PHYSICAL REVIEW A **75**, 054701 (2007)

Low-energy electron capture by Ne^{2+} ions from H(D)

B. Seredyuk,* H. Bruhns, and D. W. Savin
Columbia Astrophysics Laboratory, Columbia University, New York, New York 10027-6601, USA

D. Seely
Albion College, Department of Physics, Albion, Michigan 49224-1831, USA

H. Aliabadi, E. Galutschek, and C. C. Havener
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6372, USA
(Received 12 March 2007; published 2 May 2007)

Using the Oak Ridge National Laboratory (ORNL) ion-atom merged-beams apparatus, the absolute, total single-electron-capture cross section has been measured for collisions of Ne^{2+} with deuterium (D) at center-of-mass (c.m.) collision energies of 59–949 eV/u. With the high-velocity ion beams now available at the ORNL Multicharged Ion Research Facility, we have extended our previous merged-beams measurement to lower c.m. collision energies. The data are compared to all four previously published measurements for Ne^{2+}+H(D) which differ considerably from one another at energies $\lesssim$600 eV/u. We are unaware of any published theoretical cross-section data for Ne^{2+}+H(D) at the energies studied. Early quantal rate coefficient calculations for Ne^{2+}+H at eV/u energies suggest a cross section many orders of magnitude below previous measurements of the cross section at 40 eV/u which is the lowest collision energy for which experimental results have been published. Here we compare our measurements to recent theoretical electron-capture results for He^{2+}+H. Both the experimental and theoretical results show a decreasing cross section with decreasing energy.

DOI: 10.1103/PhysRevA.75.054701 PACS number(s): 34.70.+e, 95.30.Dr, 98.38.Bn, 98.58.Bz

I. INTRODUCTION

Studies of electron capture (EC) by ions from atomic hydrogen are of fundamental interest for atomic and molecular physics and are also important for astrophysical and fusion research [1,2]. Much theoretical and experimental work has been performed in order to provide the EC data needed to model and interpret the spectra of these laboratory and astrophysical plasmas. However, many significant issues remain unresolved.

In astrophysics, EC cross sections are important for calculating the ionization balance of planetary nebulae and H II regions [3,4]. Of particular interest are spectral emission lines from Ne ions which are commonly observed in these photoionized objects but for which significant discrepancies exist between models and observations [5,6]. For example, Pequinot *et al.* [5] suggested that not accounting for EC of Ne^{2+} on H was the cause of the difference between photoionization models and observed spectra of the planetary nebula NGC 7027. This was followed up by quantal calculations from Butler *et al.* [7,8] which implied that the rate coefficient for Ne^{2+}+H EC was far too small to remove the discrepancy. However, their calculations considered only transitions from the initial ground state $[Ne^{2+}(2s^2 2p^4\,{}^3P)+H]$ to the strongly exoergic final state $[Ne^{2+}(2s^2 2p^5\,{}^2P)+H^+]$. These states are far apart at all internuclear distances, with a separated atom limit of 27.2 eV. This results in a sharply decreasing cross section toward thermal energies. Further investigation by Forster *et al.* [9] considered initial metastable excited states of Ne^{2+} and slightly exoergic final states of Ne^{+}, within the doublet manifold of adiabatic states. Their results indicated that the EC rate coefficients are still much too low to explain the discrepancies between observations and models of planetary nebulae. But the issue of the Ne-line intensities remains unresolved. Pottasch and Beintema [6] have noted factor of 3 differences among the various Ne abundance determinations for the planetary nebula NGC 6302. They proposed that this may be due to errors in the underlying atomic data. Along these lines, subsequent investigation of the electronic potential-energy curves for Ne^{2+}+H by Mroczkowski *et al.* [10] suggests that rotational coupling to slightly endoergic quartet states, which Butler *et al.* [7,8] and Forster *et al.* [9] did not account for, may enhance the Ne^{2+} EC rate coefficient.

In fusion energy research, EC cross sections at collision energies of eV/u to hundreds of eV/u are needed for the accurate modeling and diagnostics of the plasma edge. An issue of particular interest for fusion research is the effect that impurity ions have on the plasma [11]. Neon is of special interest as it is often injected into magnetic fusion devices to enhance the confinement in the core plasma and to reduce the heat flux to the plasma-facing surfaces [12]. Accurately modeling the Ne charge balance and radiative cooling in these plasmas requires reliable EC cross sections for the various ionization stages of Ne over a wide range in energies.

Our present work is partly to follow up the implications of Mroczkowski *et al.* [10] and to provide data needed for fusion devices. To be specific, here we report absolute measurements for the total EC cross section of

*Electronic address: seredyuk@astro.columbia.edu

$$Ne^{2+} + H(D) \rightarrow Ne^{+} + H^{+}(D^{+}) \quad (1)$$

in the collision energy range of 59–949 eV/u. Previous experimental studies for this system have been carried out by Can *et al.* [13] in the energy range 40–100 eV/u, by Huber [14] in the range 80–270 eV/u, by Mroczkowski *et al.* [10] in the range 139–1490 eV/u, and by Seim *et al.* [15] in the range 200–1400 eV/u. These data show good agreement for energies $\gtrsim$600 eV/u, but at lower collision energies there are considerable differences. Additionally, the early quantal rate coefficient calculations by Butler *et al.* [7,8] for Ne^{2+}+H at eV/u energies suggest a cross section many orders of magnitude below the previous measurements of Can *et al.* [13] at 40 eV/u which is the lowest collision energy for which experimental results have been published.

To help resolve this situation we have extended the previous Oak Ridge National Laboratory (ORNL) merged-beams measurements by Mroczkowski *et al.* [10] to lower energies. Their measurements had a low-energy limit of 139 eV/u due to the limited acceleration potential of the CAPRICE electron cyclotron resonance (ECR) ion source [16] at the Multicharged Ion Research Facility (MIRF). Recently the ion-atom merged-beams apparatus has been upgraded [17] to accept the higher-velocity beams from a new 250 kV high-voltage (HV) platform [18] at MIRF.

The rest of this paper is organized as follows: A brief description of the improvements to the apparatus is given in Sec. II. In Sec. III we present our measurements. Conclusions are given in Sec. IV. Throughout this paper, collision energies are quoted using the center-of-mass (c.m.) energy divided by the reduced mass of the colliding particles—i.e., eV/u where u is the atomic mass unit.

II. EXPERIMENTAL APPARATUS

The main features of the ORNL ion-atom merged-beams apparatus have been described in detail elsewhere [19,20]. Using the merged-beams technique, relatively fast (keV) beams are colinearly merged, allowing for a large dynamic range of relative c.m. collision energies [19]. Merged-beams measurements typically span from meV/u to keV/u. However, the previous ORNL merged-beams measurements of Mroczkowski *et al.* [10] for Ne^{2+}+D could not access collision energies below 139 eV/u due primarily to the limited acceleration potential of the CAPRICE ECR ion source. For those measurements where the D beam is faster than the ion beam, lower c.m. collision energies can potentially be achieved by using either a slower D beam or a faster ion beam. However, operation of the D^- source at voltages lower than 6 kV or of the ECR at voltages near 22 kV led to poor quality or unstable beams. To extend our previous measurements to lower c.m. energies, we have used higher-velocity Ne^{2+} beams from the new HV platform at MIRF. Our measurements are absolute with the cross section determined by measurement of the beam-beam EC signal, beam-beam overlap, and intensity of the primary beams [19,20].

At MIRF, ions from the new HV platform are accelerated at 25–250 kV and are now available for experimental investigations of their collisions with electrons, atoms, molecules, and solid surfaces. Details of the HV platform can be found elsewhere [18]. Multicharged ions are produced by an all-permanent magnet 12.75–14.5-GHz ECR ion source, designed and fabricated at CEA/Grenoble [21].

The upgraded ion-atom merged-beams apparatus and associated beamline [17] are only briefly discussed here. The transport beamline from the HV platform to the ion-atom merged-beams path has been designed for maximum transmission and is equipped with three sets of horizontal and vertical slits and two sets of electrostatic quadrupoles to control the beam divergence and shape in the merge path. In the present investigation, a Ne^{2+} beam with an energy in the range of 40–72 keV is merged with a D beam with an energy in the range of 8.25–11.5 keV, thereby allowing relative collision energies in the range of 15–949 eV/u. Ne^{2+} ion beams of 5–10 μA, 2–4 mm full width at half maximum (FWHM), and 0.15° half-angle divergence in the merge path are typical.

The possible presence of metastables in the Ne^{2+} beam extracted from an ECR ion source was investigated by Bannister [22] through measurements of the electron-impact ionization cross section. No ionization signal was observed below the ground-state ionization threshold of 63.45 eV, indicating no detectable population of metastables in the Ne^{2+} beam. Though we are using a different ECR source for these measurements, based on the work of Bannister we expect no significant metastable fraction in our ion beam.

A neutral ground-state atomic D beam is obtained by photodetachment of a D^- beam produced using a duoplasmatron ion source. The photodetachment occurs inside the multimode optical cavity of a 1.06-μm cw Nd:YAG laser where kilowatts of continuous power circulate. The resulting D beam is nearly parallel with a divergence of less than 0.15°. The beam has a diameter of 2–4 mm and intensities ranging from 10 to 20 nA. For our measurements reported here D was used instead of H to maximize the angular acceptance of the apparatus [19,23]. Isotope effects from the use of D instead of H, due to differences in trajectories of the colliding particles, are not expected to be significant at the energies studied [23].

The Ne^{2+} beam is electrostatically merged with the neutral D beam. We have upgraded our merge chamber to use spherical deflectors to merge the beams. Electrostatic spherical deflectors can handle the higher-energy beams of the new ion source and provide focusing in both the horizontal and vertical dimensions. This is a major improvement from the previous arrangement which used parallel-plate deflectors.

The ion and atom beams interact along a field-free region of 32.5 cm (reduced from the previous merge-path length of 47 cm). Afterwards the D^+ product ions are magnetically separated from the primary beams and detected by a channel electron multiplier. Since only the D^+ product is measured, the apparatus actually measures electron loss, the sum of electron capture, and neutral target ionization. However, ionization at these energies is negligible compared to electron capture [24].

Features of the system also include a dual wire scanner in the merge path. The signal of this dual-wire scanner, designed at ORNL [25], is acquired by a Tektronix digital oscilloscope [21] and read by a computer through TCP/IP using

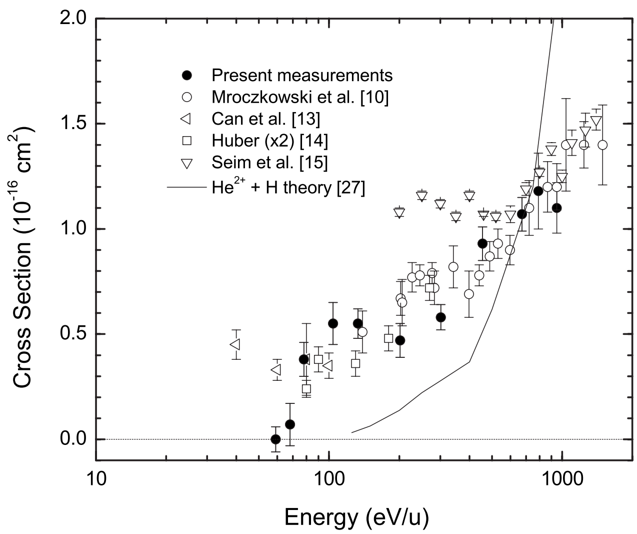

FIG. 1. Present and previous [10] ion-atom merged-beams measurements of the EC cross section for $Ne^{2+}+D \rightarrow Ne^{+}+D^{+}$ as a function of collision energy. The error bars on the merged-beams data denote the statistical uncertainties at a 90% confidence level. Measurements of the EC cross section for $Ne^{2+}+H \rightarrow Ne^{+}+H^{+}$ of Can *et al.* [13], Huber [14], and Seim *et al.* [15] are also shown. See these cited references for a discussion of the meaning of their error bars. A comparison is shown with theoretical calculations for $He^{2+}+H$ by Havener *et al.* [27].

the LabView [21] programming environment. This gives a real-time measurement of the beam shapes, used to determine the overlap of the beams [26]. As compared to the single-wire scanner, the dual-wire scanner provides a more accurate beam-beam overlap measurement as well as an additional overlap measurement in the merge path. Currently the average form factor is calculated from four beam profiles along the merge-path length of 32.5 cm. As referenced from the exit of spherical deflectors, beam profiles are measured at 3.4 and 29.3 cm using mechanical slits and also at 18.4 and 24.4 cm using the dual-wire wire scanner.

The neutral D beam is determined using secondary electron emission from a stainless steel plate. A procedure is used for *in situ* calibration of the detector [19]. The intensity of the Ne^{2+} beam was measured using a biased Faraday cup. The signal rate (hertz) is extracted from backgrounds (kilohertz) by a two-beam modulation technique [19].

III. RESULTS AND DISCUSSIONS

Figure 1 shows our present total absolute EC cross section for $Ne^{2+}+D$ as a function of collision energy compared to previously published measurements. The data are plotted showing the statistical uncertainty. Our data are also given in Table I along with the statistical uncertainty and the combined statistical and systematic uncertainty added in quadrature. All uncertainties are quoted at a 90% confidence level. A detailed discussion of our systematic errors is given elsewhere [19].

The agreement between our present data and the previous ORNL merged-beams data of Mroczkowski *et al.* [10] is within the total uncertainties of the respective measurements over the entire energy range measured. At energies above 600 eV/u, the data of Seim *et al.* [15], the previous ORNL merged-beam measurements, and the present measurements are all in good agreement. All three measurements show a decreasing cross section with decreasing energy. At energies of 200–600 eV/u the data of Seim *et al.* show a plateau. This lies significantly above the merged-beams data which continue to decrease with decreasing energy.

TABLE I. Ion-atom merged-beams cross-section data for $Ne^{2+}+D \rightarrow Ne^{+}+D^{+}$ as a function of c.m. collision energy. The last two columns give the statistical uncertainty and the total combined (statistical plus systematic) uncertainty, each at an estimated 90% confidence level. See text for details.

Collision energy (eV/u)	Cross section (10^{-16} cm^2)	Statistical uncertainty (10^{-16} cm^2)	Total uncertainty (10^{-16} cm^2)
59	0.00	0.06	0.06
68	0.07	0.10	0.10
78	0.38	0.08	0.09
104	0.55	0.10	0.12
133	0.55	0.07	0.10
202	0.47	0.08	0.10
302	0.58	0.06	0.09
456	0.93	0.08	0.14
673	1.07	0.08	0.15
790	1.18	0.18	0.23
949	1.10	0.12	0.18

In the energy range 80–270 eV/u the cross-section data of Can *et al.* [13] and the data of Huber [14] are consistent with the merged-beams data. The Huber data shown in Fig. 1 are corrected as proposed by Can *et al.* Both Huber and Can *et al.* normalized their $Ne^{2+}+H$ data to their respective $Ne^{2+}+H_2$ results. Can *et al.* used their $Ne^{2+}+H_2$ results to renormalize the data of Huber, essentially multiplying the original data by a factor of 2. This brings the data of Huber into agreement with those of Can *et al.* and both of our merged-beams measurements.

At energies below 80 eV/u, the only previous results are those of Can *et al.* [13] which show a nearly constant cross section with a possible slight increase with decreasing energy. Together with our previous results at higher energies a flattening out of the cross section was suggested possibly due to rotational coupling to endoergic quartet states [10]. Extending our merged-beams measurements to lower energies to investigate this contribution was one of the motivations behind this work. As can be seen in the figure, at energies below 80 eV/u, our present data decrease sharply with decreasing energy, in contrast to the data of Can *et al.* The statistical error bars at 59 eV/u indicates the sensitivity of the new appratus.

We are unaware of any published theoretical calculations of the EC cross section for $Ne^{2+}+H(D)$ collisions that overlap with the energy range for which measurements exist. So here we compare the experimental data to hidden-crossing coupled-channels calculations for He^{2+}+H [27], a collision system with the same incident charge state but with no electrons on the ion core. Any observed differences can be attributed to interactions with the multielectron, open-shell Ne^{2+} core. Our present results indicate that the Ne^{2+} system decreases sharply toward lower energies. Hidden-crossing coupled-channels calculations by Krstić [28] at even lower energies for He^{2+}+H show that the cross section decreases seven orders of magnitude from 60 to 1 eV/u. Such a sharp decrease for Ne^{2+} would confirm the early quantal estimates of Butler *et al.* [7,8].

IV. CONCLUSIONS

Using the higher-velocity Ne^{2+} beams from the new HV platform at MIRF and an upgraded ion-atom merged-beams apparatus, we present independent, absolute, total EC cross sections for Ne^{2+} on D for the c.m. collision energy range of 59–949 eV/u. This extends our previous merged-beams measurements to lower energies. A consistent set of experimental data now exists for collision energies between 59 and 1490 eV/u. The cross section is observed to decrease sharply below 100 eV/u, unlike the suggested flattening out of the cross section suggested by the previous data of Can *et al.* [13] and the possibility of a significant contribution from rotational coupling to quartet states [10]. We are unaware of any theoretical calculations of the EC cross section for Ne^{2+}+H(D) collisions that overlap with this energy range. Comparison of our experimental results to the theoretical calculations for the doubly charged He^{2+}+H system shows only qualitative agreement, but suggests a sharply decreasing cross section at lower energies. More accurate theoretical models for Ne^{2+} are needed to provide a more detailed comparison with experimental results. Last, our results support previous work that the Ne^{2+} EC thermal rate coefficient is too small to explain the discrepancy between observed and model line intensities for Ne in planetary nebulae. Thus, it is likely that the discrepancies are due to errors in other relevant atomic data or due to unaccounted astrophysical processes.

ACKNOWLEDGMENTS

Work performed at ORNL was supported by the Division of Chemical Sciences, Office of Basic Energy Sciencs, and the Division of Applied Plasma Physics, Office of Fusion Energy Sciences, U.S. Department of Energy under Contract No. DE-AC05-00OR22725 with UT-Batelle, LLC. From Columbia University, B.S., H.B., and D.W.S. were supported in part by NSF Stellar Astronomy and Astrophysics Grant No. AST-0606960 and by NASA Astronomy and Physics Research and Analysis Grant No. NNG06WC11G.

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