FREE-BOUND TRANSITIONS IN LiH MOLECULE

V.K. KHERSONSKII, A.A. LIPOVKA

Special Astrophysical Observatory of the Russian AS,
St.Petersburg brunch, Pulkovo, Russia

ABSTRACT. *The method and results of calculations of the radiative asso-
ciation and photodissociation cross-sections for LiH molecule are discus-
sed. We consider the free-bound vibrational transitions in the ground
electron state* $^1\Sigma^+$.

*The calculations of the radiative association cross-sections are carried
out for the interval of the colliding atom velocities from* 10^3 *to* 10^7 *cm/s.
The photodissociation cross-section are calculated for the photon wave-
length region from* 10^{-4} *to* 10^{-2} *cm. It is shown that the cross-sections of
both processes depend on the vibrational quantum number substantially; they
grow strongly if this quantum number increases.*

В работе обсуждается метод и результаты расчета сечений радиативной ас-
социации и фотодиссоциации молекулы Li H при свободно-связанных колебатель-
ных переходах в пределах основного электронного состояния $^1\Sigma^+$. Расчеты се-
чений радиативной ассоциации охватывают область изменения относительных
скоростей сталкивающихся атомов от 10^3 до 10^7 см/с, фотодиссоциации расчи-
таны для области длин волн фотонов $10^{-4} - 10^{-2}$ см. Показано, что сечения
обоих процессов существенным образом зависят от величины колебательного
квантового числа и сильно возрастают с его увеличением.

1. INTRODUCTION

As it is widely known, data on the elementary processes in the interstellar molecules including the radiative processes have the fundamental importance for the development of physical models of the interstellar medium. These data permit us to calculate the equilibrium content of different molecules in the gas clouds near IR stars, hot young stars and in many other objects if the radiation can have the pronounced effects on the chemical compositions.

Another important point of the study of the molecule and radiation interactions is the investigation of the molecular content in the primordial cosmological gas. This field is of particular interest because the molecular spectroscopic methods allow us to develop effective and, in some cases, unique possibilities for testing physical conditions in the primordial gas.

In this paper the free-bound vibrational radiative transitions are considered for LiH molecule. Actually these processes are photo dissociation and association which are connected with the transitions of molecule from the continuum of the ground electron state to the vibrational levels of the same electron state and vice versa.

The radiative association of such kind will occur in the case when the excited Li and H atoms are absent in the medium and the temperature does not exceed several hundreds of K. In this case LiH molecule can't be formed in the excited electron state. Thus the radiative association through the upper electron state is forbidden. Similarly, if the radiation field temperature in the medium is low, the short wavelength photons, which correspond to the electron transitions in LiH, are practically absent in the radiation spectrum. In this case the photodecay of LiH molecule through the upper electron state is actually forbidden. Therefore the main way for the photodissociation will be connected with the transitions from the vibrational levels of the ground state to the continuum of the same state.

The mentioned physical conditions are widely available in the sufficiently dense clouds where the kinetic temperature is about some scores of K and the cloud interior is shielded from the ultraviolet and optical radiation of the nearest stars.

Similar conditions occur also in the primordial gas in the epochs which correspond to the pregalactic stage and are characterized by the redshifts z < 100. Therefore the data on the cross-section and rate coefficients for the radiative association and photo dissociation connected with the free-bound vibrational transitions in the ground electron state are of particular interest for a wide field of the astrophysical problems.

In part 2 we consider the methods of calculation of both photo association and dissociation cross-sections. Part 3 is devoted to the discussion of calculation results.

2. GENERAL STATEMENTS OF THE CALCULATION METHODS OF ASSOCIATION AND PHOTO DISSOCIATION CROSS-SECTIONS

Let us consider cross-section of $A+B=AB(vJM)+h\nu$. The process takes place at collision of A and B atoms and lead to the AB molecule formation in rotational-vibrational state characterized by vibrational quantum number v, angular momentum J, projection of that on quantization axis M, photon polarization ρ, and wave number k. Differential cross-section of such process is (Sobelman, 1977).

$$d\sigma_{\rho vJM}(qk) = \frac{\mu}{2\pi h}\frac{k^3}{q}\left|e_{\rho k}\int\left(\Psi_q^+\right)^* d\Psi_{vJ} dV\right|^2 d\Omega_k,$$ (1)

hq is the momentum of the relative movement of the colliding atoms, and its absolute value is caused by the emitted photon frequency

$$h\nu = \frac{h^2 q^2}{2\mu} + E_{vJ}.$$ (2)

Here μ is the reduced mass of the colliding atoms and E_{vJ} is the ro-vibrational level energy

$$E_{vJ} = -D_e + h\nu_e\left(v+\frac{1}{2}\right) - x_e h\nu_e\left(v+\frac{1}{2}\right)^2 + BJ(J+1).$$ (3)

Here, D_e is the dissociation energy of the molecule, ν_e is the main vibrational frequency, x_e is the constant of unharmonity. $d\Omega_k$ is the solid angle in which photon with momentum k is emitted, $e_{\rho k}$ is the polarization vector of the photon, d is the dipole momentum vector of the system of colliding atoms, Ψ_{vJM} is the wave function of electronic ro-vibrational molecule state, Ψ_q is the wave function which describes the atom motion in the continuum.

Now we define these functions. Functions Ψ_{vJM} in Born–Oppenheymer approximation may be presented by the sum of three wave functions:

$$\Psi_{vJM} = \Phi_{AB}(r_e)\Phi_{vJ}(r)\Psi_{JM}(\vartheta\varphi),$$ (4)

where $\Psi_{AB}(r_e)$, $\Psi_{vJ}(r)$, $\Psi_{JM}(\vartheta\varphi)$ are the electron, vibrational and rotational wave functions respectively. The electron wave function depends on the electron coordinate r_e, the vibrational wave function depends on the distance between atoms r, Ψ_{JM} is the function of polar angles which determine the direction of radius-vector r in the chosen frame of reference. Notice that rotational wave function of diatomic molecule is merely spherical harmonics $Y_{JM}(\vartheta\varphi)$. The vibrational wave function is the solution of Schroedinger equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\Phi_{vJ}(r) + \left[E_{vJ} - u(r) - \frac{J(J+1)}{r^2}\right]\Phi_{vJ}(r) = 0,$$ (5)

where $u(r)$ is the internuclear potential of the interaction in the molecule. These functions are normalized by condition :

$$\int_0^\infty \Phi_{vJ}(r)\Phi_{v'J}(r)r^2 dr = \delta_{vv'}. \tag{6}$$

Electronic wave functions are normalized by

$$\int_{r_e} |\Phi_{AB}|^2 dV = 1, \qquad \int_{r_e} |\Phi_A|^2 = 1, \qquad \int_{r_e} |\Phi_B|^2 dV = 1. \tag{7}$$

The wave function of continuous motion of colliding atoms may be presented in form (Landau and Livshits, 1963):

$$\Psi_q^+ = \Phi_A \Phi_B \frac{(2\pi)^{3/2}}{q} \sum_{\lambda\mu} i^\lambda e^{i\eta_\lambda} Y_{\lambda\mu}^*(\vartheta_q, \phi_q) Y_{\lambda\mu}(\vartheta, \phi) R_{q\lambda}(r). \tag{8}$$

In this formula $R_{q\lambda}$ is the radial wave function of free motion, which must satisfy the Schroedinger equation:

$$\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) R_{q\lambda}(r) + \left[q^2 - u(r) - \frac{\lambda(\lambda+1)}{r^2}\right] R_{q\lambda}(r) = 0, \tag{9}$$

and η_λ is the phase of this function.

Function $R_{q\lambda}$ is normalized by condition

$$\int_0^\infty R_{q\lambda}(r) R_{q'\lambda}(r) r^2 dr = \delta(q-q'), \tag{10}$$

and at large r it has the asymptotic form:

$$R_{q\lambda}(r) \to \sqrt{\frac{2}{\pi}} \frac{\sin(qr - \frac{\lambda\pi}{2} + \eta_\lambda)}{r}. \tag{11}$$

The explicit form of these functions will be presented below.

Perform now the following transformations required to calculate both differential and total cross-sections of the processes being investigated. The decomposition of the polarization and dipole momentum vectors in terms of spherical basis vectors $e_\nu (\nu = \pm 1)$ is (Varshalovich et al., 1975):

$$e_{\rho k} = \sum_\mu g_{\rho\mu} e'_\mu(\vartheta_k, \phi_k) = \sum_{\mu\nu} g_{\rho\mu} D_{\nu\mu}^1(\phi_k, \vartheta_k, 0) e_\nu, \tag{12}$$

$$d = \sum_\nu d_\nu e_\nu, \tag{13}$$

where $D_{\nu\mu}^1$ is the D-function of Wigner which defines the transformation of different quantities in cases of the coordinate system rotations and depends on the corresponding Eulerian angles (Varshalovich et al., 1975), $g_{\rho\mu}$ is the matrix defining the photon polarization state and satisfying the normalization relations

91

$$\sum_{\rho} g_{\rho\mu} g^*_{\rho\mu'} = \delta_{\mu\mu'}, \qquad \sum_{\mu} g_{\rho\mu} g^*_{\rho'\mu} = \delta_{\rho\rho'}, \tag{14}$$

d_ν is the spherical components of the dipole moment vector (this spherical components are defined in the laboratory coordinate system). It is convenient to connect them with the spherical components of the dipole moment vector defined in the molecular coordinate system. It may be done using relation:

$$d_\nu = \sum_\lambda d_\lambda(r_e) D^1_{\lambda\nu}(\alpha, \vartheta, \varphi), \tag{15}$$

where r_e are the coordinates of particles in the molecule, determined in the relative molecular coordinate system, α, ϑ, φ – are the Eulerian angles defining the turn from the laboratory coordinate system to the molecular one for the diatomic molecule under consideration. This turn may be performed merely by alignment of z axis of the laboratory coordinate system with the molecule axis. In this case one may choose the Eulerian azimuth angle α equal to zero. Since only the dipole moment component $d_z = d_0$ is nonzero for the diatomic molecule in the molecular coordinate system, one can write

$$d_\lambda(r_e) = d_0(r_e)\delta_{\lambda 0}. \tag{16}$$

Using wave functions (4), (8) and decomposition of d_ν and taking into account orthogonality of the spherical basis vectors, the expression involved into the modulus sign in (1) may be represented in form

$$S = e_{\rho k}\int \left(\Psi^+_q\right)^* d\Psi_b dV = \sum_{\mu\nu\lambda} g_{\rho\mu} D^1_{\nu\mu}(\varphi_k, \vartheta_k, 0)\frac{(2\pi)^{3/2}}{q}\sum_{lm} i^{-1} e^{-i\eta_1} Y_{lm}(\eta_q, \varphi_q),$$

$$\int_0^{2\pi}\int_0^\pi\int_0^\infty\int_e \phi^*_A \phi^*_B d_\lambda(r_e)\phi_{AB}dV_e R^*_{ql}(r)\Phi_v(r)r^2 dr D^1_{\lambda\nu}(0, \vartheta, \varphi), \tag{17}$$

$$Y^*_{lm}(\vartheta, \varphi)Y_{JM}(\vartheta, \varphi)\sin\vartheta d\vartheta d\varphi.$$

The quantity $d_\lambda(r) = \int\phi^*_A\phi^*_B d_\lambda(r_e)\phi_{AB}dV_e$ is the ro-vibrational transition momentum. This is the internuclear distance function calculated usually by the quantum chemistry methods and for the molecule under consideration it will be discussed below.

To simplify the quantity S, let us take into account the relation between $D^1_{0\nu}$ and spherical harmonics (Varshalovich et al., 1975)

$$D^1_{0\nu}(0, \vartheta, \varphi) = (-1)^\nu\sqrt{\frac{4\pi}{3}} Y^*_{1\nu}(\vartheta, \varphi) = \sqrt{\frac{4\pi}{3}} Y_{1-\nu}(\vartheta, \varphi), \tag{18}$$

and after the integration over the angular variables ϑ and φ, S may be represented as

92

$$S = \frac{4\pi^2}{q}\sqrt{\frac{2}{3}} \sum_{\mu\nu} g_{\rho\mu} D^1_{\nu\mu}(\varphi_k, \vartheta_k, 0) \sum_{1m} i^{-1} e^{-i\eta_1} Y_{1m}(\vartheta_q, \varphi_q) I_{q1vJ}^* \cdot \sqrt{\frac{3(2J+1)}{4\pi(2I+1)}} \, C^{10}_{J010} C^{1m}_{JM1-\nu}, \tag{19}$$

where the following specification is introduced

$$I_{q1vJ} = \int_0^\infty R^*_{q1}(r) d_0 \Phi_{vJ}(r) r^2 dr, \tag{20}$$

and $C^{1m}_{JM1\nu}$ is the Clebsh-Gordan coefficient.

In correspondence with the summation rule of the moments in quantum mechanics, in this expression the sum over 1 involves only two terms corresponding to $1 = J\pm1$, and the sum over m is absent because $m = M-\nu$.

To make the further rearrangement more convenient we introduce the following designations:

$$\mathfrak{M}_{J+1} = e^{-i\eta_{J+1}} \sqrt{\frac{2J+1}{2J+3}} \, C^{J+10}_{J010} \, I_{qJ+1vJ}, \tag{21}$$

$$\mathfrak{M}_{J-1} = e^{-i\eta_{J-1}} \sqrt{\frac{2J+1}{2J-1}} \, C^{J-10}_{J010} \, I_{qJ-1vJ}. \tag{22}$$

Then the photo association differential cross-section may be rewritten in form

$$d\sigma_{\rho vJM}(q,k) = (2\pi)^2 \frac{\mu}{h^2} \frac{k^3}{q^3} \cdot \left| \sum_{\mu\nu} g_{\rho\mu} D^1_{\nu\mu}(\varphi_k, \vartheta_k, 0) \cdot \right.$$

$$\left. \left[Y_{J+1,m-\nu}(\theta_q, \varphi_q) C^{J+1M-\nu}_{JM1-\nu} \mathfrak{M}_{J+1} - Y_{J-1m-\nu}(\theta_q, \varphi_q) C^{J-1M-\nu}_{JM1-\nu} \mathfrak{M}_{J-1} \right] \right|^2. \tag{23}$$

In order to obtain the total cross-section of the radiative association, it is necessary to average the available differential cross-section over the relative momentum distribution of the colliding atoms, and to perform integration over the photon momentum directions and summation over two possible orthogonal polarization directions of the photon.

To obtain the total cross-section, it is necessary also to carry out summation over M, because the states corresponding to different angular momenta of the molecule are degenerated. Using the properties of matrix $g_{\rho\mu}$ (see (14)), the rules of integration of Wigner D-functions, and summation of Clebsh-Gordan coefficients (Varshalovich et al., 1975) one can obtain the following expression for the total cross-section of radiative association which takes place with the transition from the continuum spectrum of the ground electronic state to ro-vibrational state characterized by quantum numbers v and J.

$$\sigma_{vJ}(q,k) = \frac{8\pi^2}{3} \frac{\mu}{h^2} \frac{k^3}{q^3} \left\{ \frac{J+1}{2J+3} \left| I_{qJ+1vJ} \right|^2 + \frac{J}{2J-1} \left| I_{qJ-1vJ} \right|^2 \right\}. \tag{24}$$

The dependence of quantities I_{qJvJ} on the rotational quantum number is involved into expression due to parameters of the radial ro-vibrational functions Φ_{vJ}. This dependence, however, is very weak because the rotational energy is only a little addition to the vibrational one. That is why, if we are interested in the results, the errors of which are within 5-10% (this is sufficient for the astrophysical applications), this dependence in the quantities I_{qJvJ} may be neglected and hence one can believe that they are dependent on vibrational quantum numbers alone. In this case the expression (24) can be simplified and

$$\sigma_{vJ}(q,k) = \frac{8\pi^2}{3}\frac{\mu}{h^2}\frac{k^3}{q^3} Q_J |I_{qv}|^2, \tag{25}$$

where

$$Q_J = \frac{4J^2+4J+2}{(2J+1)(2J-1)}. \tag{26}$$

It should be noted that for high quantum numbers J $Q_J \approx (1+\frac{3}{4J^2})$, thus, even for small values of J we have $Q_J \approx 1$.

Further we will take $Q_J = 1$, for it is easy to correct for this factor in the final result.

Thus in order to calculate the total radiative association cross-section of the process under consideration the quantities I_{qv} must be calculated.

For this aim it is necessary to have the wave functions of both discrete and continuous vibrational spectra relating to one electronic state of the molecule, and also the dependence of the dipole momentum on the internuclear distance.

In their turn the wave functions, as mentioned above, may be defined as solutions of the Shroedinger equation with the potential corresponding to the potential interaction energy of atoms in the molecule.

It is well known that the curve of the potential function of the diatomic molecule may be approximated by different types of potential functions. In our calculations the Pöshle-Teller potential function is used to approximate the molecular one.

The one-dimensional Schroedinger equation with the Pöshle-Teller potential

$$V(R_e) = D_e \left[\frac{sh^4(\alpha r_e)}{sh^2(\alpha r)} - \frac{ch^4(\alpha r_e)}{ch^2(\alpha r)} \right], \tag{27}$$

(where r_e is the equilibrium internuclear distance and α is a constant) has normalized solutions for the discrete and continuum spectra in form:

$$\Psi_v(r) = N_v z^{(2\gamma-1)/4}(1-z)^{(a-\gamma)/2-v}F(-v, a-v, \gamma; z), \tag{28}$$

$$\Psi_q(r) = C_q z^{(2\gamma-1)/4}(1-z)^{iq/2\alpha}F\left(\frac{a+\gamma}{2} + \frac{iq}{2\alpha}, \frac{\gamma-a}{2} + \frac{iq}{2\alpha}; \gamma; z\right).$$

Here $F(a,b;c;z)$ is hypergeometric function of $z = th^2(\alpha r)$,

$$N_v = \frac{1}{\Gamma(\gamma)}\left[\frac{2\alpha(a-\gamma-2v)}{v!}\frac{\Gamma(a-v)\Gamma(\gamma+v)}{\Gamma(a-\gamma-v+1)}\right]^{\frac{1}{2}},$$

$$C_q = \frac{1}{\sqrt{2\pi}\Gamma(\gamma)}\left|\frac{\Gamma\left(\frac{a+\gamma}{2}+\frac{iq}{2\alpha}\right)\Gamma\left(\frac{\gamma-a}{2}+\frac{iq}{2\alpha}\right)}{\Gamma\left(\frac{iq}{2\alpha}\right)}\right|, \tag{29}$$

where $\Gamma(x)$ is gamma-function, and parameters a and γ are defined by expressions

$$a=\left[\frac{1}{4}+\frac{2MD_e}{h^2\alpha^2}ch^4(\alpha r_e)\right]^{\frac{1}{2}}, \quad \gamma=1+\left[\frac{1}{4}+\frac{2MD_e}{h^2\alpha^2}sh^4(\alpha r_e)\right]^{\frac{1}{2}}. \tag{30}$$

In order to calculate the dipole moment matrix element the explicit form of the function $d(r)$ must be given. This function may be expanded into Burman-Lagrange series:

$$d(R)=\sum_{r=0}^{\infty}d_r'w^r=\sum_{r=0}^{\infty}d_r'\beta^r(th^2(\alpha r)-th^2(\alpha r_e))^r, \tag{31}$$

where $\beta = ch^4(\alpha r_e)/(\alpha\, sh(2\alpha r_e))$. In this case the matrix element is calculated analytically (Khersonskij, 1977), and we obtain the next result:

$$I_{qv}=\frac{1}{\alpha}\left[\frac{a-\gamma-2v}{v!}\frac{\Gamma(a-\gamma-v+1)}{\Gamma(a-\gamma)\Gamma(\gamma+v)}\right]^{\frac{1}{2}}\varphi_{a\gamma}(q)S_{a\gamma}^v(q), \tag{32}$$

$$\varphi_{a\gamma}(q)=\left\{\frac{qsh(\pi q/\alpha)}{[(a-\gamma)^2+q^2/a^2][\sin^2(\pi(a-\gamma)/2)+sh^2(\pi q/2\alpha)]}\right\}^{\frac{1}{2}}\times$$

$$\times\left|\Gamma\left(\frac{a+\gamma}{2}+\frac{iq}{2\alpha}\right)\Gamma\left(\frac{\gamma-a}{2}+\frac{iq}{2\alpha}\right)\right|, \tag{33}$$

$$S_{a\gamma}^v(q)=\sum_{r=1}^{\infty}\sum_{s=1}^{r}\eta_{rs}\sum_{\lambda=1}^{s-1}(-1)^{\lambda+1}\left(\frac{v}{\lambda+v-s+1}\right)\frac{\Gamma(a+\lambda-s+1)}{\Gamma(a+\lambda+1)\lambda!}\frac{4^{-(\lambda+1)}}{\Gamma(a-\gamma-v+\lambda-s+2)}\times$$

$$\times\prod_{\sigma=0}^{\lambda}[(a-\gamma+2\sigma)^2+q^2/\alpha^2], \tag{34}$$

$$\eta_{rs}=d_r'\beta^r\left(\frac{r}{s}\right)[1-th^2(\alpha r_e)^{r-s}]. \tag{35}$$

If we restrict series (31) by "p" members we have to substitute in (34) the upper limit of the sum over r by p. In this case the obtained expression does not contain the infinite sum and becomes convenient for calculations. Besides that for a great number of molecules the quantities $a-\gamma$ and $a+\gamma$ are large enough, and hence the modu-

lus of the product of Γ-functions entered into $\varphi_{a\gamma}(q)$ may be changed by factor

$$\Gamma\left(\frac{a+\gamma}{2}\right)\Gamma\left(\frac{a-\gamma}{2}\right)\left\{\frac{(a^2-\gamma^2)^2+2(a^2+\gamma^2)q^2/\alpha^2+q^4/\alpha^4}{(a^2-\gamma^2)^2}\right\}^{\frac{a-1}{4}} \times \qquad (36)$$

$$\times\left\{\left(\frac{a-\gamma}{a+\gamma}\right)^2\frac{(a+\gamma)^2+q^2/\alpha^2}{(a-\gamma)^2+q^2/\alpha^2}\right\}^{\frac{\gamma}{4}}\exp\left\{-\frac{q}{2\alpha}\arccos\left[\frac{a^2-\gamma^2-q^2/\alpha^2}{\sqrt{(a^2-\gamma^2)^2+2(a^2+\gamma^2)q^2/\alpha^2+q^4/\alpha^4}}\right]\right\}.$$

The cross-section of the inverse process, photo dissociation, can be obtained using the derived results on the radiative association cross-section by Milne relationship:

$$\sigma^d(k)=2\left(\frac{q}{k}\right)^2\sigma^a(q). \qquad (37)$$

3. RESULTS OF NUMERICAL CALCULATIONS

The potential curve for the LiH molecule has been calculated in a number of works (Stwalley et al., 1977) and is shown in Fig. 1. Here the straight lines show the location of the discrete vibrational levels, the arrows indicate the free-bound (radiative association) and bound-free (photo dissociation) transitions.
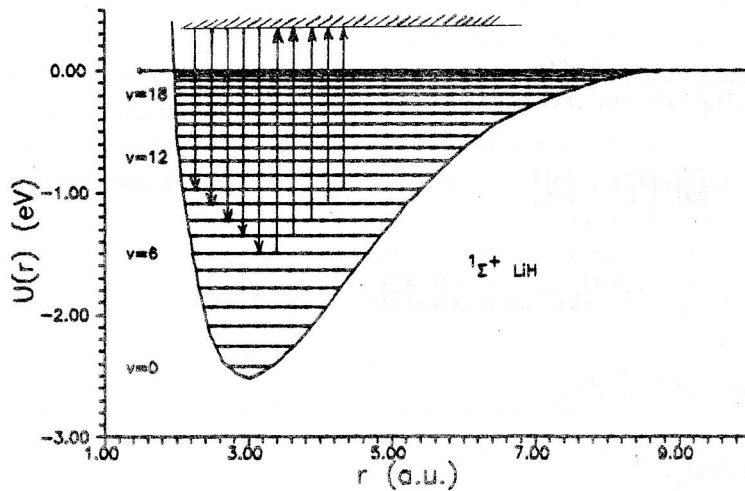

Fig. 1. *A scheme of the free-bound vibrational transitions within the ground* $^1\Sigma^+$ *electron state of LiH molecule. The potential curve is taken from Stwalley et al. (1977).*

As it was mentioned above one can approximate this potential function by the

Pöshle-Teller one. For this aim it is necessary to set three quantities: the dissociation energy D_e, internuclear distance r_e, and quantity α defining curvature of the potential function.

It should be noted that the parameters of the potential, selected by using the approximation curve formed within a predetermined range of the internuclear distance, are not sufficiently good to be applied to the other region. In other words, in spite of the good agreement of the true potential and Pöshle-Teller one, in order to describe correctly the energy spectrum of the vibrational state for low, medium and high vibrational quantum numbers we have to use several different approximations.

The summary of the Pöshle-Teller potential parameters for the corresponding regions of the vibrational quantum number variations is given in Table 1. The suggested values allow us to make further calculations of cross-sections under the conditions of the known functional dependence of the dipole momentum on the internuclear distance. The calculations of this function were carried out by Zemke and Stwalley (1980), and the results are presented in Fig. 2. In order to make calculations analytically in correspondence with the technique suggested in Section 2, we approximate this function by the following polynomials: $d(z) = d_0 + a(z-z_e) + b(z-z_e)^2 - c(z-z_e)^9$ (all these approximations are shown in Fig. 2). They were made so that the dipole moment function behaviour should be represented correctly in the internuclear distance region which is most important in the calculation of the integral I_{qv} corresponding to the defined values of the quantum number v. For instance, for low values of the quantum number the region of internuclear distance R=(2.25-4.5) is most significant, therefore in this region we use the approximation polynomial with coefficients given in the first column of Table 1. As quantum number values will increase the range in the region of the large values of r must be taken into account.

Table 1. Pöshle-Teller potential parameters and coefficients of the polynomial approximating the function of the dipole momentum of LiH molecule for different vibrational levels.

$v=$	0÷5	6÷11	12÷17	18÷24
α_e	0.31	0.329	0.36	0.403
D_e	2.515	2.65	2.89	3.245
r_e	3.015	2.99	2.96	2.925
a	4.0	4.6	5.33	6.2
b	7.7	7.75	7.79	7.7
c	2.8×10^3	8.5×10^3	3.7×10^4	3×10^5

The derived approximations allow to make complete calculations of the radiative association and photo dissociation cross-sections.
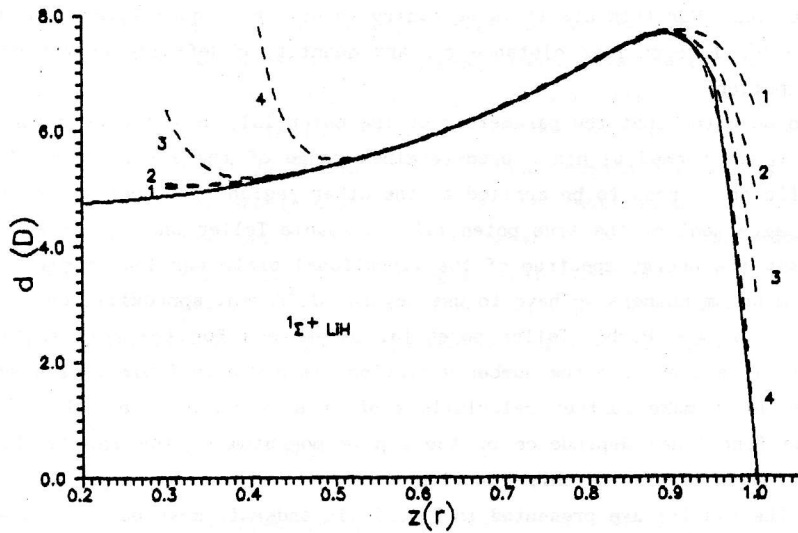
Fig. 2. *Approximation of the dipole momentum function of LiH molecule in the ground* $^1\Sigma^+$ *electron state at different intervals of internuclear distances. The dipole momentum function is taken from Zemke and Stwalley (1980).*

Now we proceed to a discussion of calculation results. The results of calculations of partial radiative photo association cross-sections as a function of relative velocities of the colliding atoms in the region $v = 10^3- 10^7$ cm/s are given in Table 2 and presented partly in Fig 3. Analysis of the data reveals the following important features of behaviour of the cross-section under investigation.

Fig. 3. *The depen-dence of radiative association cross-section of LiH mo-lecule (free-bound transitions in* $^1\Sigma^+$ *electron state) on velocity of atoms for different vib-rational states.*

98

Table 2. Logarithm of photoassociation cross-section
of LiH molecule (cm^2)

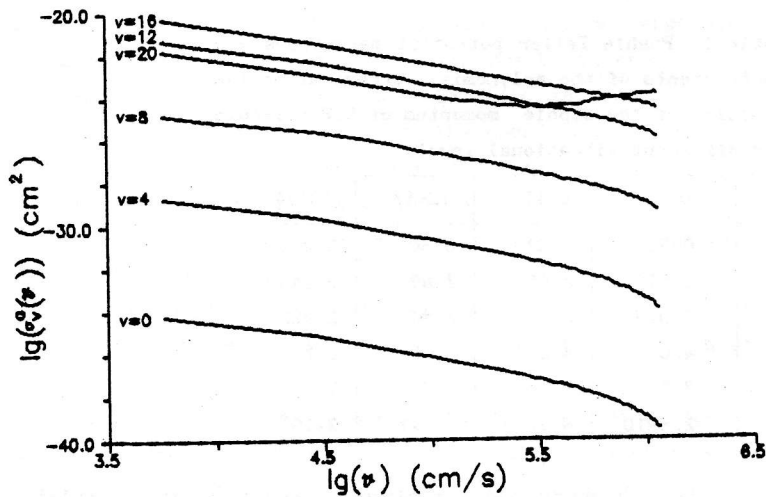| Lg(ω) (cm/s)	v=0	v=1	v=2	v=3	v=4	v=5
3.4	-33.858	-32.144	-30.724	-29.479	-28.363	-27.352
3.5	-33.970	-32.257	-30.837	-29.593	-28.477	-27.467
3.6	-34.061	-32.348	-30.930	-29.686	-28.571	-27.562
3.7	-34.164	-32.450	-31.030	-29.785	-28.668	-27.657
3.8	-34.270	-32.556	-31.137	-29.892	-28.777	-27.767
3.9	-34.372	-32.657	-31.236	-29.991	-28.874	-27.862
4.0	-34.491	-32.778	-31.358	-30.113	-28.998	-27.988
4.1	-34.602	-32.888	-31.467	-30.222	-29.105	-28.094
4.2	-34.730	-33.016	-31.597	-30.352	-29.237	-28.226
4.3	-34.871	-33.158	-31.738	-30.494	-29.378	-28.368
4.4	-35.013	-33.299	-31.878	-30.633	-29.517	-28.506
4.5	-35.178	-33.465	-32.046	-30.803	-29.688	-28.678
4.6	-35.350	-33.637	-32.217	-30.970	-29.853	-28.843
4.7	-35.539	-33.826	-32.407	-31.163	-30.047	-29.037
4.8	-35.725	-34.010	-32.590	-31.344	-30.227	-29.215
4.9	-35.921	-34.207	-32.787	-31.542	-30.426	-29.415
5.0	-36.132	-34.418	-32.998	-31.753	-30.636	-29.625
5.1	-36.335	-34.620	-33.200	-31.955	-30.839	-29.829
5.2	-36.538	-34.824	-33.404	-32.159	-31.043	-30.032
5.3	-36.760	-35.045	-33.624	-32.378	-31.261	-30.249
5.4	-36.975	-35.260	-33.839	-32.594	-31.478	-30.466
5.5	-37.205	-35.489	-34.068	-32.822	-31.704	-30.692
5.6	-37.457	-35.740	-34.318	-33.071	-31.953	-30.940
5.7	-37.740	-36.021	-34.597	-33.348	-32.228	-31.213
5.8	-38.077	-36.354	-34.927	-33.675	-32.553	-31.535
5.9	-38.475	-36.746	-35.314	-34.059	-32.933	-31.912
6.0	-39.059	-37.319	-35.878	-34.615	-33.482	-32.454
6.1	-39.887	-38.129	-36.673	-35.397	-34.253	-33.214
6.2	-41.178	-39.394	-37:917	-36.623	-35.461	-34.406

Table 2 (continued). Logarithm of photoassociation cross-section
of LiH molecule (cm^2)

Lg(ω)	v=6	v=7	v=8	v=9	v=10	v=11
3.4	-25.922	-25.149	-24.412	-23.741	-23.195	-22.594
3.5	-26.018	-25.245	-24.506	-23.838	-23.285	-22.684
3.6	-26.110	-25.335	-24.596	-23.924	-23.374	-22.774
3.7	-26.222	-25.450	-24.713	-24.042	-23.495	-22.896
3.8	-26.318	-25.543	-24.804	-24.132	-23.583	-22.983
3.9	-26.430	-25.658	-24.921	-24.250	-23.705	-23.104
4.0	-26.529	-25.755	-25.016	-24.344	-23.794	-23.194
4.1	-26.639	-25.864	-25.125	-24.454	-23.905	-23.304
4.2	-26.770	-25.999	-25.262	-24.591	-24.045	-23.444
4.3	-26.883	-26.109	-25.369	-24.697	-24.147	-23.547
4.4	-27.013	-26.240	-25.501	-24.830	-24.281	-23.681
4.5	-27.165	-26.391	-25.653	-24.982	-24.433	-23.833
4.6	-27.321	-26.548	-25.809	-25.137	-24.589	-23.988
4.7	-27.514	-26.743	-26.006	-25.336	-24.790	-24.190
4.8	-27.691	-26.919	-26.182	-25.512	-24.965	-24.366
4.9	-27.870	-27.096	-26.356	-25.684	-25.133	-24.532

Table 2 (continued). Logarithm of photoassociation cross-section of LiH molecule (cm^2)

Lg(ω)	v=6	v=7	v=8	v=9	v=10	v=11
5.0	-28.084	-27.310	-26.572	-25.901	-25.352	-24.752
5.1	-28.286	-27.513	-26.774	-26.103	-25.554	-24.954
5.2	-28.470	-27.694	-26.955	-26.283	-25.731	-25.133
5.3	-28.687	-27.910	-27.171	-26.499	-25.946	-25.348
5.4	-28.891	-28.114	-27.375	-26.702	-26.148	-25.550
5.5	-29.107	-28.329	-27.592	-26.920	-26.365	-25.769
5.6	-29.332	-28.553	-27.815	-27.144	-26.586	-25.992
5.7	-29.560	-28.775	-28.036	-27.363	-26.796	-26.205
5.8	-29.832	-29.043	-28.304	-27.631	-27.056	-26.470
5.9	-30.125	-29.328	-28.586	-27.909	-27.322	-26.739
6.0	-30.545	-29.736	-28.987	-28.303	-27.700	-27.117
6.1	-31.142	-30.318	-29.560	-28.865	-28.242	-27.655
6.2	-32.133	-31.292	-30.518	-29.809	-29.165	-28.568

Table 2 (continued). Logarithm of photoassociation cross-section of LiH molecule (cm^2)

Lg(ω)	v=12	v=13	v=14	v=15	v=16	v=17
3.4	-20.873	-20.497	-20.214	-20.057	-19.956	-19.994
3.5	-20.972	-20.596	-20.312	-20.154	-20.052	-20.088
3.6	-21.076	-20.701	-20.417	-20.259	-20.158	-20.195
3.7	-21.182	-20.807	-20.523	-20.366	-20.265	-20.302
3.8	-21.300	-20.924	-20.641	-20.483	-20.382	-20.419
3.9	-21.404	-21.029	-20.745	-20.587	-20.486	-20.523
4.0	-21.541	-21.166	-20.882	-20.725	-20.624	-20.662
4.1	-21.692	-21.317	-21.034	-20.877	-20.777	-20.817
4.2	-21.813	-21.437	-21.152	-20.994	-20.891	-20.927
4.3	-22.004	-21.629	-21.345	-21.188	-21.087	-21.125
4.4	-22.169	-21.794	-21.510	-21.351	-21.250	-21.286
4.5	-22.364	-21.988	-21.705	-21.546	-21.444	-21.481
4.6	-22.566	-22.191	-21.907	-21.748	-21.646	-21.682
4.7	-22.785	-22.409	-22.124	-21.966	-21.863	-21.899
4.8	-22.996	-22.620	-22.335	-22.177	-22.075	-22.111
4.9	-23.185	-22.810	-22.525	-22.367	-22.264	-22.299
5.0	-23.382	-23.007	-22.722	-22.562	-22.458	-22.491
5.1	-23.595	-23.220	-22.933	-22.772	-22.668	-22.698
5.2	-23.808	-23.430	-23.144	-22.982	-22.875	-22.905
5.3	-24.002	-23.624	-23.335	-23.169	-23.057	-23.079
5.4	-24.194	-23.814	-23.522	-23.351	-23.233	-23.244
5.5	-24.396	-24.014	-23.718	-23.540	-23.413	-23.412
5.6	-24.617	-24.231	-23.929	-23.741	-23.602	-23.583
5.7	-24.827	-24.437	-24.127	-23.925	-23.768	-23.724
5.8	-25.072	-24.675	-24.353	-24.132	-23.953	-23.877
5.9	-25.332	-24.928	-24.592	-24.346	-24.140	-24.026
6.0	-25.649	-25.235	-24.885	-24.612	-24.378	-24.224
6.1	-26.088	-25.664	-25.297	-24.995	-24.734	-24.540
6.2	-26.770	-26.333	-25.949	-25.621	-25.335	-25.106

Table 2 (continued). Logarithm of photoassociation cross-section
of LiH molecule (cm^2).

Lg(ω)	v=18	v=19	v=20	v=21	v=22	v=23
3.4	-20.196	-20.739	-21.297	-22.063	-23.237	-25.483
3.5	-20.299	-20.843	-21.401	-22.167	-23.341	-25.587
3.6	-20.423	-20.972	-21.532	-22.298	-23.473	-25.715
3.7	-20.552	-21.106	-21.667	-22.433	-23.605	-25.845
3.8	-20.693	-21.253	-21.816	-22.582	-23.754	-25.988
3.9	-20.813	-21.373	-21.938	-22.704	-23.874	-26.107
4.0	-20.957	-21.517	-22.081	-22.847	-24.017	-26.245
4.1	-21.075	-21.626	-22.186	-22.952	-24.122	-26.346
4.2	-21.238	-21.790	-22.350	-23.115	-24.284	-26.497
4.3	-21.477	-22.041	-22.605	-23.369	-24.533	-26.723
4.4	-21.649	-22.205	-22.767	-23.529	-24.690	-26.857
4.5	-21.855	-22.409	-22.968	-23.728	-24.883	-27.010
4.6	-22.097	-22.659	-23.220	-23.976	-25.119	-27.183
4.7	-22.265	-22.811	-23.364	-24.114	-25.244	-27.227
4.8	-22.488	-23.036	-23.587	-24.330	-25.434	-27.295
4.9	-22.696	-23.243	-23.788	-24.519	-25.587	-27.291
5.0	-22.890	-23.438	-23.976	-24.687	-25.703	-27.219
5.1	-23.063	-23.590	-24.111	-24.792	-25.734	-27.031
5.2	-23.259	-23.778	-24.279	-24.918	-25.767	-26.843
5.3	-23.408	-23.904	-24.373	-24.956	-25.691	-26.558
5.4	-23.573	-24.043	-24.470	-24.980	-25.587	-26.271
5.5	-23.682	-24.107	-24.478	-24.905	-25.389	-25.932
5.6	-23.769	-24.139	-24.443	-24.781	-25.155	-25.594
5.7	-23.816	-24.124	-24.360	-24.603	-24.897	-25.266
5.8	-23.829	-24.057	-24.220	-24.402	-24.620	-24.945
5.9	-23.816	-23.962	-24.060	-24.185	-24.358	-24.660
6.0	-23.804	-23.873	-23.919	-24.003	-24.147	-24.441
6.1	-23.843	-23.841	-23.847	-23.901	-24.030	-24.322
6.2	-24.092	-24.039	-24.016	-24.051	-24.168	-24.462

First of all there is a strong dependence of the cross-section on the vibrational
quantum number v. In the region of low vibrational quantum numbers the growth of v
leads to increase in the photo association cross-section by several orders of magni-
tude (see curves $v = 0, 4, 8, 12$ in Fig.3), however, there is a range of vibrational
quantum numbers in which the partial cross-sections have maximum, and further in-
crease of v will result again in a decrease of partial cross sections. It must be
stressed that similar dependences of partial cross-section on the vibrational quantum
number have been noted in a number of works (see for example Khersonskij, 1977). On
the whole it is due to the fact that the bound molecule can be formed easier out of
atoms in such quantum states which correspond to the larger vibrational amplitude.
For quantum number values near the dissociation threshold the connection between dis-
crete vibrational states and the continuum ones is very strong therefore the photo
association cross-section decreases for these vibrational quantum numbers. Hence the
region of vibrational quantum numbers, for which the partial cross-sections are lar-
gest, is clearly expressed and for the LiH molecule being investigated this region
includes quantum numbers $v = (15-17)$.

The dependence of cross-section on velocity of the colliding particles on the

whole tends to decrease, which is always characteristic of cross-section of this kind of processes, because the particles which have the large velocities of relative motion spend relatively little time within the integration region. However, as one can see from Fig.3, for the partial cross-sections of radiative association into high vibrational levels this dependence is somewhat violated, which is connected with the peculiarity of behaviour of the dipole momentum function. The matter is that this is the region of internuclear distances, where the dipole momentum function has a large derivative value, that yields the main contribution into the matrix element of the dipole momentum (corresponding to the free-bound transition) for high vibrational levels.

Thus, if atoms interacting at large velocities spend longer time at large distances, this region (due to the above mentioned circumstance) enhances the matrix element value and hence the cross-section on the whole. It must be added that with further growth of velocity the cross-sections values will decrease.

The results of the calculations of partial photo dissociation cross-sections as a function of wavelength of incident photons in the region $\lambda = 10^{-2} - 5.10^{-5}$ cm are given in Table 3 and Fig. 4. As it was noted above, these data have been obtained by the use of the Milne relationship and radiative association cross-sections. The presented results show the following important peculiarities which partly repeat similar features in the behaviour of the radiative association cross-sections.
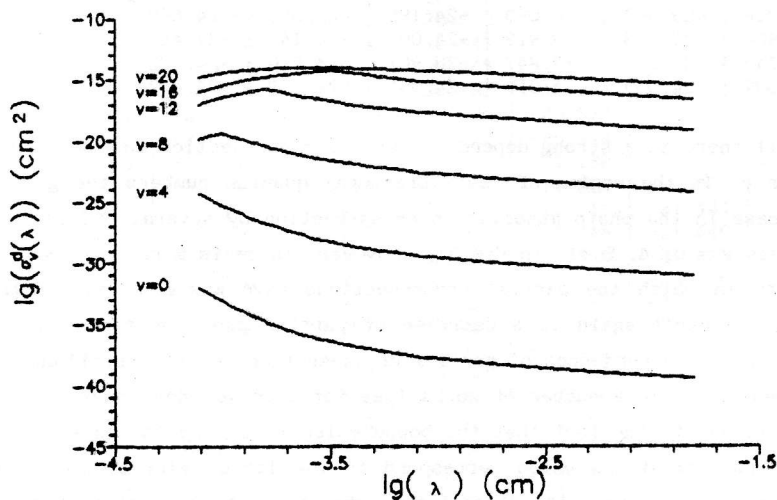

Fig. 4. *The dependence of photodissociation of LiH molecule (bound-free transitions in $^1\Sigma^+$ electron state) on wavelength of photons.*

102

Table 3. Logarithm of photodissociation cross-section of LiH molecule (cm^2).

Lg(λ) (cm)	v = 0	v = 1	v = 2	v = 3	v = 4	v = 5
-1.5	-39.752	-37.269	-35.132	-33.216	-31.467	-29.859
-1.6	-39.647	-37.165	-35.027	-33.111	-31.363	-29.755
-1.7	-39.541	-37.058	-34.921	-33.005	-31.257	-29.649
-1.8	-39.435	-36.953	-34.816	-32.900	-31.152	-29.544
-1.9	-39.328	-36.846	-34.709	-32.793	-31.045	-29.437
-2.0	-39.219	-36.737	-34.600	-32.684	-30.937	-29.329
-2.1	-39.108	-36.626	-34.490	-32.574	-30.826	-29.219
-2.2	-38.990	-36.509	-34.373	-32.457	-30.710	-29.102
-2.3	-38.877	-36.395	-34.260	-32.344	-30.597	-28.990
-2.4	-38.753	-36.272	-34.137	-32.221	-30.475	-28.869
-2.5	-38.626	-36.145	-34.010	-32.095	-30.349	-28.743
-2.6	-38.492	-36.011	-33.877	-31.963	-30.217	-28.612
-2.7	-38.347	-35.867	-33.733	-31.820	-30.075	-28.470
-2.7	-38.191	-35.712	-33.579	-31.667	-29.923	-28.319
-2.8	-38.190	-35.711	-33.578	-31.666	-29.924	-28.318
-2.9	-38.020	-35.543	-33.411	-31.500	-29.757	-28.155
-3.0	-37.832	-35.356	-33.225	-31.315	-29.574	-27.974
-3.1	-37.621	-35.147	-33.018	-31.110	-29.371	-27.772
-3.2	-37.382	-34.910	-32.784	-30.878	-29.142	-27.546
-3.3	-37.109	-34.640	-32.516	-30.614	-28.882	-27.289
-3.4	-36.788	-34.322	-32.203	-30.306	-28.577	-26.989
-3.5	-36.411	-33.951	-31.838	-29.946	-28.223	-26.641
-3.6	-35.971	-33.517	-31.411	-29.526	-27.812	-26.237
-3.7	-35.438	-32.994	-30.898	-29.024	-27.319	-25.755
-3.8	-34.799	-32.368	-30.286	-28.426	-26.737	-25.188
-3.9	-34.040	-31.628	-29.565	-27.726	-26.058	-24.526
-4.0	-33.120	-30.737	-28.703	-26.894	-25.254	-23.750
-4.1	-32.036	-29.696	-27.707	-25.936	-24.329	-22.841
-4.2	-30.794	-28.520	-26.586	-25.048	-24.200	-23.455
-4.3	-29.639	-28.254	-27.157	-26.232	-25.435	-24.733
-4.3	-31.208	-29.878	-28.838	-27.965	-27.212	-26.549
-4.4	-31.235	-29.902	-28.863	-27.990	-27.237	-26.575

Table 3 (continued). Logarithm of photodissociation cross-section of LiH molecule (cm^2).

Lg(λ)	v = 6	v = 7	v = 8	v = 9	v=10	v=11
-1.5	-27.010	-25.712	-24.512	-23.402	-22.390	-21.444
-1.6	-26.907	-25.608	-24.409	-23.299	-22.283	-21.339
-1.7	-26.804	-25.505	-24.304	-23.196	-22.182	-21.236
-1.8	-26.699	-25.400	-24.199	-23.092	-22.076	-21.128
-1.9	-26.594	-25.296	-24.096	-22.988	-21.973	-21.025
-2.0	-26.487	-25.188	-23.989	-22.883	-21.866	-20.919
-2.1	-26.380	-25.082	-23.882	-22.775	-21.758	-20.814
-2.2	-26.268	-24.972	-23.775	-22.662	-21.649	-20.703
-2.3	-26.155	-24.858	-23.658	-22.551	-21.536	-20.602
-2.4	-26.038	-24.741	-23.542	-22.435	-21.425	-20.477
-2.5	-25.915	-24.619	-23.422	-22.316	-21.303	-20.356
-2.6	-25.790	-24.495	-23.297	-22.191	-21.181	-20.232
-2.7	-25.657	-24.361	-23.164	-22.062	-21.048	-20.102
-2.8	-25.513	-24.221	-23.025	-21.922	-20.911	-19.968
-2.9	-25.359	-24.068	-22.873	-21.771	-20.764	-19.824

Table 3 (continued). Logarithm of photodissociation cross-section of LiH molecule (cm^2).

Lg(λ)	v = 6	v = 7	v = 8	v = 9	v=10	v=11
-3.0	-25.194	-23.903	-22.712	-21.610	-20.603	-19.662
-3.1	-25.009	-23.722	-22.531	-21.433	-20.435	-19.489
-3.2	-24.806	-23.520	-22.335	-21.240	-20.240	-19.296
-3.3	-24.576	-23.296	-22.113	-21.023	-20.023	-19.092
-3.4	-24.312	-23.038	-21.859	-20.769	-19.785	-18.848
-3.5	-24.009	-22.741	-21.573	-20.494	-19.510	-18.574
-3.6	-23.663	-22.406	-21.243	-20.169	-19.197	-18.273
-3.7	-23.257	-22.013	-20.860	-19.803	-18.841	-17.907
-3.8	-22.786	-21.559	-20.428	-19.383	-18.428	-17.479
-3.9	-22.252	-21.054	-19.943	-18.916	-17.981	-17.430
-4.0	-21.653	-20.486	-19.438	-18.803	-18.331	-17.852
-4.1	-21.128	-20.465	-19.862	-19.317	-18.868	-18.439
-4.2	-21.746	-21.132	-20.586	-20.097	-19.673	-19.283
-4.3	-22.757	-22.196	-21.692	-21.245	-20.846	-20.487
-4.4	-24.292	-23.769	-23.298	-22.878	-22.502	-22.167

Table 3 (continued). Logarithm of photodissociation cross-section of LiH molecule (cm^2).

Lg(λ)	v=12	v=13	v=14	v=15	v=16	v=17
-1.5	-19.515	-18.774	-18.111	-17.536	-17.003	-16.569
-1.6	-19.415	-18.679	-18.011	-17.431	-16.907	-16.488
-1.7	-19.307	-18.573	-17.908	-17.332	-16.812	-16.384
-1.8	-19.204	-18.469	-17.813	-17.233	-16.703	-16.257
-1.9	-19.103	-18.373	-17.704	-17.114	-16.591	-16.158
-2.0	-18.999	-18.270	-17.603	-17.019	-16.477	-16.068
-2.1	-18.892	-18.152	-17.492	-16.905	-16.376	-15.945
-2.2	-18.786	-18.048	-17.385	-16.803	-16.279	-15.845
-2.3	-18.676	-17.936	-17.273	-16.689	-16.165	-15.737
-2.4	-18.560	-17.829	-17.161	-16.576	-16.046	-15.633
-2.5	-18.441	-17.712	-17.052	-16.467	-15.930	-15.501
-2.6	-18.324	-17.592	-16.923	-16.343	-15.806	-15.388
-2.7	-18.200	-17.478	-16.801	-16.215	-15.689	-15.277
-2.8	-18.073	-17.342	-16.669	-16.097	-15.558	-15.141
-2.9	-17.933	-17.209	-16.536	-15.942	-15.407	-14.983
-3.0	-17.784	-17.058	-16.392	-15.797	-15.264	-14.822
-3.1	-17.626	-16.889	-16.220	-15.627	-15.101	-14.682
-3.2	-17.458	-16.714	-16.043	-15.451	-14.908	-14.483
-3.3	-17.269	-16.523	-15.838	-15.253	-14.699	-14.260
-3.4	-17.051	-16.300	-15.605	-15.007	-14.450	-14.111
-3.5	-16.805	-16.039	-15.341	-14.735	-14.282	-14.199
-3.6	-16.508	-15.726	-15.015	-14.557	-14.404	-14.272
-3.7	-16.169	-15.366	-14.967	-14.753	-14.569	-14.444
-3.8	-15.839	-15.486	-15.218	-15.011	-14.794	-14.670
-3.9	-16.118	-15.793	-15.509	-15.278	-15.079	-14.942
-4.0	-16.496	-16.164	-15.898	-15.671	-15.475	-15.330
-4.1	-16.988	-16.678	-16.407	-16.189	-16.004	-15.859
-4.2	-17.652	-17.360	-17.111	-16.898	-16.722	-16.581
-4.3	-18.589	-18.317	-18.080	-17.880	-17.710	-17.575
-4.4	-19.894	-19.636	-19.415	-19.225	-19.065	-18.936

Table 3 (continued). Logarithm of photodissociation cross-section of LiH molecule (cm^2).

Lg(λ)	v=18	v=19	v=20	v=21	v=22	v=23
-1.5	-15.975	-15.929	-15.847	-15.799	-15.849	-16.000
-1.6	-15.870	-15.835	-15.771	-15.677	-15.730	-15.915
-1.7	-15.776	-15.727	-15.629	-15.637	-15.634	-15.786
-1.8	-15.657	-15.614	-15.517	-15.535	-15.559	-15.688
-1.9	-15.598	-15.494	-15.425	-15.380	-15.380	-15.623
-2.0	-15.481	-15.448	-15.337	-15.285	-15.315	-15.509
-2.1	-15.360	-15.298	-15.199	-15.212	-15.238	-15.434
-2.2	-15.249	-15.226	-15.082	-15.109	-15.080	-15.328
-2.3	-15.140	-15.104	-15.051	-15.035	-15.042	-15.242
-2.4	-14.998	-14.970	-14.964	-14.836	-14.948	-15.106
-2.5	-14.919	-14.904	-14.803	-14.767	-14.835	-14.993
-2.6	-14.814	-14.844	-14.699	-14.660	-14.742	-14.938
-2.7	-14.732	-14.663	-14.609	-14.599	-14.646	-14.844
-2.8	-14.600	-14.567	-14.500	-14.510	-14.565	-14.779
-2.9	-14.479	-14.529	-14.371	-14.380	-14.501	-14.713
-3.0	-14.318	-14.345	-14.384	-14.346	-14.361	-14.616
-3.1	-14.184	-14.283	-14.228	-14.241	-14.330	-14.551
-3.2	-14.079	-14.182	-14.139	-14.169	-14.253	-14.498
-3.3	-14.013	-14.099	-14.129	-14.131	-14.236	-14.442
-3.4	-14.020	-14.040	-14.047	-14.076	-14.173	-14.402
-3.5	-13.994	-14.023	-14.030	-14.061	-14.127	-14.384
-3.6	-13.996	-14.026	-14.007	-14.031	-14.135	-14.401
-3.7	-14.022	-14.063	-14.011	-14.054	-14.164	-14.451
-3.8	-14.130	-14.118	-14.090	-14.132	-14.240	-14.535
-3.9	-14.268	-14.248	-14.226	-14.255	-14.391	-14.669
-4.0	-14.490	-14.458	-14.444	-14.486	-14.614	-14.905
-4.1	-14.823	-14.783	-14.775	-14.825	-14.951	-15.256
-4.2	-15.299	-15.262	-15.260	-15.310	-15.443	-15.749
-4.3	-15.983	-15.947	-15.949	-16.004	-16.140	-16.446
-4.4	-16.948	-16.915	-16.917	-16.974	-17.116	-17.426

First of all there is a strong dependence of the cross-section on the vibrational quantum number v; when v grows the cross-sections increase by several orders of magnitude. Physically this corresponds to the fact that the molecule in the high vibrational state (i.e. the molecule having large vibrational amplitude) can easily be destroyed by even small additional energy imparted to it. Low vibrational states are considerably more stable, and require substantial energies to destroy the molecule.

As the wavelength of the photon grows the cross-section of photo dissociation decreases. Naturally, it is associated with the reduced capability of low energy photon to destroy the molecule. The cross-section tends to zero as the photon frequency approaches the threshold frequency $\nu_{th} = (D_e - E_v)/h$. If $\nu \gg \nu_{th}$ the cross-section decreases too; it was already noted in the previous papers (see for example Khersonskij, 1977). Thus in some region of wavelengths the partial cross-sections have maxima which can distinctly be seen for quantum numbers $v \geq 8$. Maxima for the partial cross-sections corresponding to low values of v lie outside the wavelength region under consideration.

On the whole as one can see from the presented results, the partial cross-

sections of both radiative association and photo dissociation may achieve large va-
lues especially for high quantum numbers v. It should be noted again, this is a con-
sequence of the fact that the dipole momentum function for LiH molecule depends
strongly on the internuclear distance, i.e. it possesses large derivatives in the
most important region of internuclear distances.

REFERENCES

Khersonskij V.K.: 1977, *Optika i Spectroscopiya* (Soviet), **43**, 1, 39.

Landau L.D., Livshits E.M.: 1963, *Kvantovaya mekhanika. Relativistskaya teoriya* (Soviet), M.: Fizmatgiz, 767.

Sobelman I.I.: 1977, *Vvedenie v teoriyu atomnykh spektrov* (Soviet), M.: Nauka, 319.

Stwalley W., Zemke W., Way K. et al.: 1977, *J. Chem. Phys.*, **66**, 5412.

Varshalovich D.A., Moskalev A.N., Khersonskij V.K.: 1975, *Kvantovaya teoriya uglovogo momenta,* (Soviet), L.: Nauka, 439.

Zemke W.T., Stwalley W.C.: 1980, *J. Chem. Phys.*, **73**, 5583.