Charge transfer processes in collisions of slow highly charged ions with polar molecules CO and $C_3H_8$

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Abstract. Charge transfer processes resulting from low energy collisions of polar molecules CO and $C_3H_8$ with highly charged $Be^{2+}$ and $B^{2+}$ ions have been investigated experimentally and theoretically. The potential for the one–electron exchange interaction between a polar molecule and highly charged atomic ion were obtained in closed analytical form in the framework of a semiclassical approach. Obtained results were used for close–coupling calculations of total cross sections for single electron transfer in the studied reactions.

1. Introduction

Electron transfer processes in collisions of neutral molecules with slow highly charged ions are of great importance both for theoretical atomic physics and also for applied fields such as fusion plasmas and astrophysics. Much attention has been very recently called to the charge exchange processes involving polar molecules [1, 2]. In the present work we have studied single and double electron capture reactions in low energy collisions of atomic ions $Be^{2+}$ and $B^{2+}$ with polar molecules CO and $C_3H_8$ experimentally as well as charge transfer reactions,

$$C_3H_8 + Be^{2+} \rightarrow C_3H_8^+ + Be^+,$$

$$CO + A^{Z_A+} \rightarrow CO^+ + A^{(Z_A-1)+},$$

where: (a) $A^{Z_A+} = B^{2+}(1s^22s)$, and (b) $A^{Z_A+} = Be^{2+}(1s^2)$, theoretically. Our theoretical analysis is carried out as an extension of the asymptotic theory of electron transfer in slow ion–atomic collisions [3] to processes involving a non–central target particle with a permanent dipole moment.

2. Experiment

A portion of the experimental cross sections reported here has been published in our previous paper [4], and more recently cross section data have been measured with almost the same
procedure [5]. Only major parameters are therefore reported here. The experiment was performed using the Van de Graaff Accelerator Facility of the Quantum Science and Engineering Center, Kyoto University. A schematic view of the experimental apparatus is given in figure 1. Incident ions were obtained by an Ion–Impact–Ion–Source [6], in which a pump beam of 0.8 MeV CO$_2^+$ impacts a target of glassy beryllium or boron containing alloy in wire shape, and fractions of sputtered ions were extracted and accelerated to desired energies of 15–32 keV. Extracted ions were velocity-analyzed by a combination of an E × B filter (Wien filter) and a ‘neutral particle rejector’, and collided with a target gas (CO and C$_3$H$_8$) in a gas cell, whose pressure was monitored with a high-sensitivity Pirani gauge calibrated with a capacitance manometer (MKS Baratron). Outgoing ions were electrostatically separated and detected with a Position–Sensitive Detector utilizing Micro–Channel Plate (MCP–PSD). Cross sections were derived by the growth method under so–called single–collision condition with target gas pressure of 10$^{-2}$ – 10$^{-1}$ Pa, while the base pressure of the collision chamber was kept below 1 × 10$^{-5}$ Pa. The measured cross sections $\sigma^{(21)}$ and $\sigma^{(20)}$ are presented in table 1. Total uncertainties are estimated to be 9 – 20 %, which mainly come from the effect of residual gases and the uncertainty of Pirani gauge readings.

![Figure 1. The experimental setup.](image.png)

| Incident Ion | Target Gas | Collision Energy (keV) | $\sigma^{(21)}$ (cm$^2$) | $\sigma^{(20)}$ (cm$^2$) | Ref. |
|--------------|------------|------------------------|-------------------------|-------------------------|-----|
| Be$^{2+}$    | CO         | 15                     | 1.16 × 10$^{-15}$       | 4.16 × 10$^{-17}$       | [5] |
|              | C$_3$H$_8$ | 16                     | 2.1 × 10$^{-15}$        | 1.1 × 10$^{-16}$        | [4] |
|              |            | 24                     | 1.9 × 10$^{-15}$        | 1.4 × 10$^{-16}$        | [4] |
|              |            | 32                     | 1.8 × 10$^{-15}$        | 1.4 × 10$^{-16}$        | [4] |
| B$^{2+}$     | CO         | 20                     | 1.2 × 10$^{-15}$        | 4.3 × 10$^{-16}$        | [4] |
3. Theoretical method

Further we shortly outline the theoretical model used to describe the process of one–electron transfer. The theory for two–electron processes will be represented in our further publications.

We shall consider the charge transfer process within the 'one–electron approximation'. The active electron is considered as moving in the combined field of the molecular core $M^{Z_{M}+}$, which has permanent dipole moment $d$, and the atomic ion $A^{Z_{A}+}$, respectively. Thus, the corresponding Schrödinger equation reads

$$\left( -\frac{\Delta}{2} + V_A(|r-R|) + V_M(r) - \frac{d \cdot r}{r^3} - E \right) \Psi(r) = 0,$$

where $\Psi(r)$ and $E$ are the electronic wave function and energy, $r$ and $R$ are the position vectors of the electron and atomic ion $A^{Z_{A}+}$ with respect to the centre of mass of the molecule. We denote the energy and the wave function by $E_M$ and $\Psi_M$ when the electron is bound to core $M^{Z_{M}+}$ (quasimolecule $M^{Z_{M}+}A^{Z_{A}+}$) and by $E_A$ and $\Psi_A$ when it is bound to atomic center $A^{Z_{A}+}$ (quasimolecule $M^{Z_{M}+}A^{Z_{A}+}$), respectively. The effective potentials $V_A$ and $V_M$ of the electron interaction with corresponding core $M^{Z_{M}+}$ and $A^{Z_{A}+}$ have the following asymptotic behavior $V_A(|r-R|) = -Z_A/r - |R|$ and $V_M(r) = -Z_M/r$. In the limit $R \to \infty$, the eigenvalue spectrum of system $[AM]^{Z_{A}+Z_{M}+}$ is the sum of the eigenenergies $E_M^{(0)}$ or $E_A^{(0)}$ of the isolated $M^{Z_{M}+}$ or $A^{Z_{A}+}$ particles, respectively, the corresponding wave functions being $\Psi_M^{(0)}$ and $\Psi_A^{(0)}$. The exchange interaction $H_{ef}$ responsible for electron transfer processes (1), (2) can be given in terms of a surface integral [3]

$$H_{ef} = \frac{1}{2} \int_S dS \left( \Psi_A^* \nabla \Psi_M - \Psi_M^* \nabla \Psi_A \right),$$

where the $S$-plane divides the electronic location in the initial and final channels of the reactions (1), (2). For calculation of the wave functions $\Psi_A$ and $\Psi_M$ we employ a standard semiclassical approach [3]. In the tunneling region between interacting particles the approximate analytical representation of the wave function $\Psi_M$ can be expressed as [5]

$$\Psi_M(r) = r^{-1}Q(r) \sum_{r \sim R/2} \sum_{\ell=|m|}^{+\ell} a^{m_1}_\ell (d) D^{\ell}_{km_1} (0, \beta, 0) Y^\ell_k (\theta, \varphi),$$

where $m_1$ is the projection of the orbital momentum of the tunneling electron on the axis $d$, expansion coefficients $a^{m_1}_\ell (d)$ are given in [5], $D^{\ell}_{km_1}$ are the Wigner $D$–functions, $\beta$ being the angle between vectors $R$ and $d$, and $\{\theta, \varphi\}$ are the spherical angles of the vector $r$ in the spherical coordinate system with axis $z$ oriented along the vector $R$. Introduce the cylindrical coordinates $\{\rho, z, \varphi\}$ ($\rho = r \sin \theta$). The main contribution to the electron capture probability gives a small region of the surface $S$ near axis $R$, where $\rho \ll z$.

We shall obtain the wave function $\Psi_M$ in this classically forbidden (under–barrier) region of the electronic motion along the coordinate $z$, ($z_1 \leq z \leq z_2$, where $z_1$, $z_2$ are the turning points). In terms of the quasi momentum $p^2(r) \approx p^2(z) = 2 [E - Z_M/z - Z_A/(R-z)]$, the semiclassical expression for $Q(r)$ has the following form

$$Q(r) = \frac{n_1^{-1}}{\sqrt{(n_1 Z_M/e)}} \left( \frac{n_1 Z_M}{e} \right)^{n_1 Z_M} \exp \left( -\frac{p^2(z)}{2z} - \int_{z_1}^{z} p(z') dz' \right) \text{, \ \ } e = 2.718....$$

The asymptotic expansion for barrier integral in equation (6) is given in [3]. The wave function $\Psi_A$ can be obtained in the same manner. Calculating the surface integral in (4) using the expressions for the one–electron wave functions $\Psi_M$, $\Psi_A$ one can obtain the final expression for exchange interaction $H_{ef}$ [5].
4. Results, discussion and concluding remarks

The dynamical treatment of the collision was carried out using the impact parameter method with straight–line trajectories. The resulting cross sections were then averaged over the different orientations of the dipole vector \( \mathbf{d} \) with respect to the incident velocity vector. The measured and calculated results for total cross sections \( \sigma^{(21)} \) are plotted in figure 2(a). Reactions (1) and (2b) take place without any changes in the \( 1S \) ionic core \( \text{Be}^{2+}(1s^2) \), and we treated these colliding systems within the approximation of a single active electron interacting with frozen ionic core and corresponding polar ion. The most important products of the reaction (1) is \( \text{Be}^+(2s) \) ions and for reaction (2b) are \( \text{Be}^+(2s) \) and \( \text{Be}^+(2p) \) ions. Corresponding partial cross sections are plotted in figure 2(b). The \( \text{CO} + \text{B}^{2+}(1s^22s) \) system (reaction (2a)) was considered in the two–electron approximation (active 'transient' molecular electron and the 2s electron of the atomic core). Since no spin interaction was considered, the total spin was conserved and thus the calculations were carried out separately for the spin singlet and spin triplet symmetries. The total cross section were obtained by summation of the singlet and triplet cross sections with 1/4 and 3/4 weighting factors, respectively. Corresponding total cross sections are plotted in figure 2(c). For reaction (1) our calculations reproduced the measured energy behavior of the total cross section, but slightly (\( \sim 15–20% \)) overestimated the experimental data. Measured cross sections for reactions (2a) and (2b) are in good accord with the present calculations.

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