PHYSICAL REVIEW A VOLUME 45, NUMBER 3 1 FEBRUARY 1992

Simple formula for the cross sections of resonant charge transfer between atoms and their positive ions at low impact velocity

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(Received 7 June 1991; revised manuscript received 16 September 1991)

The cross sections of resonant charge transfer between atoms and positive ions for all non-transition-elements in the range of low collision velocities ($<10^8$ cm/sec) have been calculated by the impact-parameter and close-coupling methods. The calculated results are in fairly good agreement with the experimental results for the elements for which data are available. In these results the relation between the cross sections and the ionization potentials of elements was found, and based on this relation a useful and simple formula for the cross section was successfully obtained.

PACS number(s): 34.70.+e, 82.30.Fi

A knowledge of resonant-charge-transfer cross sections between atoms and atomic ions is of importance not only in atomic physics, but also in astrophysics and fusion research. Much experimental work on charge transfer has established the cross-section–impact-energy curves. However, the elements studied have been limited mainly to the rare gases and alkali metals because of experimental difficulties. To know the cross sections of an element not measured, therefore, a complicated calculation must be made, and to know those of measured elements, a detailed investigation of the literature is also required. It is useful not only for experimentalists but also for theorists to have a simple formula for the cross section available for all non-transition-elements. In this paper the experimental data of the resonant-charge-transfer cross sections between elements and their positive ions in the low-velocity range ($<10^8$ cm/sec) have been calculated using the impact-parameter and close-coupling methods. In the calculation results, the relation between the cross section and the ionization potential was found and shows fairly good agreement with experimental results. From this relation and the calculated dependence of the cross section on the impact velocity, a simple formula for the cross section, which has only the ionization potential and the impact velocity as parameters, has been obtained. Here we should note that concerning the transition elements, our recent experimental results for gadolinium [1,2] and yttrium and those of Ref. [3] for uranium show larger cross sections and a different velocity dependence compared to those of non-transition-elements, and these results cannot be explained by widely used theoretical models for resonant processes. Therefore they are not presented here, but a more detailed discussion on the charge-transfer process for transition elements is required in the future [4].

The present calculation assumes the impact-parameter treatment (linear-trajectory approximation), which is valid above approximately 100 eV [5]. The cross sections are obtained by solving the time-dependent, nonrelativistic, spinless Schrödinger equation. In this, we used the method of Bates and McCarroll [6], while expanding the electronic wave function in terms of a set of "traveling" atomic orbitals centered about each nucleus [7]. The wave function used for each atom is calculated by Herman and Skilman [8] with the Hartree-Fock-Slater method. The detailed procedure for the cross-section calculation is discussed in Ref. [9]. The inherent numerical errors were 10% and 5% in the ranges of 10^6–10^7 and 10^7–10^8 cm/sec, respectively.

Figure 1 shows the calculation result and the experimental data on the cross section of helium atoms as a function of impact velocity. Helium is the most abundantly studied element, and there are many other older experimental data; however, the old data seem to be scattered more and to be less accurate than the new data (Ref. [9]). Therefore, they are not included here. The calculated results show fairly good agreement with the experimental results [10–28], especially in the low-velocity range of $<10^8$ cm/sec, though there is some discrepancy in the intermediate-velocity region. Thus the cross-section–impact-velocity curve used in the following discussion is limited to the low-velocity range. For elements for which experimental data are less abundant, it is difficult to discuss the agreement with calculated results. Therefore, it is more useful to compare all data as a function of a parameter that is closely related to the charge-transfer process and is commonly known for all elements. The cross section for resonant charge transfer at low velocities in the collision of an ion X^+ with the corresponding neutral atom X is determined mainly by the potential curves of the low-lying states of the molecule $X_2{}^+$, which is formed temporarily during the collision. The Hamiltonian of the two-atom system (the molecule) $X_2{}^+$ consists of the potential energy for each atom. Therefore, these potential curves may be closely related to the ionization potential of the neutral atom X. Figure 2 shows cross sections obtained experimentally and calculated cross sections as a function of the ionization potentials of non-transition-elements, at the impact velocities of 1×10^6 and 1×10^7 cm/sec. It is inferred that the calculated results are reliable to a degree of 15–25 %. As in Ref. [9], the experimental data exhibit scattering of typically $\pm50\%$ and this is still the *status quo* of absolute cross-section studies because of experimental difficulties.

Given this experimental accuracy, the calculated results are seen to be in fairly good agreement with the measured data. The relation between the cross section and the ionization potential can be clearly seen.

From Fig. 1, it is seen that both the experimental data and the theoretical results are well fit by a curve of the form

$$\sigma_{He}(v) = A' - B' \log_{10} v \ , \tag{1}$$

in cm^2, where $A' = 7.45 \times 10^{-15}$, $B' = 8.72 \times 10^{-16}$, and v is the impact velocity in cm/sec. Note that it may be possible for a better fitting formula to be expressed by using another function, for example, a secondary degree of

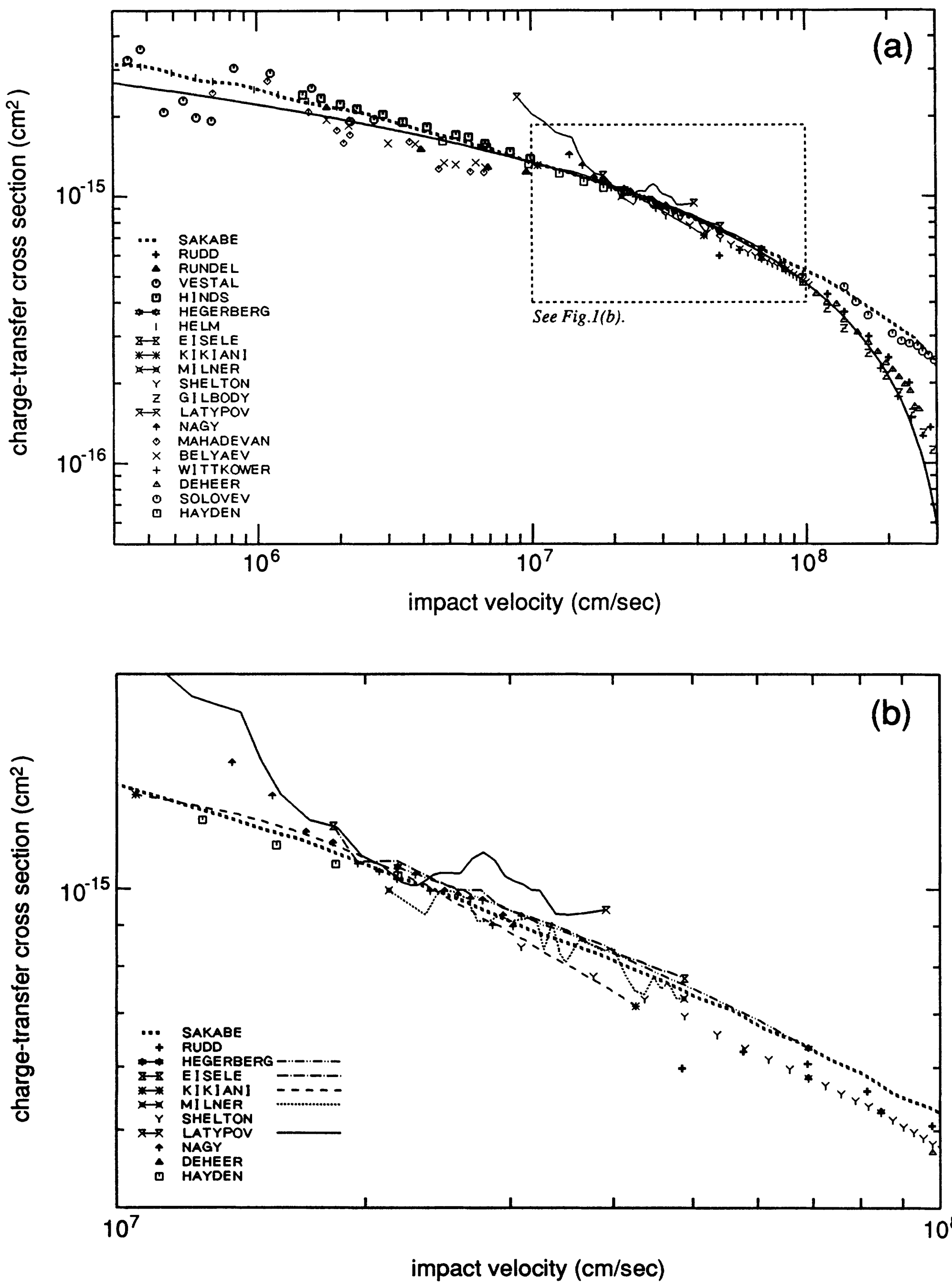

FIG. 1. Cross-section–impact-velocity curve for resonant-charge transfer of a helium atom. Experimental data are given by symbols and thin lines (Refs. [10–28]). Data given by a line in a source reference are indicated by a thin line with two symbols at the end. The data by Milner and Parker, Eisele and Nagy, and Hegerberg, Sefasson, and Elford, although originally published as plotted points, are given as lines to avoid excessive crowding. A thick dashed line is the present calculation result (Ref. [9]), and a thick solid line is the result obtained by the formula presented. (b) is the graph magnified partially from (a). In (b) the formula curve is not shown to avoid crowding.

$\log_{10}v$. However, the most simple formula is used here, and it is sufficiently accurate, given the scattering of the experimental data. From Fig. 2, the cross section σ can be related to the ionization potential I by

$$\sigma \propto I^{-1.5} . \quad (2)$$

From both relations above we can obtain the simple formula for the charge-transfer cross section for any arbitrary non-transition-element as follows:

$$\sigma(v)=(A-B\log_{10}v)(I/I_0)^{-1.5} , \quad (3)$$

where $A=1.81\times10^{-14}$, $B=2.12\times10^{-15}$, and I_0 is the ionization potential of hydrogen 13.6 eV. In Fig. 2 the cross section obtained by this formula is shown by a solid line.

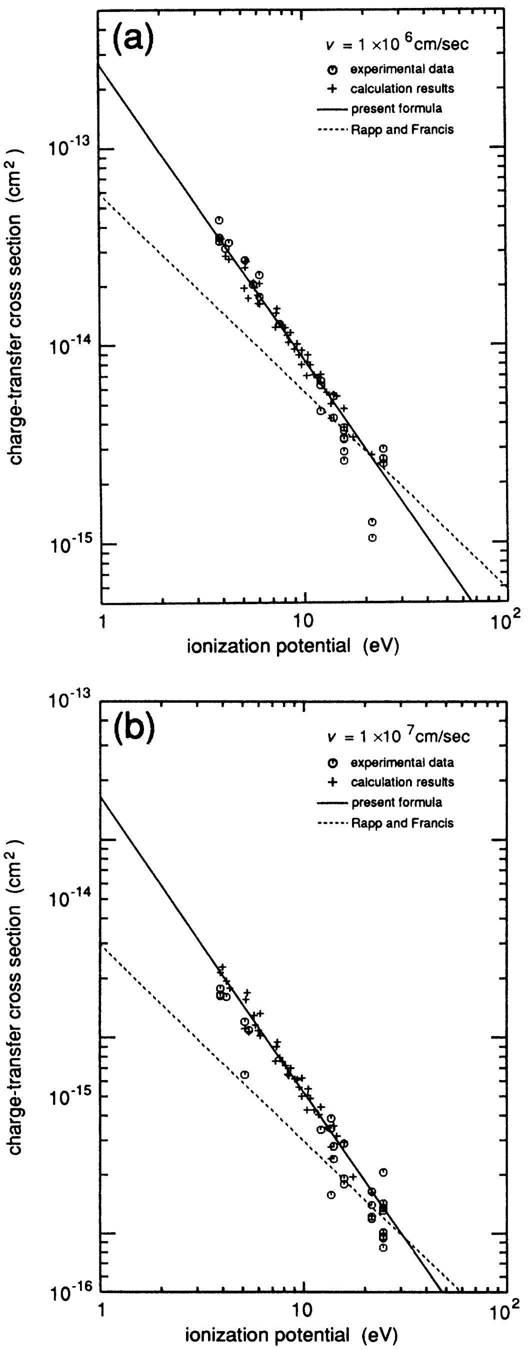

FIG. 2. Cross sections of non-transition-elements investigated in the past as a function of their ionization potentials, at the impact velocities of (a) 1×10^6 and (b) 1×10^7 cm/sec. Open circles and cross symbols are experimental data and the present calculation results, respectively. A solid line and a dashed line are obtained by the present simple formula and by Rapp and Francis (Ref. [29]), respectively.

It should be noted that Rapp and Francis have calculated the resonant-charge-transfer cross sections for a selection of atoms [29]. This calculation method has been widely used because of its simplicity, though it is less accurate. The cross section is given by

$$\sigma=\frac{\pi}{2}b_1^2 , \quad (4a)$$

$$\left[\frac{2\pi}{\gamma a_0}\right]^{1/2}\left[\frac{I}{\hbar v}\right]b_1^{3/2}\left[1+\frac{a_0}{\gamma b_1}\right]\exp\left[-\frac{\gamma b_1}{a_0}\right]=\frac{\pi}{6} , \quad (4b)$$

where I is the ionization potential of an atom in eV, $\gamma=(I/I_0)^{1/2}$, and a_0 is the Bohr radius. Using this relation we can obtain the relation $\sigma\propto I^{-1}$ as follows:

$$v=\frac{6\sqrt{2}a_0I_0}{\sqrt{\pi}\hbar}\left[\frac{\gamma b_1}{a_0}\right]^{3/2}\left[1+\frac{a_0}{\gamma b_1}\right]\times\exp\left[-\frac{\gamma b_1}{a_0}\right]=F(\gamma b_1) , \quad (5a)$$

$$\sigma=\frac{\pi}{2}\left[\frac{F^{-1}(v)}{\gamma}\right]^2\propto I^{-1} . \quad (5b)$$

The cross section obtained by this formula is also shown in Fig. 2 by a dashed line. For atoms with ionization potentials much lower than that of hydrogen, the Rapp-Francis calculation compares poorly with experimental results.

In summary, the cross sections of resonant charge transfer between atoms and positive ions for all non-transition-elements in the range of low collision velocities ($<10^8$ cm/sec) have been calculated by the impact-parameter and close-coupling methods. The calculated results are in fairly good agreement with the available experimental results. In these results the relation between the cross section and the ionization potential was found, and using this relation coupled with the cross-section–impact-velocity curve of the helium atom, which was obtained by fitting the calculation result and experimental data, the useful and simple formula for the cross section was successfully obtained.

The authors are grateful to Professor S. Nakai, Professor Y. Kato, Professor T. Yamanaka, and Professor C. Yamanaka for their encouragement and comments. They thank Professor K. Mima, Dr. H. Niki, and Professor M. Nakashima for their discussions and comments, and C. Frantz for reading the manuscript. This work was done in collaboration with the Institute for Laser Technology, and supported in part by the Matsuo Foundation.

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