Electron loss by atomic and molecular hydrogen in collisions with $^3He^{++}$ and $^4He^+$ ‡

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Total cross sections for single-electron capture by $^4He^+$ and $^4He^{++}$ incident on atomic and molecular hydrogen have been measured in the velocity range $(1–6) \times 10^8$ cm/sec. A classical-trajectory Monte Carlo method was also used to calculate the electron-capture and impact-ionization cross sections for He^{++} on H in this velocity range. The theoretical electron-capture cross sections are found to be in good agreement with the present experimental values at velocities above 2.5×10^8 cm/sec, but tend to underestimate the experimental values by roughly 25% at the lowest velocities. The experimental $He^{++} + H$ electron-capture cross sections are in excellent agreement with the measurements of Shah and Gilbody in the velocity region where the two experiments overlap. No significant isotope effect ($^4He^{++}$ versus $^3He^{++}$) could be discerned on the theoretical cross sections as a function of relative velocity.

INTRODUCTION

The investigation of electron capture by singly and multiply charged ions in collisions with atomic hydrogen is of fundamental as well as practical interest. Use of an atomic hydrogen target simplifies the theoretical approach, allowing critical comparison between theory and experiment. Also, atomic hydrogen (or deuterium) is the prime constituent of both astrophysical and thermonuclear plasmas. Electron transfer and ionization processes involving H and D are consequently of practical importance in describing particle and energy transport in such plasmas.

The simplest asymmetric collision system involving an atomic hydrogen target is that for incident He^{++} ions. Experimental measurements of the total electron-capture cross section σ_{21} for this system have been previously reported by Fite *et al.*[1] in the velocity range $(0.08–1.4) \times 10^8$ cm/s, by Shah and Gilbody[2] in the velocity range $(0.6–2.0) \times 10^8$ cm/s, and by Bayfield and Khayrallah[3] in the range $(0.6–2.6) \times 10^8$ cm/s. While the data of Shah and Gilbody and of Fite *et al.* (as renormalized by Shah and Gilbody) are in reasonable agreement, the measurements of Bayfield and Khayrallah are consistently a factor of almost 2 larger in the velocity range where the measurements overlap. This experimental discrepancy stands in the way of any conclusive test of theoretical calculations on the He^{++}-H system.

We report in this paper the results of recent measurements of the total electron-capture cross section σ_{21} for $^3He^{++}$ incident on atomic hydrogen in the relative velocity range $(1–6.2) \times 10^8$ cm/s, together with classical-trajectory calculations of this cross section in this same velocity range. Also calculated were the cross sections for impact ionization of H target atoms by incident He^{++}. (A few of these calculated values appear in a more general paper on electron loss in multicharged ion collisions.[4]) In addition, we present measurements of the electron-capture cross section σ_{10} for $^4He^+$ incident on atomic hydrogen in the velocity range $(0.7–4.4) \times 10^8$ cm/s. Experimental data on this cross section has, to our knowledge, not been published to date. In order to correct for the incomplete dissociation of molecular hydrogen in the hot-target cell, the electron-capture cross sections for $^3He^{++}$ and $^4He^+$ incident on H_2 were also measured and are presented here.

EXPERIMENTAL AND THEORETICAL METHODS

The details of the experimental apparatus and method will be presented in a subsequent paper[5] and are only briefly summarized here. Beams of $^4He^+$ and $^3He^{++}$ were produced in a simple hot-filament electron-impact ion source, and accelerated through voltages ranging from 10 to 600 kV. The ^3He isotope was used for the doubly charged ions in order to avoid the problem of preparing a $^4He^{++}$ beam free from H_2^+ contamination. Subsequent to charge and mass analysis, the desired ion beam was directed through a tungsten oven in which hydrogen could be thermally dissociated. The primary and charge-transfer components in the emergent beam were separated electrostatically and counted using a channel electron multiplier.

The directly heated tungsten-hydrogen oven is essentially the same as that previously used and described by McClure.[6] The degree of dissociation was determined by monitoring the variation with oven temperature of double-electron capture by

20 keV protons with H_2 and Ar flowing alternately through the oven (Bayfield,[7] Lockwood *et al.*[8]). For a heating current of 130 A, which resulted in a pyrometrically determined oven temperature of 2350 °K, the dissociation fraction was determined to be 0.96 ± 0.02. The gas flow rate into the target cell was determined by measuring the pressure drop across a known small conductance in the gas feed line using a capacitance manometer. The target thicknesses were determined by normalizing to the well-known cross sections for single-electron capture by 20 keV protons incident on H ($\sigma_{10} = 5.2 \times 10^{-16}$ cm^2)[6,9] and H_2 ($\sigma_{10} = 6.0 \times 10^{-16}$ cm^2).[6,10] An independent check on the target thicknesses, made by using the measured flow rate and estimating the effective length and conductances out of the target cell, yielded values in good agreement with those determined by normalization (within 8% for H_2, 2% for H).

The theoretical electron capture and impact-ionization cross sections were calculated using a classical-trajectory Monte Carlo method that has been described previously.[4,11,12] The general method of calculation involves the solution of the classical equations of motion for a three-body system. Hamilton's equations (12 coupled first-order differential equations) are numerically solved for a large number of trajectories where the impact parameters for the He^{++} ion colliding with the proton + electron target are randomly selected via the Monte Carlo method.

The major difficulty that arises is in the representation of the spherically-symmetric hydrogen ground state in a classical description. We have adopted the prescription carefully formulated by Abrines and Percival[11,12] in which the hydrogen atom is represented by a microcanonical momentum distribution.

Individual trajectories for the $He^{++} + (H^+ + e^-)$ reaction are evaluated by placing the He^{++} ion at a large distance from the H target and integrating the equations of motion until the He^{++} ion is a large distance from the proton. If at the end of the collision the electron is still in an orbit around the H^+, then there was no reaction. However, if the electron is found bound to the He^{++} ion, electron transfer occurred and is appropriately tabulated in the computer program. If the electron is found not bound to either He^{++} or H^+, then ionization occurred during the collision. In order to estimate the cross sections for electron transfer and impact ionization, it is normally necessary to calculate from one to two thousand trajectories in order to reduce the statistical error to a reasonable level. The computer time required to calculate both the electron-capture and impact-ionization cross sections at a given energy was normally approximately 25 s on a CDC 7600 computer.

We should emphasize that the classical-trajectory method incorporates all the forces between the three bodies, hence the deflection of the particles is included in the calculations. Curvilinear trajectories are needed to accurately represent the small impact parameter and low-keV energy collisions.

RESULTS

The results of the present electron-capture cross-section measurements for $^3He^{++}$ incident on atomic hydrogen are shown in Fig. 1, together with previously reported measurements.[1-3] The error bars denote total relative experimental uncertainty (statistical uncertainty at 90% confidence level combined in quadrature with the total known systematic and calibration uncertainties estimated at a comparable confidence level), and do not include uncertainties in the cross sections used for normalization. The various sources of systematic uncertainty are enumerated in Table I. The present data are in agreement with the measurements of Shah and Gilbody,[2] and with those of Fite *et al.*,[1] as renormalized by Shah and Gilbody. There is also excellent agreement with recent results by Lockwood *et al.*,[13,14] who measured σ_{21} in the velocity range $(0.8-2.2) \times 10^8$ cm/s. The measurements of Bayfield and Khayrallah,[3] however, are consistently a factor of ~1.5 larger than the present values in the velocity range where the measurements overlap. The data of Bayfield and Khayrallah are

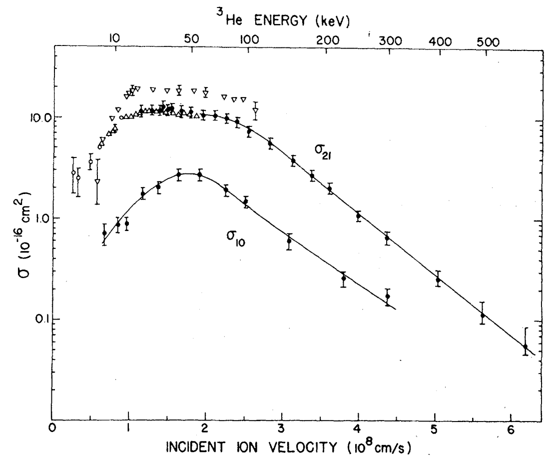

FIG. 1. Total experimental capture cross sections σ_{21} and σ_{10} for $^3He^{++}$ and $^4He^+$, respectively, incident on atomic hydrogen as a function of the relative collision velocity. Solid circles, results of this experimental study; open circles, from Fite *et al.* (Ref. 1); open triangles, from Shah and Gilbody (Ref. 2); inverted triangles, from Bayfield and Khayrallah (Ref. 3).

TABLE I. Summary of systematic uncertainties (%).

Source	$\sigma_{21}(H_2)$	$\sigma_{21}(H)$	$\sigma_{20}(H_2)$	$\sigma_{10}(H_2)$	$\sigma_{10}(H)$
Reproducibility of target thickness calibration	±3	±5	±3	±3	±5
Reproducibility of gas flow	±2	±2	±2	±2	±2
Target-gas purity (maximum effect on σ_{ij}):					
40 keV	±3	±3	$^{+15}_{-3}$	$^{+5}_{-3}$	$^{+4}_{-3}$
400 keV	$^{+12}_{-3}$	$^{+18}_{-3}$	...	$^{+7}_{-3}$	$^{+6}_{-3}$
Uncertainty in dissociation fraction (maximum effect on σ_{ij})	...	±2	...	...	±2
Reproducibility of temperature	±2	±2	±2	±2	±2
Beam collection and counting efficiency	±2	±2	±2	±2	±2
Quadrature sum:					
40 keV	±6	±7	$^{+16}_{-6}$	$^{+7}_{-6}$	$^{+8}_{-7}$
400 keV	$^{+13}_{-6}$	$^{+19}_{-7}$	...	$^{+9}_{-6}$	$^{+9}_{-7}$

normalized to their own earlier measurements of σ_{21} for He^{++}+Ar, whereas the results of Shah and Gilbody, and Fite *et al.*, as well as the present data are normalized to measurements of σ_{10} for H^++H. The consistency of existing measurements for the latter process is better than 20%, whereas discrepancies as large as a factor of 2 exist in the He^{++}+Ar data. The data of Lockwood *et al.* do not depend on any normalization.

Also shown in Fig. 1 are the results for $^4He^+$ incident on H. The cross section σ_{10} displays a velocity dependence similar to that of σ_{21} on the high-velocity side of the cross-section maximum, while being uniformly a factor of ~4 smaller in magnitude. The present data for σ_{10} are in excellent agreement with recent results by Lockwood *et al.*[14,15] for this cross section in the velocity range $(0.2-2.2)\times 10^8$ cm/s.

In Fig. 2 are shown the cross-section results for $^3He^{++}$ and $^4He^+$ incident on H_2. The present data for H_2 targets agree within experimental uncertainties with the measurements of Shah and Gilbody,[16] and of Bayfield and Khayrallah.[17] A semilogarithmic fit to the data of Pivovar *et al.*[18] for σ_{21} (which displays considerable scatter) yields values systematically 10–15% smaller than our own, while a smooth curve through the values obtained by Baragiola and Nemirovsky[19] falls a factor of almost 2 below our data. In the case of σ_{20}, the measurements of Pivovar *et al.* and of Baragiola and Nemirovsky are both a factor of 1.5–2 larger than our measurements. The systematic uncertainty in both of these experiments is estimated to be less than 15%. The measurements of σ_{10} by Barnett and Stier[20] agree with the present data within experimental uncertainties at velocities below 1×10^8 cm/s, but are consistently below our values at higher velocities. The largest discrepancy occurs near the cross-section maximum, where the present measurements are about 30% larger. We estimate the systematic uncertainties in the measurements of Barnett and Stier to be less than 15%.

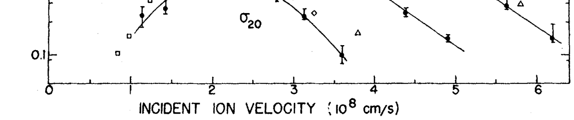

FIG. 2. Total experimental electron-capture cross sections σ_{21}, σ_{20}, and σ_{10} for $^3He^{++}$ and $^4He^+$, respectively, incident on molecular hydrogen as a function of the relative collision velocity. Solid circles, results of this experimental study; open circles, from Shah and Gilbody (Ref. 16); open squares, from Bayfield and Khayrallah (Ref. 17); open triangles, from Pivovar *et al.* (Ref. 18); open diamonds, from Baragiola and Nemirovsky (Ref. 19); inverted triangles, from Barnett and Stier (Ref. 20).

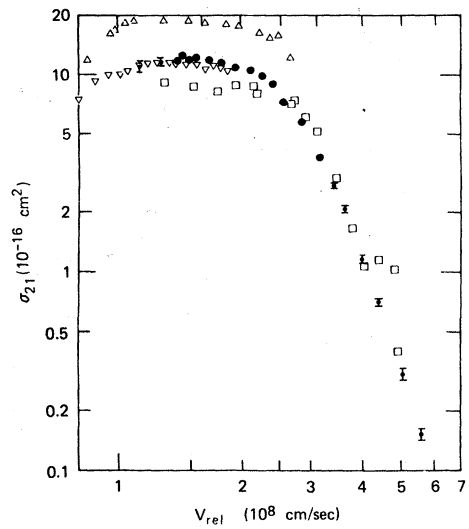

FIG. 3. Comparison of the calculated classical-trajectory electron-capture cross section for $He^{++}+H$ collisions (open squares) with the experimental results of this study (solid circles) and the work of Shah and Gilbody (Ref. 2) (inverted triangles) and the measurements of Bayfield and Khayrallah (Ref. 3) (open triangles).

The comparison between the experimental and our theoretical electron-capture cross sections is displayed in Fig. 3. We note that the agreement between our theoretical and experimental work is generally better than 25%. Only at velocities around 4.4×10^8 cm/s do the theoretical results greatly overestimate the experimental values. This velocity corresponds to the Bohr orbital velocity of the 1s electron in He^+ and it is tempting to interpret this feature as a velocity-matching phenomenon. However, within the framework of this classical model, the concept of a 1s state for the product ion has no meaning. Furthermore, no similar behavior is seen in the experimental cross sections. The cause of this structure is not understood at this time.

In Fig. 4 are presented the classical-trajectory results for the electron capture, impact ionization, and total electron-loss (capture plus ionization) cross sections along with comparisons to other calculations. There are no experimental data with which to compare our calculated impact-ionization cross sections. However, there have been recent calculations reported by Golden and McGuire[23] that are based on the Glauber and Born approximations. The agreement between the Glauber calculations and our classical-trajectory calculations is found to be good (agreement within 25%) for collision velocities greater than 3×10^8 cm/s. For velocities less than 3×10^8 cm/s, the classical-trajectory impact-ionization cross sections de-

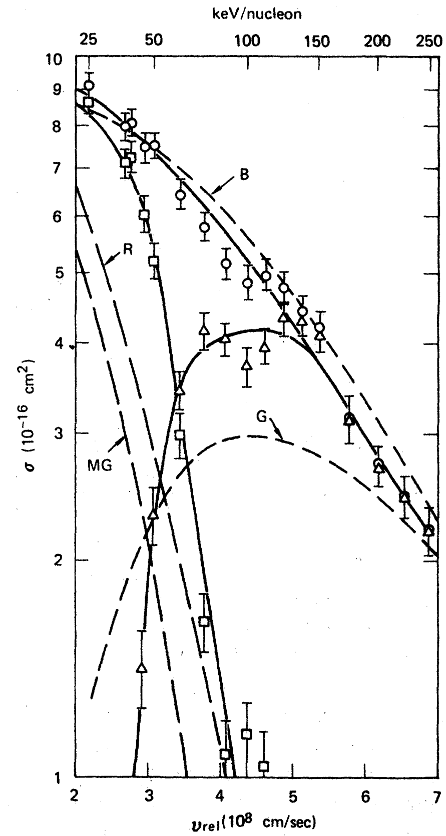

FIG. 4. Classical-trajectory calculations with one standard deviation error bars for $He^{++}+H$ collisions. Open squares, electron-capture cross sections; open triangles, impact-ionization cross sections. Open circles, total cross sections for electron loss from the H-atom target, the sum of electron-capture and impact-ionization cross sections. The solid curves corresponding to each set of cross sections were drawn in to guide the eye. Other calculations shown are the Born (B) and Glauber (G) impact-ionization cross-section calculations of Golden and McGuire (Ref. 23), short dashed lines; and the coupled-state calculations of the electron-capture cross sections of Rapp (R) (Ref. 21), and of Msezanne and Gallaher (MG) (Ref. 22), long dashed lines.

crease more rapidly than the Glauber values. Only at the higher velocities, $v\gtrsim5\times10^8$ cm/s, is there agreement between the classical-trajectory and Born calculations. However, the Born calculation does compare well with the classical-trajectory results for the total cross section for electron loss from the atomic hydrogen target. A similar result was obtained by Percival and Valentine[24] for calculations on the H^++H system.

Rapp[21] and Msezane and Gallaher[22] have made atomic expansion coupled-state calculations of the electron-capture cross sections for the $He^{++}+H$ reaction over the velocity range studied here. At

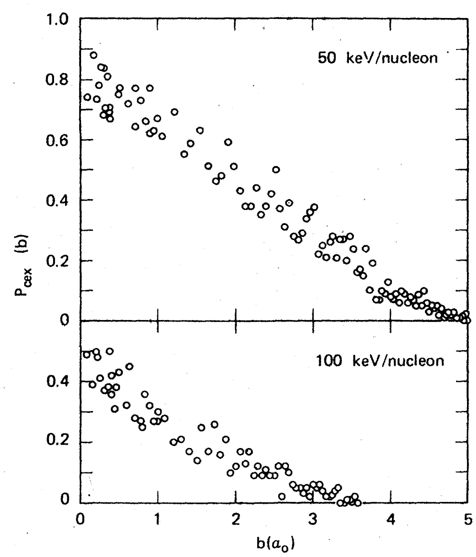

FIG. 5. Classical-trajectory calculations of the transition probabilities for electron capture vs impact parameter for $He^{++}+H$ collisions. Each circle represents the result of 100 trajectory calculations.

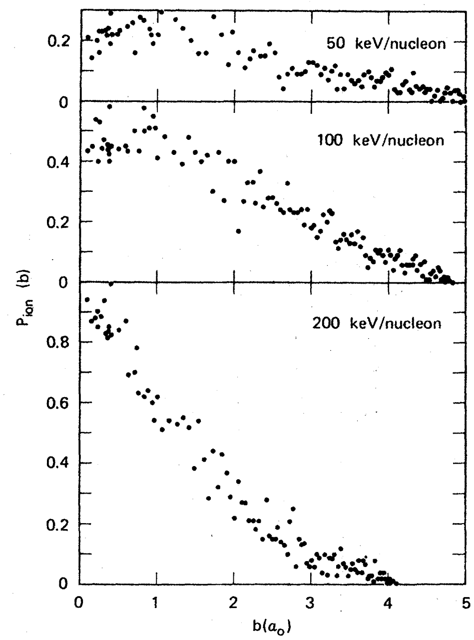

FIG. 6. Classical-trajectory calculations of the transition probabilities for impact ionization vs impact parameter for $He^{++}+H$ collisions. Each circle represents the result of 100 trajectory calculations.

the lowest collision velocity, $\sim 1\times10^8$ cm/s, these calculations are in good agreement with our results. At velocities between $(2-5)\times10^8$ cm/s, both studies report smaller cross sections. However, Rapp's eight-state calculations are within a factor of 2 of the present results whereas the values of Msezane and Gallaher are two to four times smaller.

In Figs. 5 and 6, we also present the calculated transition probabilities for electron capture and impact ionization that were obtained from the classical-trajectory studies. Each point represents 100 trajectories. By presenting these transition probabilities as a function of impact parameter, it should be easier for future workers to critically assess the details of the $He^{++}+H$ reaction.

In summary, experimental and theoretical results are presented for electron loss by atomic and molecular hydrogen for collisions with He^{++} and He^{+}. For $He^{++}+H$ collisions the agreement between our experimental and theoretical electron-capture cross sections is generally better than 25%. Our calculated impact-ionization cross section for $He^{++}+H$ also is found to be in reasonable agreement with calculations based on the Glauber approximation.[23] Other calculations[21,22] for the electron-capture cross section are significantly lower than the results presented here. However, since the cross sections calculated by the classical-trajectory method have been shown to be in good agreement with experimental data[4,5,12,24,25] for the H^+, C^{+q}($q=3$ and 4), N^{+q}($q=3-5$), O^{+q}($q=3-5$), and Fe^{+q}($q=9-22$) + H systems, we feel that the cross sections presented here are of comparable accuracy and provide a reasonable estimate of the true values.

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