Electron capture in pseudo-two-electron systems: $Ar^{8+} + He$

M. Kimura and R. E. Olson
Physics Department, University of Missouri–Rolla, Rolla, Missouri 65401
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Molecular-structure calculations using the pseudopotential method have been performed on the $(ArHe)^{8+}$ system. The cross section for single-electron capture in $Ar^{8+} + He$ collisions was calculated for energies from 20 eV/amu to 10 keV/amu. The perturbed-stationary-state method [M. Kimura, H. Sato, and R. E. Olson, Phys. Rev. A **28**, 2085 (1983)], modified to include electron translation factors appropriate to two-electron systems, was used. The total cross section is relatively energy independent with a value of approximately 2.5×10^{-15} cm^2. The $n=4$ level of Ar^{7+} is found to be preferentially populated, with the $4f$ level being dominant.

A considerable body of literature has been developed concerning collisions of multiply charged ions with atomic hydrogen. In many ways, these collisions are a mecca for theoreticians to critically test new techniques since the molecular-structure problem is reduced because there is only one electron on the target atom. However, the reverse is true for the experimentalist, since it is difficult to produce and utilize atomic hydrogen.

The opposite is true for target atoms such as the rare gases. The measurements are considerably simpler, but the calculations are much more difficult. The difficulty first arises in determining the molecular structure of the collision system, which is a many-electron problem with the inherent difficulties of basis sets, configuration lists, and correlation energies. The second difficulty facing the theoretician is more fundamental and centers about an incomplete description of the physics of collision involving multiply charged ions and many-electron atoms. For sufficiently high-charge states, the single- and multiple-electron-capture events take place on discrete states that lie in the continuum for autoionization. Thus, further approximations must be made in describing the collision dynamics.

One system in which theoretical approximations can be readily compared with experiment is on the electron-capture reaction:

$$Ar^{8+} + He \rightarrow Ar^{7+} + He^{+} \quad . \tag{1}$$

Experimental measurements have been made by Salzborn and Müller[1] and Justiniano *et al.*[2] With the use of pseudopotential techniques, this system reduces to a two-electron problem and is amenable to calculation.

The molecular-structure calculations for the pseudo-two-electron $(ArHe)^{8+}$ system were made with use of standard configuration-interaction (CI) techniques. The Slater-type-orbital basis set is given in Table I. The Ar $3s$ and He $1s$ basis sets are from Clementi and Roetti,[3] while the orbital exponents of the excited levels of Ar were obtained by quantum-defect theory. An l-dependent pseudopotential[4] was used to represent the neonlike argon-ion core. The pseudopotential parameters were obtained by a fit to spectroscopic data with dipole and quadrupole polarizabilities estimated by scaling to available values[5] in the neon isoelectronic sequence. The derived parameters are listed in Table II.

To preclude the possibility of doubly excited levels of Ar^{6+} tremendously complicating the CI calculations, we have only allowed single excitations from the $Ar^{8+} + He(1s^2)$ reference configuration in the configuration list. Such a procedure dictates that one electron will always remain in the helium $1s$ orbital. The basis set was also chosen in order to have compensating errors in the asymptotic energies of the incident $Ar^{8+} + He$ and product $Ar^{7+}(n=4) + He^{+}$ levels. The calculated exoergicities to the Ar^{7+} $4s$, $4p$, $4d$, and $4f$ electron-capture channels are 46.96, 40.75, 32.46, and 30.26 eV, respectively. These values may be compared to spectroscopic values of 47.48, 40.99, 32.40, and 30.01 eV, respectively. Thus, the maximum error in the ΔE's to the relevant Ar^{7+} $n=4$ levels is 1.1%, which translates approximately to a possible error in

TABLE I. Slater-orbital exponents (in atomic units).

Ar	$3s$	5.826	He	$1s$	1.688
		3.337		$2p$	1.688
		2.302			
	$3p$	3.042			
		2.195			
	$3d$	2.741			
		2.047			
	$4s$	2.302			
	$4p$	2.195			
	$4d$	2.047			
	$4f$	2.004			
	$5s$	1.773			
	$5p$	1.721			

TABLE II. Ar^{8+} pseudopotential parameters (in atomic units).

A_0	65.089 686
A_1	36.349 030
A_2	−11.217 802
ξ_0	5.514 980 7
ξ_1	4.938 547 2
ξ_2	7.977 459 1
d	0.412
α_d	0.094
α_q	0.0096

the position of the curve crossing point of $0.05a_0$. Figure 1 displays the molecular potential energies calculated for the $(ArHe)^{8+}$ system in the important curve crossing region of the $Ar^{7+}(n=4)+He^+$ electron-capture channels.

The scattering calculations were made with use of the perturbed-stationary-state method and straight-line trajectories.[4] Plane-wave electron translation factors were included in the coupled equations to first order in collision velocity. The inclusion of electron translation factors allows the coupling terms to dissociate properly, thus, making it possible to estimate the partial cross sections to specific (n,l) levels.

The scattering calculations included 11 molecular states consisting of the $^1\Sigma$, $^1\Pi$, and $^1\Delta$ states that dissociate to the $Ar^{8+}+He$ initial channel and to the $Ar^{7+}(n=4)+He^+$ and $Ar^{7+}(5s)+He^+$ electron-capture channels. All combinations of radial and rotational coupling terms were included in the calculations. The numerical integrations were begun at $R=10a_0$. To test the importance of trajectory effects in the low-energy results, we have employed both straight-line and Coulomb trajectories. At the lowest energy studied, the use of Coulomb trajectories decreased the calculated cross section by only 12%. The calculated cross sections are shown in Fig. 2 along with experimental results.[1,2] Our results are in reasonable accord with the data point of Salzborn and Müller[1] and the highest-velocity cross sections of Justiniano *et al.*[2] Their three lower-velocity data tend to lie lower than the calculated values. The error limits given by Justiniano *et al.* are such that it is difficult to conclude whether there is any difference in the velocity dependence of the cross section. It should be noted that the two lowest-velocity data points of Justiniano *et al.* were obtained with one apparatus configuration, while their high-velocity data were taken under a different apparatus configuration.

The experimental data shown in Fig. 2 are for single-electron capture, irrespective of the product state of the helium. Thus, the cross section is made up of the normal single-electron capture, reaction (1), and the transfer ionization reaction:

$$Ar^{8+}+He \rightarrow Ar^{7+}+He^{2+}+e^- \quad . \tag{2}$$

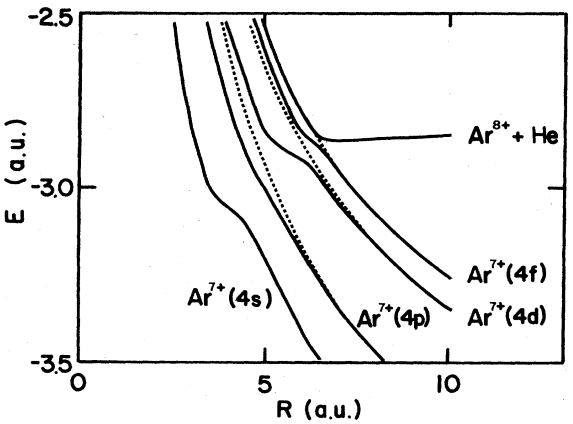

FIG. 1. Calculated interaction energies for the $(ArHe)^{8+}$ system at internuclear separations around the avoided crossings with the $Ar^{7+}(n=4)+He^+$ electron-capture channels. The solid lines are $^1\Sigma$ molecular states and the dashed lines are $^1\Pi$ molecular states. Not shown are the $^1\Delta$ states which coincide with the $^1\Pi$ states for the $Ar^{7+}(4d)$ and $Ar^{7+}(4f)$ levels.

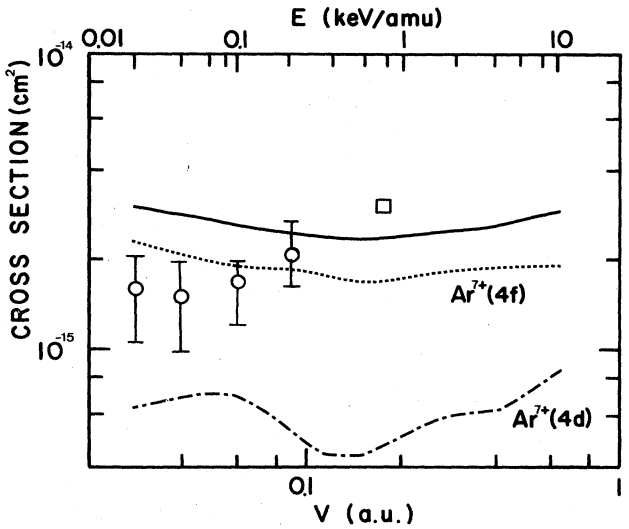

FIG. 2. Calculated total cross sections (solid line) for single-electron capture in $Ar^{8+}+He$ collisions, on a log-log scale. The dashed line is the partial cross section for capture to $Ar^{7+}(4f)+He^+$ and the dot-dashed line is for capture to $Ar^{7+}(4d)+He^+$. The open square is an experimental data point from Salzborn and Müller (Ref. 1) and the open circles are data from Justiniano *et al.* (Ref. 2) for single-electron capture without analysis of the charge state of the helium ion.

The transfer ionization process is not included in the calculations. However, Justiniano *et al.* show that the cross section for (2) has a magnitude of only 6% of that for (1) at 200 eV/amu.

The (n,l) cross sections show the dominant product is $Ar^{7+}(4f)$. At high velocities, the $n=4$ low angular momentum states increase their contribution to the total cross section.

At low velocities, we must also consider the effect of curve crossings at large internuclear separations. We find that $Ar^{7+}(5s)+He^+$ state has an avoided crossing with the initial channel at $10.1a_0$. Simple Landau-Zener calculations place the magnitude of the $Ar^{7+}(5s)$ partial cross section at $7\times10^{-18}v^{-1}$ cm^2, where the velocity v is in atomic units. At the lowest velocity studied, $v=0.03$ a.u., the coupled-channel results shown in Fig. 2 should be increased by $\sim 10\%$ to reflect the contribution from the long-range crossing with the $Ar^{7+}(5s)$ state. The adiabatic splittings at the avoided curve crossings with the higher angular momentum states of the $n=5$ manifold are much smaller than that of the $5s$ and, hence, need not be considered for this study.

In conclusion, we find the procedure of only allowing single-electron excitations in the configuration list of a pseudo-two-electron system yields eigenenergies and eigenfunctions of sufficient accuracy that they may be used in single-electron-capture cross-section calculations. Such a procedure makes the calculations feasible and removes the multitude of doubly excited levels that plague a complete two-electron CI calculation on a system with a high-charge-state ion. Further comparisons with experimental data are needed before this theoretical procedure can be considered reliable for broad classes of systems.

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