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Author

Berkner, K.H.

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September 1980

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Electron-Capture, Electron-Loss and Impact-Ionization
Cross Sections for 103- to 3400-keV/amu Multi-charged Iron Ions
Colliding with Molecular Hydrogen

K. H. Berkner, W. G. Graham⁺, R. V. Pyle, A. S. Schlachter
and J. W. Stearns

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

September 10, 1980

ABSTRACT

We report cross-section measurements for collisions of multi-charged iron ions with a molecular hydrogen target: a) electron-capture and -loss of the multi-charged ions, and b) impact ionization of the hydrogen target. Iron ions, Fe^{+q} , were used with charge states $q = 3-13$ at 103 keV/amu, $q = 9-16$ at 294 keV/amu, $q = 11-22$ at 1160 keV/amu, and $q = 20-25$ at 3400 keV/amu. We find that an empirically determined expression for the electron-capture cross section, $\sigma = (1.2 \times 10^{-8}) q^{3.15} E(\text{keV/amu})^{-4.48} \text{ cm}^2/\text{molecule}$, describes all the data at and above 275 keV/amu. These measurements are compared with recent theoretical calculations.

⁺Present Address: The New University of Ulster, Coleraine, BT52 1SA, N. Ireland

I. INTRODUCTION

A collision of a multicharged heavy ion X^{+q} with a target atom Y can result in a change of the charge state of the projectile, of the target, or of both.¹ Cross sections for electron capture,

$$\sigma_{q,q-n} : X^{+q} + Y \rightarrow X^{+(q-n)} + Y^{+n} \quad (1)$$

and electron loss by the ion,

$$\sigma_{q,q+n} : X^{+q} + Y \rightarrow X^{+(q+n)} + Y + ne \quad (2)$$

can be determined experimentally by observing the change of the charge state of the projectile.

Cross sections for charge changes of the target Y can be obtained by extracting and analyzing slow collision products.² A simpler technique, yielding less information, is to measure total or effective cross sections, σ_+ and σ_- , for producing positive and negative charge in the target. From these, one can deduce a cross section, σ_I , for the production of charge in the target in excess of that produced by electron capture or loss. This cross section for "impact ionization," which includes contributions from single and multiple ionization of the target,

is obtained by subtracting the contribution of electron-capture or -loss collisions from the charge production in the target:

$$\sigma_I(q) = \sigma_+(q) - \sum_n n \sigma_{q,q-n} \quad (3)$$

or

$$\sigma_I(q) = \sigma_-(q) - \sum_n n \sigma_{q,q+n}. \quad (4)$$

In this paper we report measurements of $\sigma_{q,q-1}$, $\sigma_{q,q+1}$ and σ_I (and in some cases $\sigma_{q,q-2}$ and $\sigma_{q,q+2}$) for collisions of multicharged iron ions, Fe^{+q} , with a molecular hydrogen target, with $q = 3-13$ at 103 keV/amu, $q = 9-16$ at 294 keV/amu, $q = 11-22$ at 1160 keV/amu and $q = 20-25$ at 3400 keV/amu. A few of these results have been reported previously.³⁻⁵

There are extensive review papers on heavy-ion electron capture and loss by Nikolaev⁶ and Betz.⁷ Published cross-section measurements for electron capture, electron loss, and impact ionization for projectiles heavier than He in H and H₂ targets are listed in Table I.^{3-5,8-37} Electron-capture and -loss cross sections for iron ions in H and H₂ have been reported by Meyer et al.²⁴ and Gardner et al.²⁵ at lower energies and charge states than we report here. We are not aware of any previous measurements for impact ionization by iron ions.

Many theoretical techniques have been used to calculate electron-capture, electron-loss, and impact-ionization cross sections for heavy projectiles colliding with atomic hydrogen.

For calculations of electron-capture cross sections the choice of the applicable theoretical model generally depends on how the projectile velocity compares with the orbital velocity of the electron to be captured. In the present paper the projectile velocity is greater than the velocity of the orbiting electron, hence a classical approach can be used in the calculation of electron-capture cross sections. Olson and Salop³⁸ have used a three-body classical approach, a classical-trajectory Monte-Carlo technique, in which all the forces between the three bodies - the projectile, the target, and the captured electron - are included. Molecular effects limit the validity of this approach to energies greater than about 25 keV/amu.³⁸ At high energies, e.g., 5000 keV/amu, the transition probabilities become so small that the technique is limited by the difficulty in obtaining good statistics for the cross-section determination.

Electron-capture cross sections relevant to the present experiment also have been calculated using quantum-mechanical methods: 1) Rule and Omidvar³⁹ have used the Oppenheimer-Brinkman-Kramers (OBK) approximation. This technique is known to overestimate the cross sections, but when modified by an empirical factor,^{40 41} yields cross sections that are consistent with experiments. 2) Chan and Eichler⁴² have used the Focke density-matrix expression in momentum space of the target electron to calculate electron-capture cross sections into arbitrary principal shells of energetic bare projectiles. From these results they have derived a scaling factor for cross sections calculated with the OBK method. 3) A unitarized distorted-wave-approximation method, based on traveling atomic orbitals, has been used by Ryufuku and Watanabe.⁴³ At

high energies, their cross sections tend to be twice as large as measured values, but they exhibit the correct charge-state and energy dependence.

Electron-loss cross sections for Fe^{+q} in H have been calculated in the first Born approximation, for energies between 0.1 and 100 MeV/amu, by Rule and Omidvar.³⁹ First-Born-approximation calculations for the loss of 1s, 2s and 2p electrons from hydrogen-like ions in hydrogen have also been reported by Dmitriev et al.⁴⁴ and Nikolaev et al.⁴⁵

Impact-ionization cross sections have been calculated with the three-body classical-trajectory Monte-Carlo technique by Olson and Salop³⁸ and by Olson.^{4,5,17} At high energies the plane-wave Born approximation may be more appropriate⁵.

Electron-capture and impact-ionization collisions of multi-charged ions with atomic hydrogen (or deuterium) are important for the fusion program. Highly ionized heavy impurity ions, such as Fe^{+25} , Mo^{+33} and W^{+35} , have been identified in magnetically confined hydrogen plasmas in tokamaks⁴⁶⁻⁴⁸. Many of these plasmas are heated by injection of 20- to 120 keV hydrogen or deuterium atoms, and the ionization (trapping) profile of the injected atoms can be altered by the presence of the multi-charged impurities.⁴⁹ In order to estimate how large an effect the impurity ions could have on the trapping profile, it is necessary to know the cross sections for the following processes:

electron capture:

impact ionization:

where A is an impurity ion in charge state q . The sum of these two cross sections is the total cross section for electron loss from the hydrogen atom.

The results presented here are for molecular hydrogen targets; we compare these cross sections with twice the theoretical cross sections calculated for an atomic-hydrogen target.

II. EXPERIMENTAL APPROACH

A. General Description

The apparatus is shown in Fig. 1. Iron ions of the desired charge state from the SuperHILAC heavy-ion linear accelerator were selected by momentum analysis and passed through the target cell described below.

Two types of measurements were made: (1) impact ionization, in which slow-electron and -ion currents in the target were collected with a parallel-plate capacitor, while the fast incident ion beam was measured with a Faraday cup; and (2) charge-transfer measurements, in which the fast ions exiting the target were analyzed by the spectrometer magnet and detected by an array of diffused-junction solid-state detectors.

B. Preparation of Projectile Beam

The iron ions from the SuperHILAC were either used directly or stripped further in a carbon foil, which was located upstream of the charge-state-selection magnet. The foil thickness chosen in each case was a compromise between a thick foil, which, at equilibrium thickness, would yield higher charge-state ions, and a thin foil to minimize energy loss in the foil.⁵⁰ Since little information exists for charge-state distributions of iron ions in carbon foils, the desired thickness had to be estimated. We used $10 \mu\text{g}/\text{cm}^2$ foils for most of the measurements; $100 \mu\text{g}/\text{cm}^2$ were used at 3400 keV/amu and for some measurements at 1160 keV/amu. We made no systematic study of the charge-state distribution as a function of beam energy or foil thickness; however, the mean charge state decreased with decreasing beam energy.

Preparation of a fast partially stripped ion beam in a foil can create metastable ions with lifetimes sufficiently long to reach the

target. These metastable ions could have different cross sections than ground-state ions, especially for electron loss, since they are less tightly bound than ground-state ions. As we prepared our projectile beams by stripping in a foil, they could contain an unknown admixture of metastable ions.

We used the charge-selection magnet to select ions in a particular charge state from the variety of charge states in the beam emerging from the carbon foil. Charge-state identification and energy measurements are discussed below. In order to ensure a unique path through the charge-selection magnet, a 12-mm-diam aperture was inserted in front of the foil.

Beyond the charge-selection magnet, the beam passed through a 3.2-mm-diam collimator C_1 . This collimator and the entrance aperture in the gas-target chamber 178 cm downbeam limited the primary beam size so that no beam was lost at the target entrance and exit nor at the Faraday cup or detectors. Since the exit collimation allowed the scattered beams to be larger than the detectors, the equal widths of the charge-transferred and the primary beams showed that there was negligible beam broadening due to scattering.

C. Charge-State Identification and Energy Measurement

Considerable care was required to determine the charge state of the primary beam, especially for high charge states, where magnetic separation of adjacent charge states was small.

The spectrometer magnet was calibrated for charge-state identification by a wire-orbit technique, in which a current-carrying wire assumes the path taken by an ion beam of fixed momentum p and

charge state q .⁵¹ The wire orbit, defined by collimators C_1 , C_2 , and a 1.25-mm-wide slit located at the exit of the magnet, was used to obtain the integral of the magnetic field over the path length as a function of the magnetic field measured with a fixed-position Hall probe. A surface barrier detector, mounted behind the slit, was used to determine the p/q ratio of the beam of interest. The beam energy could be determined to within 1% by a reference spectrometer that is maintained by the SuperHILAC; we used this measurement to normalize the energy scale for our spectrometer. When this spectrometer was not available, we relied on pulse-height measurements with solid-state detectors.

A complication in the energy determination was the use of a carbon foil to strip ions to higher charge states. The approximate energy loss to be expected in a given foil was obtained from energy-loss tables,⁵⁰ and was occasionally checked by measuring the decrease in pulse height on a solid-state detector. We used identical foils in pairs in most of our experiments: the foil located upstream of the charge-selection magnet and an identical foil which could be inserted downstream of collimator C_1 . The latter was used to measure energy loss of the incident beam without the necessity of retuning the charge-selection magnet, thus eliminating the possibility of error in charge-state or energy-loss determination. Once the energy loss in the second foil was determined, we verified that the energy loss in the original foil was comparable; subsequently, only the foil upstream of the charge-selection magnet was used during the experiment. Corrections for Hall-probe drift and offsets, uncertainties in the wire-orbit calibration, and resolution of

the slitted detector lead to a relative standard uncertainty of one percent for measurements taken near a given nominal value. Uncertainties in the relative calibration over a large energy range and in the absolute calibration of the reference spectrometer yield an absolute uncertainty of 3 - 5 percent. Since the charge-state determination depends on the square root of the energy, $\Delta q/q = \Delta E/2E$, we are able to unambiguously determine the charge states of the iron beams.

D. Beam Analysis and Detection

After passage through the target the beam traversed a 33-cm x 61-cm spectrometer magnet (maximum central field 2 T). At zero magnetic field, the fast-ion beam could be detected by a 25-mm-diam magnetically suppressed Faraday cup located on the axis of collimation. This Faraday cup was used for beam tune-up for high intensity beams; it was replaced by a 25-mm-diam solid-state detector for tune-up of low-intensity beams.

The charge-analyzed beam was detected by either of two methods: a double Faraday cup or an array of solid-state detectors. The double Faraday cup (Fig. 2a) consisted of a long rectangular open-ended box (103 mm x 35 mm x 25 mm) which collected all ions which had changed their charge in a collision in the gas target. The primary beam was collected in a small Faraday cup located behind an adjustable slit, typically 7 mm wide, in the rectangular cup. This double Faraday cup was located at the same position as the five-detector array indicated in Fig. 1. The currents from the Faraday cups were amplified by electrometers, the outputs of which were integrated.

For measurements of charge-changing cross sections with low intensity beams, or when simultaneous measurements of single and double-electron-capture and -loss cross sections were made, the double Faraday cup was replaced with an array of five diffused-junction solid-state detectors (Fig. 2b). Each detector had a sensitive area of 16×10 mm; the detectors were so arranged that each had an exposed area larger than the scattered beam, yet the spacing was such that 5 beams could be detected simultaneously: the primary beam of charge q , and secondary beams of charges $q+1$, $q+2$, $q-1$, and $q-2$. The entire array was mounted on a sliding shaft so that the position of the array could be changed within the magnet to match the spatial separation of the beams to the detector spacing. For very low values of q , only beams with charges q , $q+1$, and $q-1$ were detected, using the central and the two outer detectors. For each value of q we determined that the detected signals for the various charge states were independent of small changes in the spectrometer magnetic-field settings; this assured that there was no overlapping of adjacent charge-state beams onto neighboring detectors. The signal from each detector was amplified, discriminated and recorded with a scaler.

The maximum primary-beam intensity was maintained at an average of 10^4 particles/sec; instantaneous count rates were approximately a factor of 100 higher because of the low duty factor of the accelerator. For the primary beam a 100 MHz counting system was used; for the secondary-beam channels 1 MHz counting systems were used. Periodic checks were made to verify that cross sections were independent of counting rate up to the maximum rate used for each measurement.

E. Target

The gas cell was a differentially pumped chamber with an inner diameter of 7.5 cm, and with entrance and exit apertures (C_3 and C_4) of 3.3 mm diameter (Fig. 1). Apertures C_2 and C_5 had diameters of 2.5 and 3.8 mm and served to isolate the differentially pumped section from the beam line. Apertures C_1 and C_2 limited the beam incident on the target to a half-angle divergence of 0.093° and a beam diameter at the detectors of 6.6 mm. Some measurements were made with a slightly different geometry described in Ref. 4.

A set of parallel plates (Fig. 1 inset) inside the gas cell was used for measuring impact-ionization cross sections by the technique of slow-ion and -electron collection. The plates were 3.00 cm long, 1 cm apart, and had guard plates on each end to provide a uniform transverse electric field. Slow ions and electrons produced by impact-ionization or charge-changing collisions were swept from a well-defined length of the target chamber by the electric field and collected on one of the plates. The electric field was increased until the collected currents were insensitive to further changes; the typical field was 120 V/cm. The measurements required incident beams of sufficient intensity that current-measuring techniques could be used. Currents collected at the plates were detected with electrometers, the outputs of which were integrated. Secondary-electron emission from the collecting plates is discussed in Section II F.

The pressure in the gas cell was measured with a differential capacitance manometer whose calibration was checked, at high pressures, with an oil manometer. The uncertainty in this measurement is $\pm 4\%$; the

uncertainty in the gas-cell length and variations in ambient temperature are less than 2%, leading to an overall target-thickness uncertainty of 4 percent. One gas sample was analyzed for impurities, and was found to contain 0.06% N_2 . The effect of this N_2 admixture was negligible for ionization cross sections, but was significant for electron-capture cross sections, especially at higher energies. It is included as a source of uncertainty in II H.

Charge-transfer collisions in background gas reduce the charge-state purity of the primary beam, especially at low energies. It was therefore found necessary to maintain the pressure in the beamline between the charge-selection magnet and the gas-target cell below 10^{-6} Torr at maximum gas-cell thickness, while the pressure in the spectrometer magnet was kept below 2×10^{-6} Torr. The spectrometer magnet permitted us to verify that the incident-beam charge-state purity was better than 99 percent.

F. Electron Emission from Ion Collector

The condenser-plate method of collecting slow-ion and -electron current in the target is potentially inaccurate due to the possibility that the slow ions will produce emission of electrons from the ion-collector surface, which will be swept by the electric field to be collected at the electron collector. This effect increases the apparent current at each electrode and produces a corresponding error in the cross section being measured. We determined the magnitude of this effect in a separate experiment on a small accelerator, using the same target chamber, but with the addition of a solenoidal magnetic field coaxial with the beam to suppress secondary electrons.

A 120-150 keV D^+ beam was passed through the target chamber to produce the slow ions, and the beam-normalized ion-collector current was monitored while varying the transverse electric field, the axial magnetic field and the target pressure. The secondary electrons were considered to be suppressed when a change in the magnetic field produced no change in the normalized ion-collector current. At 100 V/cm a field of about 200 gauss was required to suppress electrons. With H_2 as the target, gas electron emission represents less than 2% of the pressure-dependent slow-ion current.

G. Data Acquisition and Analysis: Electron-Capture and -Loss Cross Sections

The slow-ion and -electron collection plates were grounded for charge-transfer cross-section measurements. A beam in charge-state q was selected by the charge-selection magnet and its charge state was verified by deflecting it onto the slitted detector in the spectrometer magnet. The primary beam was then centered on the middle detector of the 5-detector array. The correct spacing of the detectors was confirmed by observing that, with gas in the cell to produce charge-changed ions, the detector signals were independent of small variations in the analyzer field.

A measurement consisted of counting pulses from the five detectors for a time sufficient to achieve reasonable statistics; typical counting times were one minute. Each cross-section measurement consisted of at least ten such measurements at various pressures. Typical data are shown in Fig. 3. Because of the long integration times we had to consider possible variations in the target pressure. The pressure was either read during the middle of the counting period or the output from

the manometer was integrated during the counting period, then divided by the integration time, to average small pressure drifts. We were not always able to determine all four charge-transfer cross sections, either because some were too small to measure in a reasonable integration time, or because of background effects. Background was important for two-electron-transfer cross-section measurements: the primary beam was prepared in charge-state q , but collisions with background gas before the target could contaminate this beam with an admixture of ions in charge states $q \neq 1$. A single collision of an ion in charge-state $q \neq 1$ in the target then could give an ion in charge-state $q \neq 2$, which could mask the single-step, two-electron-transfer, cross section which one would like to measure.

We also measured a few charge-transfer cross sections with the Faraday-cup array: The primary beam was collected on the small cup, secondary beams (electron capture or loss) on the large cup. This technique required higher intensity beams and could be used only when one of the cross sections (either single-electron capture or loss) dominated. The dominant reaction could be determined by sweeping the secondary beams across the small cup. Several cross sections were measured with the solid-state detectors and with the Faraday-cup array. The results agreed within the estimated uncertainties.

The population of a charge state k , expressed as a fraction of the total beam F is related to the target thickness π [target density times path length through target] by the coupled equations,

$$\frac{dF_k}{d\pi} = \sum_{j \neq k} (F_j \sigma_{j,k} - F_k \sigma_{k,j}) \quad (7)$$

where $\sigma_{j,k}$ is the cross section for changing the beam ion from charge-state j to charge-state k . The complete solutions to these equations for a three-level system are listed in articles by Allison and Garcia-Munoz.⁵²

An initial approximation for the single-electron-capture and -loss cross sections is obtained using the thin-target approximation, or first-order expansion of Eq. 7. For an incident beam in charge-state j , for less than 10% beam attenuation, we have

$$\sigma_{j,j\pm 1} = \frac{\Delta F_{j\pm 1}}{\Delta \pi} \quad (8)$$

These first-order solutions were used in a second-order expansion of Eq. 7, which can be written as

$$\pi \sigma_{j,k} = \frac{2}{F_{j+1}} F_k - \frac{\pi}{2} \sum_{(k\pm 1) \neq j} F_{k\pm 1} \sigma_{k\pm 1,k} + \frac{\pi}{2} \sum_{(k\pm 1) \neq j} F_k \sigma_{k,k\pm 1}. \quad (9)$$

The factor applied to F_k is the "attenuation" correction and the other terms are the "two-step" corrections. The effect of this approximation is to linearize the data within the region of the thin-target definition. The final cross-section results were obtained from the slope of a least-squares fit of the expression on the right-hand side of Eq. 9.

H. Data Acquisition and Analysis: Impact-Ionization Cross Sections

An ion beam in charge-state q was selected by the charge-selection magnet and its charge state was verified by deflecting it onto the slit-detector in the spectrometer magnet. The small cup of the double Faraday-cup assembly was used to measure the primary beam, while beam attenuation was monitored by measuring the fraction of the beam in the large cup. The voltage on the collector plates was varied until the slow-ion and -electron currents, I^+ and I^- , did not change with further increases of voltage. Figure 4 shows a typical collector voltage sweep. Operating voltages were about 120 V. Once this operating voltage was determined, simultaneous measurements were made of collected slow-ion or -electron current, primary-beam current (small cup), and charge-transferred beam current (large cup). The electrometer outputs were integrated for 30 to 60 sec, a time long compared to the time constant of the electrometers. Primary-beam currents of 10^{-8} to 10^{-13} A were used to make these measurements. A measurement consisted of the integrated output of the three electrometers and the average pressure. We made measurements at more than ten different pressures to obtain a cross section. Typical data are shown in Fig. 5.

Secondary electrons from the double Faraday cup were suppressed by the spectrometer-magnet field. Secondary-electron emission from the ion-collection plates has been discussed in Section II F. The electrometers were calibrated against a secondary current standard.

An initial approximation for the cross section for electron production by Fe^{+q} , over a range of pressures such that the

attenuation of the primary beam, with current I_q , and ionization by electrons produced in the target are kept small (thin target), is

$$\sigma_-(q) = \frac{\Delta F_-(q)}{\Delta \pi} \quad (10)$$

where F_- is the number of electrons produced in the target per primary particle:

$$F_-(q) = \frac{I^-}{(I_q/q)} \quad (11)$$

Equation 10 was used to obtain an initial approximation of electron-production cross sections for beams of different charge states. Second order corrections were made to linearize the data:

$$\pi\sigma_-(q) = \frac{F_-(q) - a \frac{\pi}{2} [\sigma_{q,q-1} \sigma_-(q-1) + \sigma_{q,q+1} \sigma_-(q+1)]}{\frac{1 + F_q}{2}} \quad (12)$$

where q is the incident charge state, F_q is the fraction of the beam remaining in that charge state (either measured or estimated from the cross sections), and a is the ratio of the total gas-cell length to the length of the collector region. The two subtractive terms in the numerator remove, to first order, the charge produced by the incident beam admixture in adjacent charge states, while the divisor corrects for

attenuation of the primary beam. The slope of a least-squares fit to the right-hand expression was used to determine $\sigma_{-}(q)$.

Similarly, the cross section for the production of slow ions is, to first order,

$$\sigma_{+}(q) = \frac{\Delta F_{+}(q)}{\Delta \pi} \quad (13)$$

where the definition of F_{+} is analagous to Eq. 11. The second-order corrections were made with an equation analagous to Eq. 12.

Since electron capture and loss by the primary beam can also create charge in the target, the impact ionization cross section, $\sigma_I(q)$, is

$$\begin{aligned} \sigma_I(q) &= \sigma_{+}(q) - \sigma_{q,q-1} \\ &= \sigma_{-}(q) - \sigma_{q,q+1} \end{aligned} \quad (14)$$

Values of σ_I obtained from either σ_{+} or σ_{-} agreed within 2% .

H. Uncertainties

The relative standard uncertainty in our single-electron-capture and -loss cross sections is estimated to be 4 percent. This is obtained from uncertainties in the least-squares fit (3%)(which averages contributions from counting statistics, zero drift in the capacitance manometer, and corrections for second-order processes), counting errors due to intensity fluctuations in the beam (2%), and possible beam-energy drift during a sequence of measurements (2%). The cross sections for two-electron capture and loss are less certain because of corrections for two-step processes and poor counting statistics, and the estimated

relative standard uncertainties are 10%. For possible systematic errors we estimate 4% for the determination of the target thickness (calibration of the capacitance manometer and determination of the length of the gas cell), 5% for possible beam loss on collimators, and 3% due to gas impurities; the systematic error is thus estimated to be 7% . Combining the relative and systematic uncertainties, we obtain an absolute standard uncertainty of 8% for the single-electron-capture and -loss cross sections and 12% for the two-electron-capture and -loss cross sections.

The ionization cross sections have the following sources of relative uncertainty: zero drift and fluctuations in electrometers and in the capacitance manometer (3%), corrections for second-order processes (2%), scale-to-scale variations in the electrometer-integrator system (3%), correction for secondary-electron emission from the collector plates (2%), and uncertainty in the slow ion/electron collection efficiency (5%). The total standard relative uncertainty is 7%. The estimates of systematic errors are: target thickness (4%), beam loss on collimators (2%), gas impurity (1%), and differences in using σ_+ or σ_- for the determination of σ_I (2%); the systematic error is thus estimated to be 5%. Combining the relative and systematic uncertainties we estimate an absolute standard uncertainty of 8% for the ionization cross sections.

III. RESULTS AND DISCUSSION

A. Projectile Electron Capture

Our electron-capture cross-section results for Fe^{+q} projectiles in an H_2 target are given in Table II. The two-electron double-capture cross sections were often masked by competing two-step processes or poor counting statistics.

The single-electron-capture cross sections $\sigma_{q,q-1}$ vs charge state q are shown in Fig. 6. From the figure it is clear that the cross sections have a strong energy dependence, and, at a given energy, the cross sections exhibit a power-law dependence with q . In an attempt to find a general expression for the energy and charge-state dependence of the single-electron-capture cross sections, we chose a power law expression of the form

$$\sigma_{q, q-1}(q, E) = \sigma_a q^\alpha E^\beta \quad (15)$$

where σ_a , α , and β are constants. There are no values for σ_a , α , and β for which Eq. (15) describes all of our results; however, our results at 275 keV/amu and above are in excellent agreement with the expression:

$$\sigma_{q, q-1}(q, E) = (1.2 \times 10^{-8}) q^{3.15} E^{-4.48}, \quad (16)$$

where $\sigma_{q,q-1}$ is the cross section in cm^2 and E is the projectile energy in keV/amu. To demonstrate the range over which Eq. (16) describes the data, we have plotted $q^{-3.15} \sigma_{q, q-1}$ vs E in Fig. 7a

and $E^{4.48} \sigma_{q,q-1}$ vs q in Fig. 7b. We also show the scaled cross sections for Fe^{+q} in H_2 from Gardner et al.²⁵ and Meyer et al.²⁴

We observe that $\sigma_{q,q-1}$ at energies greater than 275 keV/amu fit Eq. (16), while cross sections at lower energies deviate increasingly with decreasing energy. We also point out that our results for $\sigma_{q,q-1}$ for Fe^{+q} in H_2 are in good agreement with previously reported values.^{24,25}

Other authors have observed a discontinuity in the electron-capture q -scaling at values of q corresponding to closed shells.^{29,30,36,53} Gardner et al.²⁵ observed such a discontinuity for electron capture by Fe^{+q} in H , H_2 , and Ar targets for Fe^{+8} , which is argon like. We see no discontinuity in our cross sections at $q = 8$ (argon-like), $q = 16$ (neon-like), or $q = 24$ (helium-like).

We compare our experimental results for electron capture by Fe^{+q} in H_2 with theoretical calculations for Fe^{+q} in H in Fig. 8, where we have doubled the theoretical results for comparison with molecular hydrogen. The modified OBK calculations by Rule and Omidvar³⁹ and by Chan and Eichler⁴² are in very good agreement with our results above 1000 keV/amu. Chan and Eichler have also calculated cross sections at lower energies, but the agreement gets progressively worse as the energy decreases. The results of Ryufuku and Watanabe⁴³ are about twice as large as our measured values over the entire energy range. The classical-trajectory Monte-Carlo results of Olson⁵ are within $\pm 50\%$ of our measurements at 103 and 294 keV/amu. All of the calculations predict a charge-state variation consistent with our results.

B. Projectile Electron Loss

Our electron-loss cross sections are given in Table II. Two-electron-loss cross sections were masked by competing two-step processes or poor counting statistics except at 3400 keV/amu. We are not aware of any previous electron-loss cross-section measurements for Fe^{+q} projectiles.

The single-electron-loss cross sections $\sigma_{q, q+1}$ vs charge state q are shown in Fig. 9. The cross sections have a weak energy dependence over the range reported here and decrease rapidly with increasing q . It is clear from the figure that there is no simple power-law scaling to describe the q -dependence. Previous measurements²⁷ with other projectiles with lower q 's and lower energies have been consistent with cross sections that scale as $q^{-\alpha}$, where α ranges between 2 and 3; we find that for $q \geq 10$, α ranges between 9 and 12.

A notable feature in the single-electron-loss cross sections is the pronounced discontinuity between projectiles with $q = 23$ (lithium-like) and $q = 24$ (helium-like). This can be attributed to the shell structure of the iron ion: The energy necessary to ionize Fe^{+25} (1s) or Fe^{+24} (1s²) is 9.0 and 8.5 keV respectively. The energy required to ionize Fe^{+23} (1s² 2s), Fe^{+22} (1s² 2s²), Fe^{+21} (1s² 2s² 2p) etc. is 2.0 keV or less.⁵⁴ Thus the large discontinuity in electron loss is a clear manifestation of the shell structure of Fe. We might also expect that $\sigma_{24,25}$ would be approximately twice $\sigma_{25,26}$, since there are two 1s electrons to be removed from Fe^{+24} , while only one from Fe^{+25} ; we observe cross sections with approximately this behavior.

Also shown in Fig. 9 are the first-Born-approximation results of Rule and Omidvar;³⁹ the agreement is within the experimental uncertainties. There is also good agreement with the calculations of Dmitriev et al.⁴⁴ for Fe^{+25} . For $q = 20-23$ our cross sections are only 5-20% higher than those calculated by Nikolaev et al.⁴⁵, but for Fe^{+24} our results are 30% larger than calculated. Nikolaev⁵⁵ suggests that this could be attributed to a metastable contamination of about 1%.

C. Target Impact Ionization

Impact-ionization cross sections for Fe^{+q} in H_2 are shown in Fig. 10. The impact-ionization cross sections are not monotonic with energy; there is a maximum in the ionization cross section at a few hundred keV/amu. Olson⁵ has used the classical-trajectory Monte-Carlo method to calculate impact-ionization cross sections for Fe^{+q} in atomic hydrogen. Calculated cross sections have been multiplied by a factor of 2 for comparison with our experimental results for H_2 . There is very good agreement at 1160 and 294 keV/amu. At 103 keV/amu the agreement in magnitude between theory and experiment is poor, which may reflect that the description of the H_2 molecule by 2 H atoms is becoming increasingly invalid as the collision velocities decrease and approach the molecular regime.

At high velocities, calculations based upon the Born-Binary Encounter⁵⁶ or semi-classical approximation, predict a q^2 dependence for the impact-ionization cross section. At our highest energy the ionization cross section has a $q^{1.43 \pm 0.05}$ dependence. These methods are of use in the present energy range only for collisions of light projectiles and so are not applicable to the present results.

D. Target Electron Loss

The total cross section for loss of an electron from a hydrogen target is the sum of the electron-capture cross section and the impact ionization cross section. From the measurements shown in Fig. 6 and Fig. 10 we can compute the H_2 -target electron-loss cross section for Fe^{+q} projectiles with $q = 11-22$ at 1160 keV/amu, $q = 9-16$ at 294 keV/amu and $q = 3-13$ at 103 keV/amu. These measurements are found to be in excellent agreement with the classical-trajectory calculations of Olson.⁵ We have previously found that the electron-loss cross sections can be combined into a universal scaling rule, applicable for a very wide range of projectile energies and charge states;⁵ we found that these results could be fit to an analytic expression of the form

$$\sigma_{Loss} = 4.6 \times q \times 10^{-16} [(32q/E)(1-\exp(-E/32q))], \quad (17)$$

where σ_{Loss} is the H-atom electron-loss cross section in cm^2 , q is the ion charge state and E is the energy in keV/amu. This equation is valid for $1 \leq q \leq 50$ and for energies in the range 50 keV/amu to 5000 keV/amu. The present cross sections are compared with Eq. 17 and with the Plane-wave Born-approximation cross section for ionization only^{57,58} in Fig. 11.

E. CONCLUSION

We have measured electron-capture, electron-loss, and impact-ionization cross sections for highly stripped iron ions in an H_2 target. Electron-capture cross sections are found to obey an empirical scaling rule in energy/nucleon, E , and charge state q , for energies greater than 275 keV/amu; the cross sections are proportional to $E^{-4.48} q^{3.15}$. We have compared our cross sections measured in H_2 with twice the theoretical cross sections calculated for an H target, and found good agreement with modified OBK calculations at high energies.

We have found electron-loss cross sections in H_2 to be a slow function of energy, but to decrease rapidly with projectile charge state. We also have found a pronounced discontinuity in electron loss, attributable to shell structure of the Fe projectile. There is good agreement with calculations by Rule and Omidvar and by Dimitriev et al. and Nikolaev et al. for an H target, multiplied by a factor of two.

Impact-ionization cross sections are in excellent agreement with classical-trajectory Monte-Carlo calculations of Olson, except at the lowest energy, where molecular effects make comparison of cross sections for H and H_2 questionable. It would be very desirable to measure ionization cross sections for heavy multiply charged ions colliding with atomic hydrogen.

Our results are consistent with a scaling rule based on CTMC calculations for electron loss from H in collision with a highly stripped ion, valid for a wide range of energies and charge states. We have recently found⁵⁹ a scaling rule of similar form for ionization of rare-gas targets.

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Table 1: Summary of published measurements of electron-capture, electron-loss, and impact-ionization cross sections for collisions of heavy projectiles ($Z > 2$) with H and H₂.

Authors	Ref	Projectiles	Charge states	Targets	Energy Range (keV/amu)	Electron Capture	Electron Loss	Impact Ionization
McCullough et al	8	Ba,Ti,Cd,Zn,Kr,B	2	H,H ₂	0.005-8	x		
Nutt et al	9	C,Ti	2	H,H ₂	0.01-1.2	x		
Huber and Kahlert	10	Ar, Kr	2-7	H ₂	0.012-0.25	x		
Flaks and Ogurtsov	11	N	0-3	H ₂	0.07-7	x		x
Sherwin	12	Be,B,C, Al,K,Fe,Cu	1-3	H ₂	0.09-0.4	x		x
Muller and Salzborn	13	Ne,Ar, Kr, Xe	2-8	H ₂	0.23-1.5	x		
Phaneuf et al	14	C,N,O	1-5	H,H ₂	0.5-137	x		
Crandall et al	15	C,N,O	3-6	H ₂	0.6-9.2	x		
Crandall et al	16	B,C,N,O,F,Ar	2-8	H,H ₂	0.6-9.2	x		
Phaneuf et al	17	N	1-5	H	0.6-18	x		
Gardner et al	18	B,C,N,O	2-5	H	1.0-2.9	x		
Gardner et al	19	B	2-4	H ₂	1.1-8.4	x		
Winter et al	20	Ne	1-4	H ₂	5		x	x
El-Sherbini et al	21	Ar	6	H ₂	5-30		x	x
Shah et al	22	Li	1-3	H,H ₂	9-214		x	x
Goffe et al	23	B,C	1-6	H,H ₂	9-200		x	x
Meyer et al	24	O,Fe,Mo,Ta,W,Au	1-19	H,H ₂	24-200		x	
Gardner et al	25	Fe	4-13	H,H ₂	27-290		x	
Pivovar et al	26	Li	0-3	H ₂	28.5-285	x		x
Ryding et al	27	Cl,Br,I	2-7	H ₂	32-428	x	x	
Ryding et al	28	I	1-4	H ₂	35	x	x	
Betz and Wittkower	29	I	2-18	H ₂	39-197	x	x	
Betz et al	30	Br,I	2-10	H ₂	47-187	x	x	
Kim et al	31	Si	2-9	H,H ₂	51-204	x		
Kim et al	32	Ta,Mo,W,Au	5-18	H	60	x		
Nikolaev et al	33	N	2-4	H ₂	80-751	x	x	
Moak et al	34	I	12,17	H ₂	87-1280	x		
Wittkower and Betz	35	I	5	H ₂	95	x	x	
Olson et al	5	Fe	3-15	H ₂	108-290			x
Datz et al	36	Br	6-11	H ₂	173-312	x	x	
Berkner et al	4	Fe	9-22	H ₂	260-1140	x		x
Berkner et al	3	Fe	20-25	H ₂	3400	x	x	
Tonuma et al	37	C,N	4-7	H ₂	3500-7500	x	x	

Table II. Electron-capture, electron-loss and impact-ionization cross sections. Fe^{+q} in H_2 . All units in $10^{-16} \text{cm}^2/\text{molecule}$

Energy (MeV)	keV/amu	Charge state	$\sigma_{q,q-1}$	$\sigma_{q,q-2}$	$\sigma_{q,q+1}$	$\sigma_{q,q+2}$	σ_I
190 ± 9	3400	25	0.00039		0.0000034 ^d		
		24	0.00036		0.00001 ^b		
		23	0.00030 ^a		0.00029		
		22	0.00028 ^b		0.00064 ^a	0.0000043 ^d	
		21	0.00025 ^a		0.0010	0.000018 ^b	
		20	0.00023 ^a		0.0017		
65.0 ± 1.9	1160	22	0.0430	0.00039 ^a	0.00034 ^a		95.0
		20	0.0315	0.00044 ^b	0.0012 ^a		74.0
		18	0.0250	0.00025 ^a	0.0038		63.0
		16	0.0142	0.00006 ^d	0.0090	0.00006 ^d	51.0
		14	0.0108		0.022	0.0023 ^a	43.5
		13					38.5
		12	0.0064		0.040		35.5
		11					33.0
60.0 ± 1.8	1070	21	0.051	0.005 ^a	0.0007 ^b		
		20	0.045		0.00085 ^d		
16.5 ± 0.7	294	16	5.6 ^a				
		15					83 ^a
		14	4.4				81
		13					76
		12	2.8				71
		11					65
		10	1.3				59
15.8 ± 0.5	282	9	1.21		0.10 ^b		48.5
15.4 ± 0.5	275	14	5.70	0.30 ^c			
		12	3.3	0.16 ^c			
6.16 ± 0.29	110	3	0.65		1.13		14.9
5.77 ± 0.28	103	13	43.6				
		11	31.6				50 ^a
		9	18.9				44 ^a
		7	11.3				36 ^a

Random standard uncertainties are $\pm 5\%$ unless otherwise indicated (^a $\pm 10\%$; ^b $\pm 15\%$; ^c $\pm 20\%$; ^d $\pm 30\%$). Systematic uncertainties add an additional $\pm 7\%$ to absolute magnitudes (see Sect. II.H).

FIGURE CAPTIONS

- Figure 1. Schematic diagram of the apparatus. Dimensions for C_1 - C_5 are in the text.
- Figure 2. a) Schematic diagram of Faraday-cup assembly.
b) Schematic diagram of solid-state-detector array.
- Figure 3. Charge-state fractions, F_{15} and F_{17} , as a function of target thickness, for 1160 keV/amu Fe^{+16} in H_2 .

The lines are the solution of a least-squares fit to the data (including corrections for second-order effects) from which the cross sections were obtained (Eq. 9). The F_{15} fraction (Fig. 3a) and F_{17} fraction (Fig. 3b) were used to determine the single-electron-capture and single-electron-loss cross sections, respectively.

- Figure 4. Slow-ion and -electron current (arbitrary units) to collector plates in target, as a function of bias voltage applied to the plates, for 1160 keV/amu Fe^{+16} incident on H_2 .
- Figure 5. The fraction $F_{(16)}$ of slow ions produced in the target as a function of target thickness for 1160 keV/amu Fe^{+16} in H_2 . The line is the solution of a least-squares fit to the data (including corrections for second-order effects) from which the ionization cross section was obtained (Eq. 12).

Figure 6. Single-electron-capture cross sections $\sigma_{q,q-1}$ vs q , for Fe^{+q} in H_2 : results of present experiment. The projectile energy corresponding to each symbol is defined in the figure.

Figure 7. Single-electron-capture cross sections $\sigma_{q,q-1}$ shown scaled empirically to the form $\sigma = (1.2 \times 10^{-8}) q^{3.15} E^{-4.48}$ (solid line), for Fe^{+q} in H_2 .

a. Energy dependence of $\sigma_{q,q-1}$, scaled by $q^{-3.15}$. The following symbols are used to denote the experimental results: ■, present experiment; ⊕, Meyer et al.;²⁴ ☆, Gardner et al.²⁵

b. Charge-state dependence of $\sigma_{q,q-1}$, scaled by $E^{4.48}$. The present experimental results are shown using the same symbols as in Fig. 6. In addition, results of Meyer et al.²⁴ are shown as ⊕, and results of Gardner et al.²⁵ are shown as ☆.

Figure 8. Single-electron-capture cross sections, $\sigma_{q,q-1}$ for $\text{Fe}^{+q} + \text{H}_2$ (experiment, left ordinate) and $\text{Fe}^{+q} + \text{H}$ (theory, right ordinate). The short-dashed line is the classical-trajectory calculation of Olson⁵, the solid line the modified OBK calculation of Chan and Eichler,⁴² the long-dashed line the UDWA calculation of Ryufuku and Watanabe,⁴³ and the dot-dashed line the modified OBK calculation of Rule and Omidvar.³⁹

Figure 9. Single-electron-loss cross sections, $\sigma_{q, q+1}$, for $\text{Fe}^{+q} + \text{H}_2$ (experiment, left ordinate), and $\text{Fe}^{+q} + \text{H}$ (theory, right ordinate). Present results: ●, 110 keV/amu; △, 282 keV/amu; ▲, 1070 keV/amu; □, 1160 keV/amu; ■, 3400 keV/amu.

The solid lines are the calculations by Rule and Omidvar; the dashed line is to guide the eye and has no other significance.

Figure 10. Impact ionization cross sections, σ_I , for $\text{Fe}^{+q} + \text{H}_2$ (experiment, left ordinate), and $\text{Fe}^{+q} + \text{H}$ (theory, right ordinate). The numbers indicate the energy in keV/amu. The solid lines are the classical-trajectory calculations of Olson.⁵ The dashed line is to visually connect the experimental point at $q = 3$ with the rest of the 103 keV/amu experimental points at higher q values.

Figure 11. Hydrogen electron loss cross section.

Solid line: Calculated cross section σ_{loss} for electron loss by atomic hydrogen in collision with an ion in charge state q ; this curve is valid for $1 \leq q \leq 50$ and for energies in the range 50 to 5000 keV/amu (from Ref. 5). The range of E/q values for which the curve is valid is indicated by the bars drawn in the lower portion of the figure. The uncertainty in the calculated cross sections is ± 25 . Dashed lines: Plane-wave Born-approximation cross section for ionization only (Refs. 57,58). Closed

symbols: Present experimental results for $\text{Fe}^{+q} + \text{H}_2$
divided by a number between 1.5 and 2.0 to allow comparison
with the calculations (see discussion in Ref 5). The
uncertainty is ± 30 . ■, 103 keV/amu, $q = 7-11$; ▲, 110
keV/amu, $q = 3$; ◆, 282 keV/amu, $q = 9$; ★, 294 keV/amu,
 $q = 10-15$; ●, 1160 keV/amu, $q = 11-22$.

XBL 805-918

Figure 1

XBL 806-1163

Figure 2a

XBL 806-1164

Figure 2b

Figure 3a

XBL 805 - 922

Figure 3b

XBL 805-923

XBL 805 - 925

Figure 5

XBL 805-917A

Figure 6.

XBL 805-920

Figure 7a

XBL 805 - 919A

Figure 7b

XBL 805 - 921A

Figure 8

XBL 805-926A

Figure 9

XBL 805-924A

Figure 10

XBL 783-2458B

Figure 11

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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