Charge transfer in $H^+ + Ar$ collisions from 10 to 150 keV

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Total as well as partial cross sections for single-electron capture of H^+ on Ar are calculated by the semiclassical impact parameter method, using a two-center atomic basis expansion, in the impact energy range 10–150 keV. The resulting total cross sections are in good agreement with previous experimental data. Partial cross sections agree qualitatively with measurements at high energies, while at low energies the experimental data are found to be approximately six times smaller than the present results.

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I. INTRODUCTION

Single electron capture from low to intermediate collision energies has been the subject of many experimental and theoretical investigations, because of both its fundamental importance and its applications in astro- and plasma physics [1] and in material science [2]. In spite of these continuous efforts to study the capture processes our understanding of them is still rather incomplete. Notwithstanding the increasing sophistication of the experimental techniques and theoretical models, the accurate determination of state-selected and total charge tranfer cross sections has remained a challenging task. There has been a substantial amount of experimental work on charge exchange reactions, over a wide energy range, between H^+ projectiles and a target Ar gas [3–36]. Not only have total cross sections for this process been measured, but also the formation of hydrogen excited states and most recently differential cross sections have been reported. Theoretical models used to calculate electron transfer cross sections are generally limited to single-electron systems [37,38]. There are also calculations in the literature for a few systems with more than one electron (see, for instance, Refs. [39,40]). At lower energies the two-state approximation has yielded satisfactory results for H^+ passing through Ar [6], but at intermediate energies several competing channels should be taken into account to give a meaningful picture of the reaction. No detailed theoretical treatment of the process has been made, to our knowledge, at the intermediate-energy range, because of the complexities involved in an accurate calculation of the collision.

In the present work we have calculated electron transfer total cross sections by 10–150 keV protons in Ar. We also report formation cross sections to low-lying hydrogenic excited states. The semiclassical model applied to study the capture from each *M* subshell of Ar is described in the next section.

II. MODEL

We used a semiclassical impact parameter approximation which we will describe briefly. We considered classical straight lines for the nuclear motion, while the dynamics of one active electron was found by solving the time-dependent Schrödinger equation with the two-center atomic orbital close-coupling method [41]. The interaction potential is modeled by a Coulomb potential centered at the projectile and an effective potential centered at the Ar nucleus,

$$V_A(r) = -\frac{Z_0}{r} + (Z_1 + Z_2 r)\frac{e^{-Z_3 r}}{r}. \tag{1}$$

The wave function $\Psi(r,t)$ is expanded in two-center bound atomic orbitals with the plane-wave electronic translational factors $P_{\mathrm{H,Ar}}(t)$ as

TABLE I. Orbital energies and parameters for the potentials experienced by the active electron and for even-tempered basis functions to represent the bound states of H and Ar atoms up to $n=4$.

Potential parameters					
		Z_0	Z_1	Z_2	Z_3
	H	1.0	0.0	0.0	0.0
	Ar	1.0	−17.0	−3.0	2.15

Wave function parameters						
	H			Ar		
	S	*P*	*D*	*S*	*P*	*D*
α	0.110	0.061	0.042	0.08	0.08	0.04
β	1.465	2.0	2.0	2.45	3.33	1.50

Argon orbital energies					
State	Calculated	Ref. [45]	State	Calculated	Ref. [45]
$3s$	−1.097	−1.067	$4p$	−0.087	−0.104
$4s$	−0.146	−0.151	$3d$	−0.057	−0.070
$3p$	−0.571	−0.577	$4d$	−0.0320	−0.0325

TABLE II. State-to-state single-capture cross sections at 20 keV as a function of the size of the basis at H center. The cross sections are given in $Å^2$. Note that 2(4) means 0.0002, etc.

$1s$	$2s$	$2p$		$3s$	$3p$			$3d$		$4s$	$4p$			$4d$	
Partial capture cross sections from $3p_1$															
1.77	0.23	0.21	0.14	0.08	0.070	0.023	0.014	0.008	0.014	0.029	0.026	0.004	0.010	0.003	1(4)
1.86	0.25	0.18	0.14	0.08	0.075	0.022	0.017	0.007	4(4)						
1.94	0.29	0.13	0.12												
2.01															
Partial capture cross sections from $3p_0$															
0.57	0.26	0.048	0.083	0.08	0.026	0.012	0.004	0.002	2(4)	0.026	0.012	0.002	0.004	6(4)	4(5)
0.71	0.24	0.044	0.076	0.076	0.030	0.011	0.0063	0.001	2(4)						
0.93	0.25	0.045	0.065												
1.38															
Partial capture cross sections from $3s$															
0.58	0.08	0.054	0.019	0.023	0.016	0.003	0.003	0.001	6(5)	0.008	0.005	6(4)	0.002	5(4)	1(5)
0.65	0.08	0.052	0.020	0.024	0.018	0.003	0.004	0.001	5(5)						
0.75	0.08	0.045	0.020												
1.00															

Corresponding total capture cross sections

$3p_1$	$3p_0$	$3s$
2.62	1.13	0.79
2.63	1.20	0.85
2.48	1.29	0.90
2.01	1.38	1.00

$$\Psi(r,t)=P_{\mathrm{H}}(t)\sum_i a_i^{\mathrm{H}}(b,t)\,\phi_i^{\mathrm{H}}(r) + P_{\mathrm{Ar}}(t)\sum_i a_i^{\mathrm{Ar}}(b,t)\,\phi_i^{\mathrm{Ar}}(r), \qquad (2)$$

where b is the impact parameter. The atomic states are in turn expanded in terms of even-tempered basis functions [42],

$$\phi_i^{\mathrm{H,Ar}}(r)=\sum_k c_{nk}^{\mathrm{H,Ar}} N_l(\zeta_k)\, e^{-\zeta_k r}\, r^l\, Y_{lm}(\hat{r}), \qquad (3)$$

where $i=\{n,l,m\}$ and $N_l(\zeta_k)$ is a nomalization constant. The exponential parameters ζ_k are taken to form a geometric sequence $\zeta_k=\alpha\beta^k$, $k=1,2,\ldots,k_{max}$, and Y_{lm} stands for the usual spherical harmonics. The parameters α,β and those of the potentials are determined so that the atomic energy levels of interest can be well represented by the eigenvalues of the diagonalized Hamiltonian of the H and Ar atoms. The calculated orbital energies, comparison to experimental values, and the parameters that we used are shown in Table I. Also note that the potential has the expected asymptotic behavior for small and large r and for the Ar case closely follows the potential found by Szydlik and Green [43].

We display in Table II an example of the convergence of the cross sections as a function of the size of the basis at an energy of 20 keV. The basis used for the calculations consists of all $n=1$–4 H orbitals at the hydrogenic center, as well as $3s$, $3p$, $3d$, $4s$, $4p$, and $4d$ orbitals at the Ar center. The coupled equations are integrated up to internuclear separations of 100 a.u. where all couplings have essentially vanished.

Within an independent particle model, the total electron capture cross sections are obtained by summing the cross sections for each M subshell and multiplying by 2, in order to take into account the number of equivalent target electrons available for capture in each subshell.

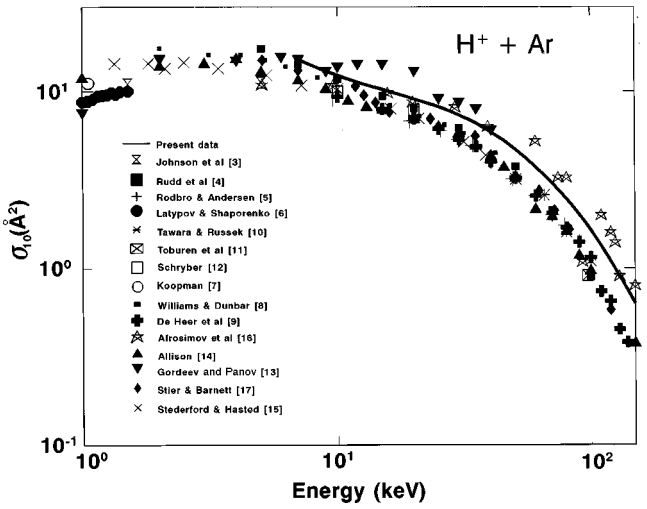

FIG. 1. Total single-electron capture cross sections in $H^+ + Ar$ collisions.

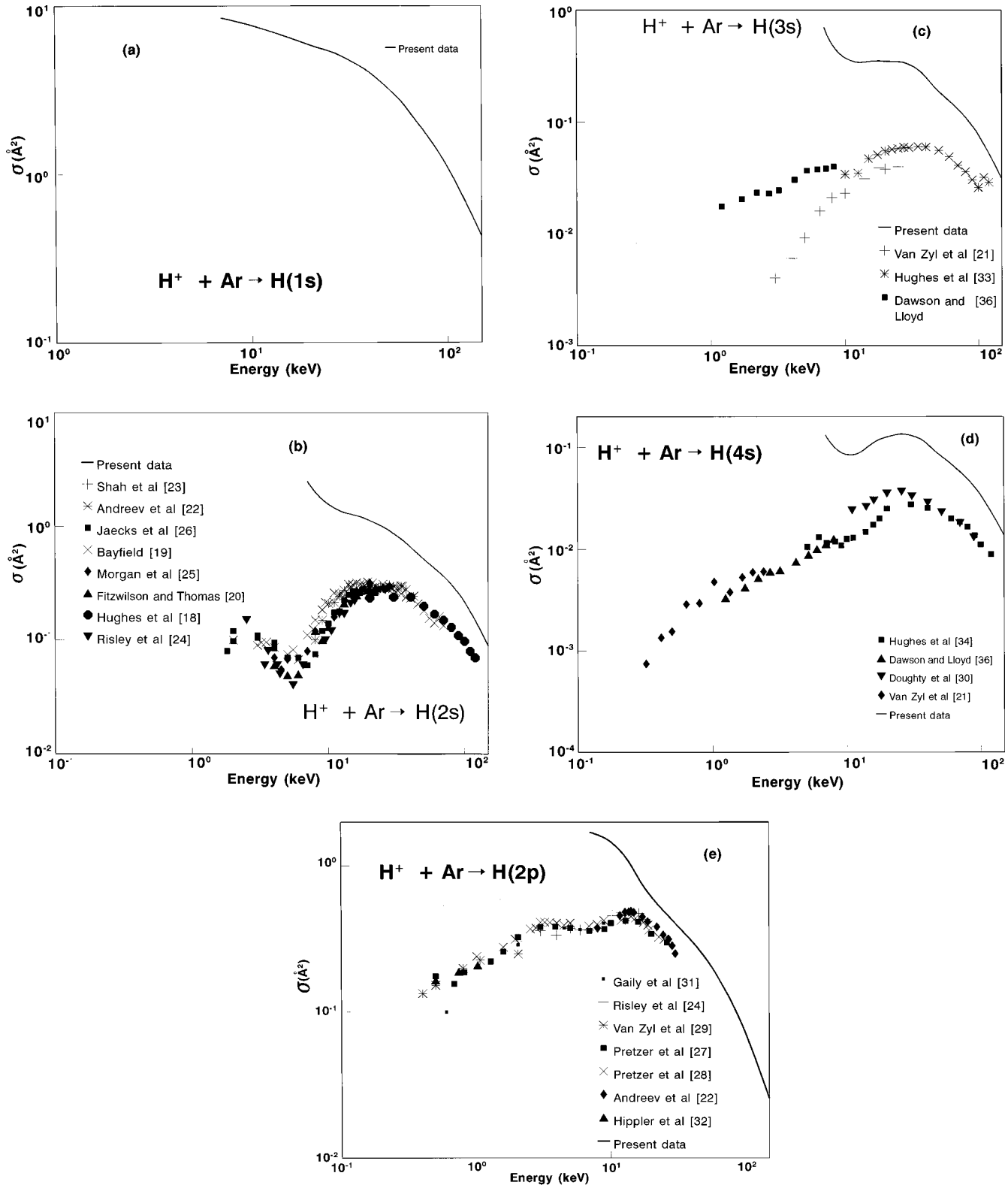

FIG. 2. Partial cross sections for single-electron capture into the state (a) H(1s), (b) H(2s), (c) H(3s) , (d) H(4s), (e) H(2p).

III. RESULTS AND DISCUSSION

Our calculated total capture cross sections are compared to a variety of experimental results in Fig. 1. There is general agreement between the calculated values and experimental data even though most of the experimental values lie slightly below our theoretical curve. At the lower-energy end ($E < 10$ keV) the slope of the theoretical curve increases whereas the experimental values are nearly constant. For the

higher-energy region the agreement is good but the calculations systematically overestimate the cross section values. As was mentioned in a previous section the one-electron probabilities that emerge from solving the close-coupling equations have to be used in conjunction with the independent electron model to take into account all of the electrons in the $3p$ shell of Ar, and the corresponding cross sections can then be compared with experiment. This independent electron model clearly neglects the electron correlation effect, which is expected to be more important at the lower energies. We thus attribute the discrepancy in the lower-energy region largely to the limitations of the independent electron model. In the present calculation, the ionization channels are not included. As demonstrated in another recent close-coupling study of charge transfer [44], leaving out the ionization channel from the wave function expansion tends to lead to larger charge transfer cross sections.

A much more stringent test of the calculations is to examine the state-specific capture cross sections, as displayed in Figs. 2(a)–2(e). The order of magnitude and the general shape of the experimental cross sections are reproduced, but the disagreement at lower energies is more apparent and with similar behavior as for the total cross section. In part the discrepancy is due to the fact that the cross sections are one or more orders of magnitude smaller than the main channel and should be more sensitive to all approximations in the calculation, in particular, the independent electron model, the size of the basis set, and the form of the potential.

Further insight into the collision can be obtained by examining the behavior of the capture probabilities p as a function of energy E and impact parameter b, as is done in Fig. 3. The smooth behavior observed at high energies changes to an oscillatory pattern as the energy and impact parameter diminish. The oscillations at small velocity reflect the oscillation of the electron between the target and the projectile when the orbiting velocity of the electron is faster than the collision velocity. Such oscillatory behavior is typical of charge transfer reactions at low energies.

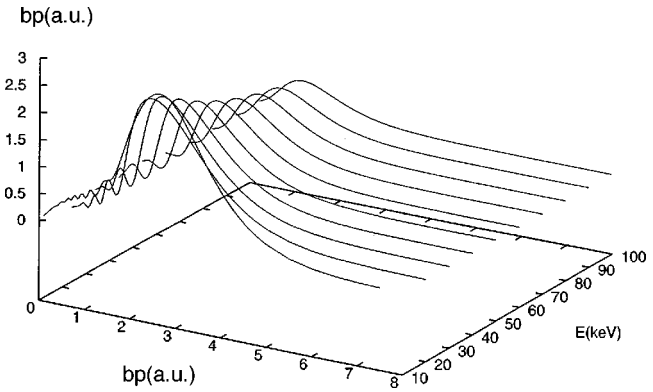

FIG. 3. Total single-electron capture probabilities as a function of collision energy and impact parameter.

In conclusion, we have calculated single-capture cross sections for $H^+ + Ar$ collision, in the impact energy range 10–150 keV. The resulting total cross sections are in good agreement with previous experimental data. Partial cross sections agree qualitatively with measurements at most energies, but at lower energies the present calculations are not adequate. In future improved calculations, it is desirable to go beyond the independent electron model and treat at least all the M-shell electrons on an equal footing. Such a calculation is expected to improve the theoretical results at lower energies.

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