



Adiabatic asymptotic theory of two-electron charge exchange involving the polar molecules

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Abstract

In the framework of asymptotic approach and semiclassical method the closed analytic expression for matrix element of the two-electron exchange interaction between polar molecular ion and neutral polar molecule, responsible for direct two-electron transfer processes, have been calculated.

1 Introduction

The process of two-electron transfer between the atomic and molecular particles remains highly attractive object of research for both the theoretical and experimental groups (see [1, 2, 3, 4] and references therein). In the theory of electron transition in the course of atomic collision the exchange interactions at large internuclear distances R between projectile and target particles are the most important ones, since they are associated with the largest cross sections. However, accurate calculation of such exchange interaction in the asymptotic region of large R still requires significant computational effort. Aiming to simplify these calculations many analytical approximate theories have been proposed (see [1, 2, 3] and references therein). Among them the asymptotic theory remains quite popular because of ability to combine the general character of proposed analytical results and relatively satisfactory numerical estimations for cross-sections of the processes under investigation. However, until now the application of asymptotic theories were limited, mainly, to studying of the one-electron processes in the collisions that involves atomic or simplest diatomic ions. The cases, where polar molecules considered as a target have been studied in [5, 6, 7, 8, 9]. The application of the asymptotic methods for studying of the two-electron exchange processes in the collisions that involves the polar molecules, to the best of our knowledge, is limited by publication [10].

In the present work the asymptotic theory [10] has been extended to the case when both of the colliding particles has a permanent dipole moment. It allows to calculate the leading asymptotic (at $R^{-1} \ll 1$) expression for the matrix element H_{ab} responsible for two-electron capture at slow collision of polar molecule $A^{(Z_a-2)+}$ with a doubly charged polar molecular ion B^{Z_b+} :

$$A^{(Z_a-2)+} + B^{Z_b+} \longrightarrow A^{Z_a+} + B^{(Z_b-2)+}, \quad (1)$$

where Z_a and Z_b are effective charges of the cores of colliding particles (further we suppose that $Z_a = Z_b = 2$).

2 The asymptotic arrangement of the problem

In the following, we shall assume the electronic configuration of the molecular cores A^{Z_a+} and B^{Z_b+} are frozen during the course of collision. Therefore, the problem is reduced to consideration of two active electrons described by the following Hamiltonian of the system $(AB)^{(Z_a+Z_b-2)+}$

$$H_{ab} = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} + V_a(r_{1a}) + V_a(r_{2a}) + V_b(r_{1b}) + V_b(r_{2b}) + r_{12}^{-1}, \quad (2)$$

where $-\Delta_i/2$ is a kinetic energy operator for the i -th electron, $V_{a(b)}$ are the potentials of electronic interaction with ionic core A^{Z_a+} or B^{Z_b+} , the r_{12} is the distance between two active electrons. At asymptotic distances ($r \rightarrow \infty$) the potentials $V_{a,b}(r)$ has the Coulomb form

$$V_{a,b}(r) \rightarrow -Z_{a,b}/r. \quad (3)$$

Let d_{1a} and d_{2a} are the dipole moments of ions $A^{(Z_a-1)+}$ and A^{Z_a+} , and d_{1b} and d_{2b} are the dipole moments of ions $B^{(Z_b-1)+}$ and B^{Z_b+} . Let us to introduce the coordinate frames $\{x, y, z\}$ and $\{\tilde{x}, \tilde{y}, \tilde{z}\}$ with common origin in the point O in the center of mass of the particle $A^{(Z_a-1)+}$, such that axis Oz directed along the vector \vec{R} and axis $O\tilde{z}$ along the vector \vec{d}_a . Transition from the $\{\tilde{x}, \tilde{y}, \tilde{z}\}$ to $\{x, y, z\}$ described by the three Euler angles $\Omega_1 = (\alpha_1, \beta_1, \gamma_1)$ [11]. Similarly, we shall introduce the frame $\{\bar{x}, \bar{y}, \bar{z}\}$ with the origin O' in the center of mass of the ion B^{Z_b+} and with the axis $O'\bar{z}$ along the vector \vec{d}_b . Mutual orientation of the frames $\{x, y, z\}$ and $\{\bar{x}, \bar{y}, \bar{z}\}$ described by Euler angles $\Omega_2 = (\alpha_2, \beta_2, \gamma_2)$, see Fig.1.

Let m_{1a} and m_{2a} (m_{1b} and m_{2b}) are the projections onto $O\tilde{z}$ ($O'\bar{z}$) the orbital momentum of the electrons in initial (final) electronic state, i.e. centered at the core A^{Z_a+} (B^{Z_b+}).

It is known from the asymptotic theories, that two-electron exchange interaction H_{ab} is determined by asymptotic of the electronic wave functions in the whole configuration space of the coordinates of both electrons [1]. As shown in [1, 10], the asymptotic, at $R \rightarrow \infty$, form of H_{ab} can be represented through the one-electronic orbitals as follows

$$H_{ab} = \langle \varphi_b^{(0)}(\vec{r}_{1b}) \varphi_{ba}(\vec{r}_{2a}) | r_{12}^{-1} | \varphi_{ab}(\vec{r}_{1b}) \varphi_a^{(0)}(\vec{r}_{2a}) \rangle. \quad (4)$$

The φ_{ab} is the wave function of the "outer" electron of the $A^{(Z_a-2)+}$ molecule in the vicinity of the ion B^{Z_b+} , and vice versa: φ_{ba} is the wave function of the "outer" electron of the $B^{(Z_b-2)+}$ near the core A^{Z_a+} . Hence, without the perturbation of ion B^{Z_b+} (A^{Z_a+}) the wave function φ_{ab} (φ_{ba}) goes over into the wave function $\varphi_a^{(0)}$ ($\varphi_b^{(0)}$), which is the wave function of a bound state of ion $A^{(Z_a-1)+}$ ($B^{(Z_b-1)+}$).

We shall calculate the wave functions φ_{ab} and φ_{ba} of the quasimolecular systems $A^{(Z_a-2)+} + B^{Z_b+}$ and $A^{Z_a+} + B^{(Z_b-2)+}$ for the asymptotic configuration which

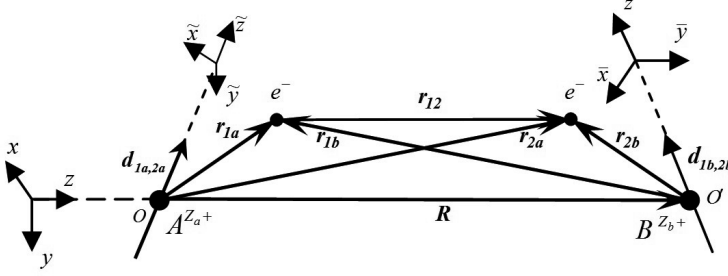


Figure 1: Geometry of the quasimolecular system

contribute mainly to the matrix element (4), i.e. in the vicinity of the cores A^{Z_a+} and B^{Z_b+} .

3 The wave functions and exchange interaction

We start from the asymptotic of the one-electron wave function φ_{ab} of the polar molecule in case the perturbation of the distant core B^{Z_b+} is small, i.e. the arrangement $A^{(Z_a-2)+} + B^{Z_b+}$ is under consideration. The wave function φ_{ab} satisfies the Shroedinger equation

$$\left(-\frac{\Delta}{2} + U_a(r_a) + V_b(r_b) - E_{1a} \right) \varphi_{ab}(\vec{r}_b) = 0, \quad (5)$$

where $U_a(r_a)$ and $V_b(r_b)$ are the interaction potentials of the electron with ions $A^{(Z_a-1)+}$ and B^{Z_b+} respectively. The electronic energy E_{1a} at $R \rightarrow \infty$ goes over into the unperturbed bound energy $E_{1a}^{(0)} = -1/2n_{1a}^2$ of the outer electron of a molecule $A^{(Z_a-2)+}$. In the framework of a point-dipole model the electronic interaction with a dipoles \vec{d}_{1a} and \vec{d}_{2b} reads:

$$U_a(\vec{r}_a) = -(Z_a - 1)/r_a - \vec{d}_{1a} \cdot \vec{r}_a / r_a^3. \quad (6)$$

$$V_b(\vec{r}_b) = -Z_b/r_b - \vec{d}_{2b} \cdot \vec{r}_b / r_b^3. \quad (7)$$

We solve equation (5) with the boundary condition [6, 10]:

$$\begin{aligned} \varphi_{ab}(\vec{r}_a) \Big|_{1 < r_a \ll R} &= \varphi_a^{(0)}(\vec{r}_a) = \\ &= \frac{(2 - n_{1a})^{n_{1a}(Z_a-1)+1}}{2(Z_a - 1)^{1/2} \sqrt{\Gamma(2n_{1a}(Z_a - 1))}} r_a^{n_{1a}(Z_a-1)} e^{-r_a/n_{1a}} Z_{Lm_{1a}}^{(1)}(\tilde{\theta}_a, \tilde{\phi}_a). \end{aligned} \quad (8)$$

The functions $Z_{Lm_{1a}}^{(1)}$ are the dipole-spherical harmonics (see [6]-[10]), which satisfies the following equation

$$\left[-\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} - 2d_{1a} \cos \theta \right] Z_{Lm}^{(1)}(\theta, \phi) = \eta_{Lm} Z_{Lm}^{(1)}(\theta, \phi), \quad (9)$$

and can be expanded over the standard spherical harmonics

$$Z_{Lm}^{(1)}(\tilde{\theta}_a, \tilde{\phi}_a) = \sum_{l \geq |m|} a_{Ll}^m(d_{1a}) Y_{lm}(\tilde{\theta}_a, \tilde{\phi}_a). \quad (10)$$

The coefficients $a_{Ll}^m(d_{1a})$ defined by the following system of recurrent equations

$$\begin{aligned} 2d_{1a} \left[\frac{l^2 - m^2}{4l^2 - 1} \right]^{1/2} a_{Ll-1}^m + [l(l+1) - \eta_{Lm}] a_{Ll}^m \\ + 2d_{1a} \left[\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)} \right]^{1/2} a_{Ll+1}^m = 0. \end{aligned} \quad (11)$$

Here m is the number of root, i.e. the number of eigensolution η_{Lm} of the equation (11) at a given quantum number L .

In the region far from each of molecules, where the potentials $U_a(r_a)$ and $V_b(r_b)$ goes over into the Coulomb asymptotic form the semiclassical solution for $\varphi_a(\vec{r}_a)$ of equation (5) reads:

$$\begin{aligned} \varphi_a(\vec{r}_a) = \frac{n_{1a}^{-1} \pi^{-1/2}}{\sqrt{\Gamma(2n_{1a}(Z_a - 1) + 1)}} \left(\frac{n_{1a}(Z_a - 1)}{e} \right)^{n_{1a}(Z_a - 1)} \\ \times \frac{F(p_a)}{z_a |p_a(z_a)|^{1/2}} \sum_{\ell \geq |m_{1a}|} \sum_{k=-\ell}^{\ell} a_{L\ell}^{m_{1a}}(d_{1a}) D_{km_{1a}}^{\ell}(\Omega_1) \\ \times \frac{1}{2^{|k|} |k|!} \left(\frac{(2\ell+1)(\ell+|k|)!}{2(\ell-|k|)!} \right)^{1/2} \left(\frac{\rho}{z_a} \right)^{|k|} e^{ik\phi_a}, \end{aligned} \quad (12)$$

where

$$p_a^2(z_a) = 2(-|E_{1a}| + (Z_a - 1)/z_a + Z_b/(R - z_a)). \quad (13)$$

Expansion for $F(p_a)$ close to axis R (i.e. at small θ_a) reads

$$F(p_a) = \exp \left(- \int_{z_{1a}}^{z_a} |p_a(z)| dz \right) \exp \left(- \frac{\rho^2 p_a(z_a)}{2z_a} \right), \quad (14)$$

where $\rho \simeq z_a \sin(\theta_a)$, and the turning points z_{1a} and z_{2a} are determined by relation

$$p_a(z_{1a}) = p_a(z_{2a}) = 0.$$

Under the condition $r_a \sim 1$ the solution (12) goes over into the asymptotic of the unperturbed wave function of the polar molecule (8).

The wave function φ_{ab} in the vicinity of ion B^{Z_b+} given in terms of a surface integral [1, 10]

$$\varphi_{ab}(\vec{r}_b) = -\frac{1}{2} \int_S d\mathbf{S} (\varphi_{ab} \nabla G_b - G_b \nabla \varphi_{ab}), \quad (15)$$

where the S -plane divides the electronic location in the initial and final channels of the reactions. The $G_b \equiv G_b(\vec{r}_b, \vec{r}_b'; E_{1a})$ is the one-electron Green's function

of the quasimolecular system $A^{(Z_a-2)+} + B^{Z_b+}$, which can be expanded over the dipole-spherical harmonic as follows

$$G_b(\vec{r}_b, \vec{r}'_b; E_{1a}) = -\frac{2}{r_b r'_b} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} g_{lm}(r_b, r'_b; E_{1a}) Z_{lm}^{(2)}(\bar{\theta}_b, \bar{\phi}_b) Z_{lm}^{(2)*}(\bar{\theta}'_b, \bar{\phi}'_b), \quad (16)$$

where $g_{lm}(r_b, r'_b; E_{1a})$ is the radial Green's function. The functions $Z_{lm}^{(2)}(\bar{\theta}_b, \bar{\phi}_b)$ satisfies the equation (9) subject to the following substitutions in the latter: $d_{1a} \rightarrow d_{2b}$, $\eta \rightarrow s(s+1)$, and assuming that $s \equiv s_{lm}$. As a result, the radial Green's function $g_{lm}(r_b, r'_b; E_{1a})$ satisfies the following equation

$$\left[\frac{d^2}{dr^2} + 2 \left(E_{1a} + \frac{Z_a - 1}{|\vec{R} - \vec{r}|} + \frac{Z_b}{r} - \frac{s(s+1)}{2r^2} \right) \right] g_{lm}(r, r'; E_{1a}) = \delta(r - r'), \quad (17)$$

and can be represented as a product

$$g_{lm}(r_b, r'_b; E_{1a}) = -\frac{n_{1a}}{2} f_{1lm}(r_{<}) f_{2lm}(r_{>}), \quad (18)$$

where $r_{<} = \min(r_b, r'_b)$, $r_{>} = \max(r_b, r'_b)$, and $f_{1lm}(r)$, $f_{2lm}(r)$ are the linearly independent solutions of the homogeneous version of the equation (17) with the boundary conditions

$$f_{1lm}(r) \underset{r \rightarrow \infty}{=} r^{-n_{1a} Z_b} e^{r/n_{1a}}, \quad f_{2lm}(r) \underset{r \rightarrow \infty}{=} r^{n_{1a} Z_b} e^{-r/n_{1a}}. \quad (19)$$

As seen, the asymptotic of the φ_{ab} on the variable r_b determined by asymptotic of the Green's function $G_b(\vec{r}_b, \vec{r}'_b; E_{1a})$ at $r'_b \sim R \gg 1$, $r_b \sim 1$ and hence, $r_{<} = r_b$, $r_{>} = r'_b$. In this region of configuration space of electronic coordinates one can neglect the term $Z_a - 1/|\vec{R} - \vec{r}| \ll 1$ in equation (17) to take approximate solution $f_{1lm}^{(0)}(r)$ of the equation

$$\left[\frac{d^2}{dr^2} + 2 \left(E_{1a} + \frac{Z_b}{r} - \frac{s(s+1)}{2r^2} \right) \right] f_{1lm}^{(0)}(r) = 0, \quad (20)$$

as a zero approximation for the solution $f_{1lm}(r)$. We note, that detailed algorithm of construction of the solutions similar to considered here $f_{1,2}$ given in [1, 10, 12].

Using obtained approximations and solving equation (20) semiclasically (see [10]) we can represent the Green's function $G_b(\vec{r}_b, \vec{r}'_b; E_{1a})$ in the region $r'_b \gg 1$, $r_b \approx 1$ as following expansion

$$\begin{aligned} G_b(\vec{r}_b, \vec{r}'_b; E_{1a}) &= \frac{n_{1a}}{4\pi} \left(\frac{n_{1a}^2 Z_b}{2e} \right)^{n_{1a} Z_b} \frac{F(p_b)}{z_b z'_b} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \sum_{\lambda \geq |m|} \sum_{\mu \geq |m|} (-1)^{\lambda+|m|} \\ &\times a_{l\lambda}^m(d_{2b}) a_{l\mu}^m(d_{2b}) B_{\lambda m}^- f_{1lm}^{(0)}(r_b) P_{\lambda}^{|m|}(\bar{\theta}_b) e^{im\bar{\phi}_b} \sum_{k=-\mu}^{\mu} D_{km}^{\mu}(\Omega_2) B_{\mu k}^+ \left[\frac{\rho}{z'_b} \right]^{|k|} \frac{e^{-ik\bar{\phi}'_b}}{2^{|k|} |k|!}, \end{aligned} \quad (21)$$

where $P_\lambda^m(\theta)$ is the associated Legendre polynomials, parameter B_{lm}^\pm reads

$$B_{lm}^\pm = \left[\frac{(2l+1)(l \pm |m|)!}{(l \mp |m|)!} \right]^{1/2}, \quad (22)$$

and

$$F(p_b) = \exp \left(- \int_{z'_a}^{z_{2a}} |p_b(z)| dz \right) \exp \left(- \frac{\rho^2 p_b(z'_b)}{2z'_b} \right), \quad (23)$$

$$p^2(z'_b) = 2(-|E_{1a}| + (Z_a - 1)/(R - z'_b) + Z_b/z'_b), \quad z'_a + z'_b = R. \quad (24)$$

The turning points z'_{1b} and z'_{2b} determined by following relations

$$p(z'_{1b}) = p(z'_{2b}) = 0, \quad z'_{1b,2b} = R - z'_{2a,1a}.$$

Finally, using the semiclassical representations (21) for the Green's function $G_b(\vec{r}_b, \vec{r}'_b; E_{1a})$ and (12) for the wave function φ_{ab} we can proceed to calculation of the surface integral (15). The integration in (15) is tedious albeit straightforward and leads to the following result for the wave function φ_{ab} of the polar molecule in the vicinity of ion B^{Z_b+} :

$$\begin{aligned} \varphi_{ab}(\vec{r}_b) = & D_a(R) \sum_{l \geq |m_{1a}|}^{\infty} \sum_{k=-l}^{+l} \frac{n_{1a}^{|k|}}{2^{|k|} |k|!} a_{Ll}^{m_{1a}}(d_{1a}) D_{km_{1a}}^l(\Omega_1) B_{lk}^+ R^{-|k|-1} \\ & \times \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{+l'} \frac{f_{1l'm'}^{(0)}(r_b)}{r_b} \sum_{\lambda \geq |m'|} \sum_{\mu \geq |m'|} a_{l'\lambda}^{m'}(d_{2b}) a_{l'\mu}^{m'}(d_{2b}) \\ & \times (-1)^{\lambda+\mu+|m'|} D_{km'}^\mu(\Omega_2) B_{\mu k}^+ B_{\lambda k}^- P_\lambda(\bar{\theta}_b) e^{im'\bar{\phi}_b}, \end{aligned} \quad (25)$$

$$D_a(R) = \frac{1}{2} \sqrt{\frac{n_{1a}}{2\pi\Gamma[t]}} \left(\frac{n_{1a}^2 Z_b}{2e} \right)^{n_{1a} Z_b} \left(\frac{n_{1a}(Z_a - 1)}{e} \right)^{n_{1a}(Z_a - 1)} \exp(-I_a(R)),$$

where $t = 2n_{1a}(Z_a - 1) + 1$, and the barrier integral $I_a(R)$ reads

$$\begin{aligned} I_a(R) = & \frac{n_{1a}^{-1}}{\sqrt{(R - z_{1a})z_{2a}}} \left\{ (-R^2 + (z_{1a} + z_{2a})R - z_{1a}z_{2a}) K(k_a) \right. \\ & \left. + (R - z_{1a})z_{2a}E(k_a) + [R^2 - (z_{1a} + 2z_{2a})R + z_{1a}z_{2a} + z_{2a}^2] \Pi(\nu_a, k_a) \right\}, \quad (26) \\ \nu_a = & (z_{2a} - z_{1a})/(R - z_{1a}), \quad k_a = \sqrt{\nu_a R / z_{2a}}. \end{aligned}$$

The $K(k)$, $E(k)$ and $\Pi(\nu, k)$ are the full elliptic integrals of the first, second and the third kind. The wave function $\varphi_{ba}(\vec{r}_a)$ can be obtained from the $\varphi_{ab}(\vec{r}_b)$ after formal substitutions: $a \leftrightarrow b$, $\Omega_1 \rightarrow \Omega_2$, $(\bar{l}, \bar{m}) \rightarrow (\bar{l}, \bar{m})$, $(\bar{\theta}_b, \bar{\phi}_b) \rightarrow (\bar{\theta}_a, \bar{\phi}_a)$. In order to calculate the H_{ab} we shall use the following representation for $f_{1lm}^{(0)}$ [5]

$$f_{1lm}^{(0)}(r_{1b}) = (2/n_{1a})^{n_{1a} Z_b} \frac{\Gamma(1 + s_{lm} - n_{1a} Z_b)}{\Gamma(2s_{lm} + 2)} M_{n_{1a} Z_b, s_{lm} + 1/2}(2r_{1b}/n_{1a}), \quad (27)$$

where $M_{k\mu}(x)$ is the Whittaker function. The normalized wave function $\varphi_b^{(0)}$ of the potential (7) reads [5]:

$$\varphi_b^{(0)}(\vec{r}_{1b}) = B_2 r_{1b}^{n_{2b}Z_b-1} e^{-r_{1b}/n_{2b}} \sum_{n \geq |m_{2b}|} a_{L'n}^{m_{2b}}(d_{2b}) Y_{nm_{2b}}(\bar{\theta}_{1b}, \bar{\phi}_{1b}), \quad (28)$$

$$B_2 = \frac{1}{2\sqrt{Z_b\Gamma(2n_{2b}Z_b)}} \left(\frac{2}{n_{2b}} \right)^{n_{2b}Z_b+1}. \quad (29)$$

In calculation of the integral for H_{ab} we use the dipole approximation for r_{12}^{-1}

$$\frac{1}{r_{12}} = -\frac{8\pi}{3R^3} \sum_{q=-1}^{+1} \sum_{j=-1}^{+1} \sum_{i=-1}^{+1} \frac{r_{2a}r_{1b}Y_{1j}(\tilde{\theta}_{2a}, \tilde{\phi}_{2a})D_{qj}^1(\Omega_1)Y_{1i}(\bar{\theta}_{1b}, \bar{\phi}_{1b})D_{-qi}^1(\Omega_2)}{(1+q)!(1-q)!}, \quad (30)$$

and finally comes the following representation for H_{ab}

$$H_{ab} = -\frac{8\pi(-1)^{S+1}}{3R^3} \sum_{q=-1}^{+1} \sum_{j=-1}^{+1} \sum_{i=-1}^{+1} \frac{D_{qj}^1(\Omega_1)D_{-qi}^1(\Omega_2)}{(1+q)!(1-q)!} H_{1b}H_{2a}, \quad (31)$$

$$H_{1b} = \int \varphi_{ab}(\vec{r}) \varphi_b^{(0)*}(\vec{r}) r Y_{1i}(\theta, \phi) d\vec{r}, \quad (32)$$

$$H_{2a} = \int \varphi_{ba}(\vec{r}) \varphi_a^{(0)*}(\vec{r}) r Y_{1j}(\theta, \phi) d\vec{r}. \quad (33)$$

Calculating the integral (32) we obtain the resulting expression for H_{1b}

$$\begin{aligned} H_{1b} = & \sqrt{3}B_2D_a(R) \sum_{l \geq |m_{1a}|} \sum_{k=-l}^{+l} \frac{a_{Ll}^{m_{1a}}(d_{1a})}{|k|!} \left(\frac{n_{1a}}{2} \right)^{|k|} D_{km_{1a}}^l(\Omega_1) R^{-|k|-1} \\ & \times \sum_{\bar{l}=0}^{\infty} \sum_{\bar{m}=-\bar{l}}^{\bar{l}} \sum_{\lambda \geq |\bar{m}|} \sum_{\mu \geq |\bar{m}|} (-1)^{-\mu} a_{\bar{l}\lambda}^{\bar{m}}(d_{2b}) a_{\bar{l}\mu}^{\bar{m}}(d_{2b}) D_{k\bar{m}}^{\mu}(\Omega_2) \sqrt{2\lambda+1} B_{lk}^+ B_{\mu k}^+ \\ & \times \sum_{n \geq |m_{2b}|} a_{L'n}^{m_{2b}}(d_{2b}) \sqrt{2n+1} T_{000}^{\lambda n 1} T_{\bar{m}m_{2b}i}^{\lambda n 1} J_b(s_{\bar{l}\bar{m}}), \end{aligned} \quad (34)$$

with $J_b(s)$ given by

$$\begin{aligned} J_b(s) = & \left(\frac{2}{n_{1a}} \right)^{n_{1a}Z_b+s+1} \left(\frac{n_{1a}n_{2b}}{n_{1a}+n_{2b}} \right)^{t_2} \frac{\Gamma(t_1)\Gamma(t_2)}{\Gamma(t_3)} {}_2F_1 \left(t_1, t_2; t_3; \frac{2n_{2b}}{n_{1a}+n_{2b}} \right), \\ & t_1 = -n_{1a}Z_b + s + 1, \quad t_2 = n_{2b}Z_b + s + 3, \quad t_3 = 2s + 2. \end{aligned}$$

Here ${}_2F_1$ is the Hypergeometric function and $T_{m_1m_2m}^{l_1l_2l}$ are the $3j$ -Wigner's symbols. The matrix element H_{2a} can be obtained from the H_{1b} by the following substitutions: $a \leftrightarrow b$, $B_2 \rightarrow A_2$, $\Omega_1 \rightarrow \Omega_2$, $(\bar{l}, \bar{m}) \rightarrow (\bar{l}, \bar{m})$. Substituting obtained H_{1b} , H_{2a} into (31) we come to the final result for the matrix element H_{ab} .

4 Concluding remarks

To conclude, we have calculated the semiclassical representation for the two-electron wave functions of the quasimolecules $A^{(Z_a-2)+} + B^{Z_b+}$ and $A^{Z_a+} + B^{(Z_b-2)+}$ under assumption of a large intermolecular separation R . The obtained results allow to construct the two-electron exchange interaction H_{ab} in a form of a leading asymptotic approximation at large R . The matrix element H_{ab} may be applied for cross section calculation of the direct two-electron capture (1) in slow collision of a polar molecule with a double charged polar molecular ion.

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