \quad t_0^{1\text{H}} = m[G_J^{71}/m_p - 2\mu_0/(eR_0m_7)], \quad (27)$$

$$t_0^{7\text{Li}} = m[G_J^{72}/m_p + 2\mu_0/(eR_0m_2)], \quad t_0^{2\text{H}} = m[G_J^{72}/m_p - 2\mu_0/(eR_0m_7)], \quad (28)$$

$$t_0^{6\text{Li}} = m[G_J^{61}/m_p + 2\mu_0/(eR_0m_1)], \quad t_0^{1\text{H}} = m[G_J^{61}/m_p - 2\mu_0/(eR_0m_6)], \quad (29)$$

$$t_0^{6\text{Li}} = m[G_J^{62}/m_p + 2\mu_0/(eR_0m_2)], \quad t_0^{2\text{H}} = m[G_J^{62}/m_p - 2\mu_0/(eR_0m_6)]. \quad (30)$$

In these equations  $g_J^{62}$  and  $g_J^{61}$  (defined by Eq. (25)) for  $J = 1$  are treated as fitted *local* parameters, whereas  $R_0$  is a fitted independent parameter. In this way instead of  $t_0^{1\text{H}}$  and  $t_0^{2\text{H}}$  we fit  $g_J^{62}$  and  $g_J^{61}$ ; the total number of free parameters remains the same.

## 4. Applications

In this work we apply the DSC procedure to evaluate radial parameters of LiH in four isotopic variants, working in a scheme with dependent local parameters  $t_0^{a(b)}$ . As input data we use 594 pure rotational and vibration-rotational transitions [18–24] of  ${}^7\text{Li}^1\text{H}$ ,  ${}^6\text{Li}^1\text{H}$ ,  ${}^7\text{Li}^2\text{H}$  and  ${}^6\text{Li}^2\text{H}$ .

TABLE I

Mass-independent radial parameters of LiH  $X^1\Sigma^+$ .

$i$	$c_i$	$t_i^{\text{H}}$	$u_i^{\text{Li}}$ [ $\text{cm}^{-1}$ ]	$u_i^{\text{H}}$ [ $\text{cm}^{-1}$ ]
0	65728.935(76) $\text{cm}^{-1}$			
1	-0.8972918(46)	1.5080(24)		-52058.5(95)
2	0.348279(22)	-2.156(41)	-12006(718)	33305(102)
3	-0.088424(90)	2.609(74)		-6510(671)
4	-0.04518(25)			
$R_0$	1.594963675(62) Å			
$g_{J=1}^{62}$	-0.279032(88)			
$g_{J=1}^{61}$	-0.661020(32)			

Normalized standard deviation of the fit of 594 data was  $\hat{\sigma} = 1.140$ , standard deviation  $\sigma = 0.000575 \text{ cm}^{-1}$  and  $F$  value  $7.7 \times 10^{14}$ .

Table I presents the radial parameters and values of  $g_{J=1}^{62}$  and  $g_{J=1}^{61}$  obtained according to the DSC scheme with dependent local parameters  $t_0^{\text{Li}}$  and  $t_0^{\text{H}}$ ; all other parameters were constrained to zero. The uncertainty in parentheses is one estimated standard deviation in units of the last quoted digit of the fitted values.

Fitted parameters in various sets were tested according to the criteria:

- (i) minimum number of fitted parameters  $N$ ;
- (ii) optimum value of the normalized standard deviation  $\hat{\sigma} \approx 1$ ;
- (iii) maximum value of the  $F$  statistic [25];
- (iv) optimum values of standard errors  $\sigma_i$  of fitted parameters and correlation coefficients  $cc(i, j)$ .

In calculations we used the vibrational Dunham coefficients

$$Y_{k0} = \sum_{h=0}^3 Y_{k0}^{2h}, \quad (31)$$

up to sixth order for  $0 \leq k \leq 4$ , including  $a_n$ ,  $0 \leq n \leq 6$  potential parameters. Consequently, the expansion for the effective potential energy (17) contains derivatives up to eighth order.

The proposed iterative DSC procedure is rapidly convergent and in the case of LiH requires ten iterations to evaluate parameters in a final set such that values alter less than their standard errors, and affect insignificantly the precision of

TABLE II

Mass-dependent deformational parameters  $x_J = (R_J^{\text{ad}} - R_0)/R_0$ .

$J$	${}^7\text{Li}^1\text{H}$	${}^7\text{Li}^2\text{H}$	${}^6\text{Li}^1\text{H}$	${}^6\text{Li}^2\text{H}$
0	0.0002155853	0.0001078689	0.0002155858	0.0001078692
1	0.0004442349	0.0002366796	0.0004490142	0.0002414605
2	0.0009014868	0.0004942859	0.0009158216	0.0005086269
3	0.0015872467	0.0008806575	0.0016159100	0.0009093357
4	0.0025 013754	0.0013957493	0.0025491341	0.0014435386
5	0.0036436906	0.0020395019	0.0037153042	0.0021111717
10	0.0127690897	0.0071851666	0.0130310139	0.0074475592
15	0.0275539125	0.0155314250	0.0281234484	0.0161026476
20	0.0479551435	0.0270599547	0.0280970638	0.0280569710
25	0.0739473958	0.0417521194		0.0432910541
30		0.0595945993		

calculations. Initial values of fitted parameters were taken from Ogilvie's calculations [11].

In Table II parameters  $x_J = (R_J^{\text{ad}} - R_0)/R_0$  for LiH in four isotopic variants are reported; they are evaluated with an accuracy  $\epsilon = 10^{-20}$  to be achieved in 60 bisections. The quantity  $R_0^{\text{ad}}$ , appearing in Table II for  $J = 0$ , denotes the adiabatic reference conformation defined according to a criterion of a minimum of potential energy  $U_0(R) = V(R) + V'(R)$ .

### 5. Results and discussion

In preliminary fits of the data, we discovered that inclusion  $u_1^{\text{Li}}$  in the fit leads to large magnitudes (over 0.99) of correlation coefficients  $cc(i, j)$  linking  $u_1^{\text{Li}}$  with  $R_0$  as well as other parameters. Because the value of  $u_1^{\text{Li}}$  was relatively small ( $u_1^{\text{Li}} = 88(1747)$ ) and associated with a relatively large error, we constrained  $u_1^{\text{Li}}$  to zero during fitting. In further fits with  $u_1^{\text{Li}}$  constrained to zero, the number of entries in the parameter correlation matrix with magnitudes greater than 0.90 decreased to two:  $cc(R_0, t_0^{\text{H}}) = 0.9177$  and  $cc(u_2^{\text{H}}, u_3^{\text{H}}) = -0.9270$ .

Inspection of Table I reveals the absence of  $c_5$ ,  $c_6$ ,  $t_1^{\text{Li}}$ ,  $u_4^{\text{H}}$  and  $u_5^{\text{H}}$  appearing in the fitting the same data in the standard scheme [11]; instead parameters  $t_3^{\text{H}}$  and  $u_3^{\text{Li}}$  appear. In the DSC approach the presence of  $c_5$ ,  $c_6$  and  $u_5^{\text{H}}$  in the fit is superfluous. Also worth mentioning is the value of the determined reference conformation  $R_0 = 1.594963675(62)$  Å, more precise (by two orders of magnitude), than the standard method yielding  $R_0 = 1.5949107(14)$  Å<sup>†</sup>. A difference in values of  $R_0$  as well as  $c_0 = 65728.935(76)$  cm<sup>-1</sup> and  $c_0 = 65724.833(99)$  cm<sup>-1</sup> (obtained in the standard approach [11]) suggest nonequivalence of both treatments; the mass-dependent parameters  $t_0^{\text{a(b)}}$  result in the values of the fitted radial para-

<sup>†</sup>Ogilvie's value was calculated from the fitted value of the parameter  $U_{0,1} = 1000\hbar^2 N_A / (2cR_0^2)$  with uncertainty estimated by taking into account the errors in the fundamental constants  $\hbar$  and  $N_A$  [14].

meters. A question arises what is the source of such mass-dependence. Comparing the generating expression for  $\alpha(R)$  [9]

$$\alpha(R) = \hbar^2 \left( \frac{1}{m_a} + \frac{1}{m_b} \right) \sum_{\lambda' \neq \lambda} \frac{\langle \lambda | \partial / \partial R | \lambda' \rangle \langle \lambda' | \partial / \partial R | \lambda \rangle}{E_{\lambda'} - E_{\lambda}}, \quad (32)$$

in which  $E_{\lambda'}$ ,  $E_{\lambda}$  are BO eigenvalues of the electronic wave equation in  $\lambda'$  and  $\lambda$  electronic state, with (6) we see that a mass-dependence of  $E_{\lambda}$  may be a potential source of this peculiar property. Such an effect has been found, for example, for dissociation energy of  $^1\text{H}_2$ ,  $^1\text{H}^2\text{H}$ , and  $^2\text{H}_2$  [26] that is strictly related to eigenvalues  $E_{\lambda}$ .

A detailed analysis of results obtained indicates that working in the DSC scheme with locally dependent parameters we are able:

- (i) To reproduce 594 rotational and vibration-rotational transitions of LiH with  $\hat{\sigma} = 1.14$  (comparable to  $\hat{\sigma} = 1.12$  in the standard approach [11]) by making use of only 13 independent and four locally dependent parameters (comparable to 18 independent and two constrained parameters in the standard scheme [11]);
- (ii) To estimate with great precision values of rotational  $g$ -factors of  $^6\text{Li}^2\text{H}$   $g_{J=1} = -0.279032(88)$  and  $^6\text{Li}^1\text{H}$   $g_{J=1} = -0.661020(32)$  in the rotational state  $J = 1$ , for which neither experimental nor theoretical values are reported.

The obtained theoretical values of  $g$ -factors should be treated as predictions requiring an experimental verification. At this stage one may show only that their values undergo a general qualitative rule: the magnitudes of values of  $g_J$  and  $\mu_J$  for lighter  $^6\text{Li}$  isotope are greater than for heavier  $^7\text{Li}$ . The same rule is for  $^1\text{H}$  and  $^2\text{H}$  isotopes.

TABLE III

Mass-dependent  $t_0^{\text{Li}}$  and  $t_0^{\text{H}}$  parameters of four isotopic variants of LiH.

$^k\text{Li}^l\text{H}$	$t_i^{^k\text{Li}}$	$t_i^{^l\text{H}}$
$^7\text{Li}^1\text{H}$	0.7537956	-0.7677280
$^7\text{Li}^2\text{H}$	0.7519498	-0.7695768
$^6\text{Li}^1\text{H}$	0.7361294	-0.7853941
$^6\text{Li}^2\text{H}$	0.7216020	-0.7999246

Having evaluated  $g_{J=1}^{61}$  and  $g_{J=1}^{62}$  one may calculate  $t_0^{\text{a(b)}}$  for four isotopic variants of LiH. Their values are reported in Table III that shows that for a given nuclear centre the values of parameters  $t_0^{\text{a(b)}}$  vary significantly confirming their unexpected dependence on mass.

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