Low-energy electron capture by Cl^{7+} from D using merged beams

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Measurements of the absolute total cross section for single-electron capture in collisions of Cl^{7+} with ground-state atomic deuterium are reported in the energy range 4.6–428 eV/amu. These measurements represent the highest charge state yet reported using the Oak Ridge National Laboratory ion-atom merged-beams apparatus. The electron-capture cross section for Cl^{7+} is observed to decrease at lower energies, in contradiction to what is expected from a popular simple model and speculation from previous measurements for highly charged $(7+)$ ions with multielectron cores. The observed low-energy behavior is interpreted using coupled-channel molecular-orbital hidden-crossing calculations for $N^{7+}+D$.

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I. INTRODUCTION

Low-energy electron capture (LEEC) from neutral atoms plays an important role in charge and energy transport in astrophysical and laboratory plasmas [1]. For example, the need for benchmark low-energy electron-capture cross section data for calculations used in modeling the dynamics of the edge plasma and diverters in tokamak designs has been demonstrated [2,3]. Spectral modeling of astrophysical plasmas can be significantly influenced by electron capture, since it plays a critical role in establishing the ionization balance [4].

Experimental data for electron capture from atomic hydrogen (deuterium) by *heavy* multicharged ions have been relatively scarce, due in part to the difficulty in making sufficiently intense beams at low energies. This lack of data is evident in particular for highly charged ions with multielectron ionic cores at low (eV/amu) collision energies. However, some general characteristics have been observed. A time-of-flight technique by Phaneuf [5] used a pulsed-laser-produced plasma to produce beams of heavy multicharged ions at low (eV/amu) energies which were directed through a thermal dissociation atomic hydrogen oven. When compared to other hydrogen oven measurements by Crandall *et al.* [6] at higher energies (300–2000 eV/amu), obtained with beams using a Penning discharge ion source, the capture cross sections were found to be approximately independent of energy for the systems studied. This behavior of the cross section was thought [5] to be representative for collisions with highly charged ions in which the number of bound electrons exceeds the ionic charge. However, only a limited number of cross section measurements were taken over a large energy range. The measurements by Phaneuf [5] at $E<100$ eV/amu energies indicate that the cross section for $Fe^{q+}+H, q=3-14$, can be estimated by $q\times10^{-15}$ cm^2 within 25%.

This behavior is in contrast to the observed [7] Z oscillations in the electron-capture cross section for fully stripped and H-like (one-electron core) projectile ions at collision energies near the peak of the cross section. Furthermore, merged-beams measurements for the ions B^{4+}, C^{4+}, N^{4+}, O^{4+}, and Si^{4+} with D [8–12] show that the cross sections for these relatively light $4+$ ions vary by as much as a factor of 10 at 1 eV/amu.

Fully quantal coupled-channel molecular-orbital (MOCC) theory is considered most appropriate at low collision energies, but it requires accurate molecular potentials and wave functions, appropriate electron translation factors (ETF's), and appropriate choice of the basis of molecular electronic wave functions. All these conditions are difficult to meet when used with a heavier ion projectile, having many electrons in the core. Simple theoretical methods have been used to explain the cross section, including the absorbing-sphere model of Olson and Salop [13], the tunneling model of Grozdanov and Janev [14], the classical overbarrier model of Ryufuku and Watanabe [15], the Landau-Zener (LZ) model [16], and hidden-crossing (HC) theory [17]. In general, when quasiresonant conditions for tunneling or overbarrier transitions between the electronic states of the two potential wells are fullfilled, as they are in the case of hydrogen (deuterium) colliding with a highly charged ion, the cross sections are expected to stay mostly flat at low collision energies. Still, in dealing with a finite charge q of the ionic projectiles A^{q+}, the detailed behavior of LEEC cross sections depends on the actual quasimolecular structure of the $(AH)^{q+}$ system. This may involve, for example, interference between various reaction paths and trajectory acceleration effects, causing deviations of the flat behavior, like local dips, oscillations, or increases in the cross sections at low energies. When the ionic core of charge q is a closed shell and the collision energy is sufficiently low that small internuclear distances

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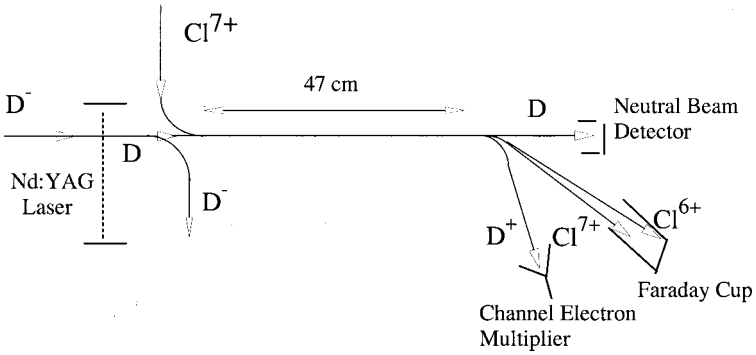

FIG. 1. Schematic diagram of the ORNL ion-atom merged-beams apparatus. See text for details.

play a minor role in the transition dynamics, a possible simplification is to consider an analog bare ion projectile with the same charge q. Such an approach enables one to reach accuracy in all required aspects of the calculation, sacrificing possibly unimportant ion core effects. This is the theoretical approach we adopt here.

II. EXPERIMENT

The ORNL ion-atom merged-beams apparatus [18–20] in conjunction with the ORNL ECR Caprice ion source [21] has been used in recent years to perform benchmark electron-capture cross section measurements for collisions of various multicharged ions with H and D at relative energies from 20 meV/amu to 5000 eV/amu. In this approach [20], beams of neutral atoms and multicharged atoms having energies in the keV range are merged onto a common axis. By adjusting the kinetic energies of the beams, the relative velocity of the two beams can be ''tuned'' over a very large range of collision energies. Figure 1 is a simplified schematic of the apparatus. A 1–5 μA Cl^{7+} multicharged ion beam with an energy of $q\times(9-18)$ keV was merged electrostatically with an 8.2 keV neutral deuterium beam. The merged beams interacted in a field-free region for a distance of 47 cm, after which the primary beams were magnetically separated from each other and from the product or ''signal'' D^+ ions. The Cl^{6+} product of the reaction was not measured separately, but was collected together with the primary Cl^{7+} ions in a large Faraday cup. The neutral beam intensity was measured by secondary-electron emission from a stainless steel plate, and the signal D^+ ions were recorded by a channel electron multiplier operated in pulse counting mode. The ground state beam of D atoms was produced by passing an 8.2 keV beam of D^- ions through the optical cavity of a 1.06 μm Nd:YAG lyttrium aluminum garnet laser, where kilowatts of continuous power circulated. The D^- beam was produced with a duoplasmatron ion source.

Electron-capture cross sections were determined absolutely by measuring the rate of D^+ ion production by the beam-beam interaction over the merge path. Production of D^+ ions due to ionization was assumed negligible for the energies used here. The electron-capture cross section value was determined at each velocity from directly measurable parameters by the formula

$$\sigma=\frac{R\gamma q e^2 v_1 v_2}{I_1 I_2 v_r F}, \tag{1}$$

where R is the signal count rate, q the charge of the ion, e the electronic charge, I_1, I_2 the intensities of the two beams, v_1, v_2 the velocities of the D and Cl^{7+} ions, v_r the relative velocity between the D and Cl^{7+} ions, γ the secondary-electron emission coefficient of the neutral detector, and F the form factor that quantifies the overlap of the beams. The integrated three-dimensional form factor was estimated from two-dimensional measurements of the overlap at three different positions along the merge path. The secondary-electron emission coefficient in the neutral detector, γ, was measured *in situ* as described previously [20] and found to be 0.98 ± 0.03.

The signal rate R was extracted from the background by using a two-beam modulation technique [20]. Backgrounds on the order of 10 kHz were produced by collisional ionization of D on the background gas in the merged path where pressures were on the order of 1.3×10^{-8} Pa. Backgrounds on the order of 80 Hz were a result of the photons emitted during collection of the Cl^{7+} ions in the Faraday cup. Signal rates of 30 Hz were observed at the higher collision energies, the signal decreasing to a few hertz at the lower energies due not only to the observed decrease in cross section but also to the fact that the number of collisions along the merge path scales as v_r.

Even though the neutral beam was estimated to be 99.99% pure ground state, the signal due to excited states comprised a few percent $(6\%\pm2\%)$ of the measured signal. The excited states of D are formed by collisional detachment of D^-. To correct for the signal due to the excited states, the signal was measured with and without the laser on. The difference between the signals corresponded to the signal due to the ground state collisions.

One advantage of the merged-beams technique is the large angular collection in the center-of-mass frame due to the kinematic transformation to the laboratory frame. The low-energy electron-capture collisions under study are exoergic and both products are positively charged. Therefore significant angular scattering can occur in the center-of-mass frame [22]. However, due to the kinematic frame transformation, this angular scattering is significantly compressed in the laboratory frame in which the products are collected. No quantal calculations for $Cl^{7+}+D\rightarrow Cl^{6+}+D^+$ angular scattering exist, but a multichannel LZ estimate indicates that capture to the $n=5$ and 4 shells is the most probable. From the determined [23] angular collection of the apparatus in the laboratory frame of 2.3°, one can estimate the maximum

TABLE I. The hidden-crossing parameters for the $N^{7+}+D$ (or H) system in the considered subset of molecular adiabatic states.

$N\ell m \leftrightarrow (N+1)(\ell+1)\ell m$	$\mathrm{Re}\{R_c\}$	$\mathrm{Im}\{R_c\}$	Δ
$6h\sigma \leftrightarrow 7i\sigma$	31.84	<0.001	$<10^{-4}$
$5g\sigma \leftrightarrow 6h\sigma$	11.585	0.594	0.011
$4f\sigma \leftrightarrow 5g\sigma$	6.090	1.354	0.253
$3d\sigma \leftrightarrow 4f\sigma$	3.045	1.334	0.902
$7i\sigma \leftrightarrow 8j\sigma$	14.517	4.276	0.484

angle at which the product D^+ can be emitted in the center-of-mass frame as a function of collision energy for capture to specific states in the $n=4$ and 5 manifolds. The angular collection increases as the collision energy decreases, from an average of 10° at 100 eV/amu to 40° at 10 eV/amu.

Relative uncertainties in the measured signal are mainly due to counting statistics. Absolute uncertainties in the cross section were estimated to be 12% at the 90% confidence level and have been discussed previously [20].

III. THEORY

Assuming that the principal reaction paths for low-energy electron capture in the $Cl^{7+}+D(1s)$ system lie at internuclear distances large enough so that the [Ne] core of Cl^{7+} does not play a significant role in the collision dynamics, we consider the single-electron $(ND)^{7+}$ system as a model system for $(ClD)^{7+}$. To get insight into the LEEC dynamics, we first perform a hidden-crossing [24] analysis [17,25] of the $(ND)^{7+}$ system. A HC MOCC [26] calculation is then performed for $(ND)^{7+}$ to interpret the results of the present measurements.

The real and imaginary parts of the branch points R_c (hidden crossings) among the adiabatic molecular electronic eigenenergy surfaces of $(ND)^{7+}$ in the plane of complex internuclear distance are presented in Table I along with the corresponding Massey parameters, which we found relevant for the LEEC process. The corresponding adiabatic energy terms, as a function of internuclear distance, as well as the positions of the localized transitions induced by the hidden crossings, are plotted in Fig. 2. The molecular states are designated by the united atom spherical quantum numbers N, ℓ, and m. Thus, $7i\sigma$ is the electronic molecular state of $N^{7+}+D$ evolving from the ground state of deuterium. The hidden crossings shown are of the so-called Q type [17], associated with the top of the radial barrier between the two potential wells, localized around the deuterium and nitrogen nuclei. The exception is the branch point at $R\sim 32$ a.u. (R_{c_1} in Fig. 2) between the $7i\sigma$ and $6h\sigma$ states, which is an isolated Landau-Zener avoided crossing, describing the tunneling close to the top of the potential barrier between accidentally and locally quasiresonant atomic states. According to the parameters for the avoided crossing in Table I, a transition from the initial $N^{7+}+D(1s)$ molecular state $7i\sigma$ to the $6h\sigma$ electron-capture state $N^{6+}(n=6)+D^+$ is almost completely diabatic in the collision energy range considered (1–150 eV/amu). As a consequence, the $n=6$ excited state

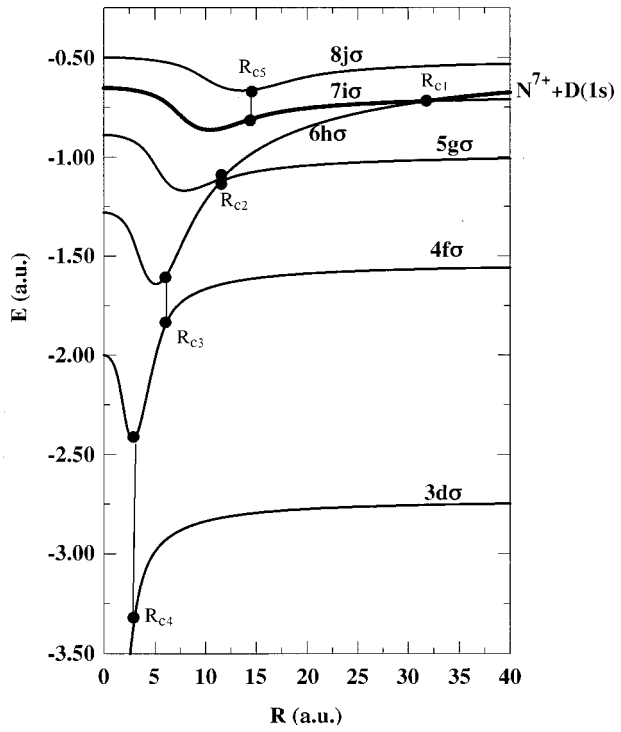

FIG. 2. Adiabatic electronic molecular terms for the $N^{7+}+D$ (or H) system. The only electronic state localized asymptotically at D is $7i\sigma$. The positions of the hidden crossings and corresponding transitions, projected to the real internuclear distance R, are shown by filled circles and vertical lines, respectively.

of N^{6+} is not expected to be populated in the electron-capture process.

As N^{7+} approaches D along the $7i\sigma$ state, it passes diabatically (at R_{c_1}) to the $6h\sigma$ term of $N^{6+}+D^+$, followed by a transition to the $5g\sigma$ $[N^{6+}(n=5)+D^+]$ state at $R_{c_2}\sim 11.5$ a.u. The $4f\sigma$ state $[N^{6+}(n=5)+D^+]$ is populated from the $5g\sigma$ state by a weaker transition around $R_{c_3}\sim 6$ a.u. The probability of this transition is exponentially small, $P\sim\exp(-2\Delta/v)$, at low collision velocities v, as long as v is smaller than the relevant Massey parameter Δ [24,17] (center-of-mass collision energy <20 eV/amu). A transition to $3d\sigma$ at $R_{c_4}\sim 3$ a.u. is too weak at the considered energies (Massey parameter close to 1, and thus $\Delta/v\gg 1$). The same is true for the $7i\sigma$-$8j\sigma$ transition: Besides the large Massey parameter, this transition (unlike the others considered here) is endoergic, having a threshold of a few eV. Thus, only $n=5$ (for $E<20$ eV/amu) and $n=4$ states of N^{6+} will be populated significantly in the LEEC process. This coincides with the corresponding LZ estimates for the $Cl^{7+}+D$ electron-capture process (see Sec. II).

In the receding phase of the collision, the probabilities of keeping the electronic populations in the charge exchange states of N^{6+} are proportional to terms of the form $1-P$. Thus, at the end of the collision, the electron-capture probability is a subtle trade-off of various $P(1-P)$ terms, leading, at least in principle, to the exponential decrease of the cross section as the velocity decreases below the values of the relevant Massey parameters. Still, the ''trajectory accel-

eration'' effects, which increase the transition probability (as $1/v$) in very slow exoergic transitions, may be in direct competition with this exponential decrease. In effect, the charge exchange cross section may experience some drop toward low collision energies before trajectory effects become important. When and whether it is going to happen obviously depends on the detail of the molecular potential surface topology for the collision system considered, as described by the hidden-crossing parameters in Table I.

To avoid uncertainty in the influence of the trajectory acceleration effects on low-energy electron capture as well as possible interference along the various reaction paths, we performed a fully quantal molecular-orbital close-coupling calculation [27], which involved the solution of a truncated set of coupled second-order differential equations for the scattering amplitudes for the partial waves of the internuclear motion. This calculation relies on matrix elements of the radial nonadiabatic perturbation $\partial/\partial R$ between the adiabatic electronic molecular states. These matrix elements, in general, do not satisfy the collision boundary conditions at large internuclear distances, which require vanishing of all couplings. In addition, they significantly depend on the choice for electron coordinate origin. The standard approach to correct for these problems is to use (nonuniquely defined) ETF's and/or to increase the size of the adiabatic basis, often resulting in additional numerical difficulties and uncertainties.

Here we propose another approach: use of the approximate nonadiabatic radial matrix elements, obtained from the hidden-crossing parameters [24,28] (HCME's), in the analytic form of the Lorentzian [26]

$$\left\langle i \left| \frac{\partial}{\partial R} \right| j \right\rangle \approx \frac{1}{2} \frac{\mathrm{Im}\{R_c\}}{(R-\mathrm{Re}\{R_c\})^2+(\mathrm{Im}\{R_c\})^2}, \qquad (2)$$

where i and j denote the sets of quantum numbers for the coupled adiabatic molecular states, and R_c is the (complex) hidden crossing of the relevant electronic eigenenergy surfaces. A time-dependent MOCC calculation with these matrix elements has already been successfully used to describe such subtle effects as small oscillations in the excitation cross section [26]. The HCME's are derived using eigenfunctions of the so-called Solov'ev Hamiltonian [24], and have two peculiar features: they already contain the ETF's and do not depend on the choice of the electronic origin. The latter also has the consequence that a relatively small expansion basis in the MOCC may lead to a physically complete description of the collision dynamics. The analytical form of the HCME's in Eq. (2) is an approximation, derived as a leading term in an expansion in the collision velocity v, and valid in the vicinity of the relevant hidden crossings. The last two conditions are the standard assumptions of the validity of HC theory and they usually overlap: If the collision velocity is low enough, transitions are localized in narrow R regions around the hidden crossings. Here we use these matrix elements in a fully quantal MOCC (FQ MOCC HC) approach. We construct a three-state diabatic basis [29] for the set of interacting $(4f\sigma,5g\sigma,6h\sigma)$ states, and the resulting MOCC partial wave equations are solved with the Johnson [30] algorithm of logarithmic derivatives, matching the solutions to the plane wave boundary conditions at $R_{\max}=200$ a.u. The transition $7i\sigma-6h\sigma$ is assumed fully diabatic. Particular attention is paid to convergence and numerical accuracy of the computation, which required several thousand partial waves in the 10 eV/amu collision energy range.

The adiabatic-diabatic transformation performed with the matrix elements in Eq. (2) has a peculiar feature: The integral of the HCME's up to numerical infinity, $R_{\max}$, decreases asymptotically too slowly, as $1/R_{\max}$. This may require use of the Coulomb rather than plane wave boundary conditions with the resulting diabatic basis. A way to avoid this implication is to introduce an arbitrary switching function, which would reduce coupling to zero at $R_{\max}$. Fortunately, the numerical algorithm for the adiabatic diabatic transformation [29] starts the transformation from $R_{\max}$ assuming zero coupling. This has the effect of a smooth switching function, and if $R_{\max}$ is chosen large enough it does not influence the resulting diabatic matrix elements and potentials in the transition active region of R.

Due to the assumptions of the validity of the HCME's in Eq. (2) as well as the use of the restricted expansion basis, our calculation is applicable only up to approximately 150 eV/amu. At higher collision energies, not only are new reaction channels opening that are not included here, but also the accuracy of the HCME's deteriorates due to loss of localization of the transitions.

IV. RESULTS AND DISCUSSION

The ion-atom merged-beams apparatus has been used to measure total electron-capture cross sections for $Cl^{7+}+D \rightarrow Cl^{6+}+D^+$ collisions. The measurements are presented in Table II and Fig. 3. In Table II the cross sections are listed along with the relative and total uncertainties in the measurements estimated at a 90% confidence level. The total uncertainty in the measurements corresponds to a quadrature sum of the absolute and relative uncertainties. In Fig. 3 the cross section is plotted with the relative uncertainty.

While no theory exists for this multielectron system, one can compare the peak, plateau values of the cross sections to the scaling proposed by Phaneuf [5]. This scaling predicts the cross section in this case to be 70×10^{-16} cm^2, which agrees well with previous measurements of Fe^{7+} [5] and Al^{7+} [31] multielectron ions with H and reasonably well with the measured plateau values of the total electron-capture cross sections above approximately 40 eV/amu ($\sim 55 \times10^{-16}$ cm^2).

A simple multichannel Landau-Zener (MCLZ) analysis of the diabatic potentials for the $(ClD)^{7+}$ system suggests that capture into the $4d$ and $4f$ orbitals dominates the electron-capture cross section in the 1000 to 20 eV/amu energy range and the $5s$ orbital begins to contribute to the cross section below 20 eV/amu. This agrees qualitatively with the HC analysis for the $N^{7+}+D$ system in Sec. III. LZ calculations using a variety of couplings [13,32] predict that the cross section is (slightly) increasing toward lower energies. The

TABLE II. The measured total electron-capture cross sections for the reaction $Cl^{7+}+D \rightarrow Cl^{6+}+D^{+}$ with collision energies. The uncertainties are listed at the 90% confidence level.

Energy (eV/amu)	Cross section (10^{-16} cm^2)	Relative uncertainty (10^{-16} cm^2)	Total uncertainty (10^{-16} cm^2)
4.6	24.4	4.3	5.2
7.1	27.1	3.1	4.5
7.9	23.5	4.2	5.1
8.3	33.3	3.5	5.3
9.0	37.0	5.1	6.8
10.2	33.9	3.0	5.0
11.7	37.4	4.7	6.5
13.0	41.3	3.6	6.1
14.1	41.8	4.0	6.4
16.1	37.8	2.2	5.0
18.3	41.9	2.5	5.6
20.6	46.8	2.6	6.2
22.0	43.6	4.0	6.6
25.5	47.0	2.2	6.0
30.5	47.1	2.6	6.2
35.5	51.9	3.2	7.0
42.6	54.1	2.1	6.8
47.4	55.8	3.4	7.5
55.4	51.2	2.1	6.5
69.6	56.3	3.5	7.6
104	57.7	2.6	7.4
150	56.4	2.4	7.2
200	55.7	4.7	8.2
263	58.6	5.4	8.9
337	60.2	2.7	7.7
428	55.4	3.9	7.7

MCLZ calculation using the couplings of Ref. [13] is shown in Fig. 3 as an illustration. It should be noted that no reasonable couplings resulted in a satisfactory fit of the MCLZ calculation to the measurements. The cross section energy behavior predicted by MCLZ theory reflects the expectation that for multielectron highly charged ions the cross section will be flat or increasing [33] with decreasing collision energy.

The present data, however, show a cross section that decreases with decreasing energy to a value of $\sim 24 \times 10^{-16}$ cm^2 at 4.6 eV/amu. To get an insight into the dominant physical processes, the measured electron-capture cross section data for $Cl^{7+}+D$ are compared in Fig. 3 to our calculation of the total electron-capture cross section for the process $N^{7+}+D \rightarrow N^{6+}+D^{+}$. Agreement of the two sets of data is obtained in the range of validity of the applied theory (see Sec. III), at collision energies below 150 eV/amu. This agreement seems to validate the assumption that at low energies electron capture occurs at large internuclear separations which do not probe the Cl^{7+} [Ne] core. The core may have an effect at larger energies, though, where the electron transfer process accesses smaller internuclear separations. The atomic orbital coupled-channel (AOCC) calculations of Fritsch and Lin [34] and the MOCC calculation of Kimura and Lane [27] for electron capture in the $N^{7+}+H$ system are in fair agreement with the plateau values of the current measurement of the $Cl^{7+}+D$ system as well as with previous experimental values of Meyer *et al.* [7] for $N^{7+}+H$. As seen in Fig. 3, although the calculations did not extend below 100 eV, they suggest a decreasing cross section toward lower energies, as obtained in the current measurement and the MOCC calculation. The present FQ-MOCC-HC calculation is also performed for $N^{7+}+H$ (not shown). A slighty larger cross section for H is due to trajectory effects which are more pronounced at the lower energies. Although not shown in the figure, the present calculation predicts a cross section that rises again at energies below 1 eV/amu.

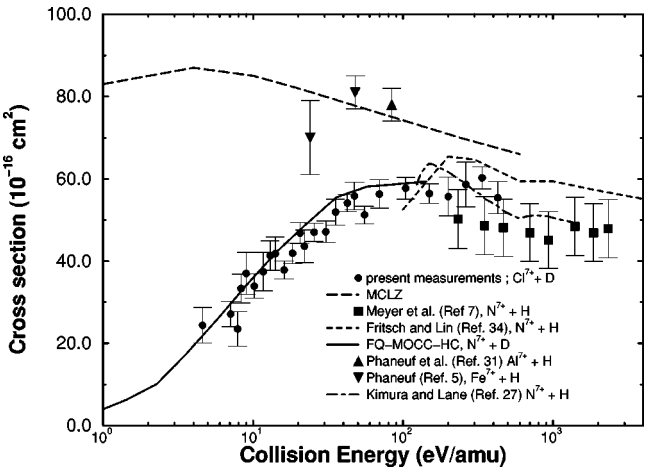

FIG. 3. Plot of total electron-capture cross section measurements for $Cl^{7+}+D \rightarrow Cl^{6+}+D^{+}$ versus collision energy (eV/amu). The error bars represent the relative uncertainty in the measured cross sections at the 90% confidence level. A comparison is shown with theory including the present fully quantal molecular-orbital coupled-channel hidden-crossing calculation for $N^{7+}+D \rightarrow N^{6+}+D^{+}$ (solid line) and with other measurements with $7+$ ions.

V. CONCLUSION

Total electron-capture cross sections for $Cl^{7+}+D \rightarrow Cl^{6+}+D^{+}$ have been measured over the energy range 4.6–428 eV/amu. The cross section has a magnitude of 55×10^{-16} cm^2 at collision energies above 40 eV/amu. Below 40 eV/amu the cross section monotonically decreases to a value of $\sim 24 \times 10^{-16}$ cm^2 at 4.6 eV/amu. A fully quantal molecular-orbital hidden-crossing calculation for the $N^{7+}+D$ system shows a similar low-energy behavior as is observed for $Cl^{7+}+D$, suggesting that the electronic structure of the closed [Ne] shell has little effect. The fact that the cross section for the highly charged mulitelectron ion Cl^{7+} does not remain flat toward decreasing energies shows that the actual quasimolecular structure and associated dynamics remain important. Future efforts will explore other highly charged multielectron ions with open and closed shells to determine for which ions, if any, simple models are inadequate.

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