Cross sections for resonant transfer and excitation in $Fe^{q+}+H_2$ collisions

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Resonant transfer and excitation (RTE) is investigated for Fe^{q+} ions ($q=23$, 24, and 25) colliding with H_2. For each charge state, cross sections for RTE were obtained from measurements of K x rays, emitted from the doubly excited intermediate state, coincident with single-electron capture by the incident ion. Additionally, for Fe^{25+} cross sections were obtained from measurements of coincidences between the two K x rays emitted from the intermediate state. These latter measurements provide information on the lifetimes of intermediate metastable states formed in the RTE process. In all cases, measured cross sections are in good agreement with calculations based on theoretical cross sections for dielectronic recombination (DR). Since RTE closely approximates DR, the results indicate that dielectronic-recombination cross sections involving K-shell excitation can be accurately predicted for highly charged iron ions. The results for Fe^{25+} show that metastable states are sufficiently short lived to be observable in the RTE (or DR) process for these hydrogenlike ions.

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I. INTRODUCTION

Resonant transfer and excitation [1] (RTE) takes place when charge transfer (electron capture) and projectile excitation occur together in a single collision due to the electron-electron interaction. The doubly excited intermediate state that is formed in the collision can subsequently decay by photon emission, thereby effecting recombination of the ion. RTE is analogous to and closely approximates [2] dielectronic recombination [3] (DR) which involves the interaction between an ion and a free electron.

Over a broad energy range DR is the primary recombination mechanism in electron-ion collisions, and is of considerable interest to astrophysical studies [4], nuclear fusion plasmas [5], and the development of storage rings. Hence, accurate knowledge of DR cross sections is needed. Until recently, DR measurements were carried out using merged-beam or crossed-beam techniques for which the counting rates were often quite low, thus making the experiments difficult. The development of ion traps [6], electron coolers [7], high-intensity ion and electron sources [8], and storage rings [9] and their use to measure DR is alleviating this latter difficulty and the results obtained are providing stringent new tests of theory.

Because of the close relationship between RTE and DR, the former can be used as a test of theoretical DR cross sections. Since RTE is measured using static gas targets with pressures of several mTorr, absolute experimental cross sections are readily obtained without requiring normalization to radiative recombination cross sections [6] or to ionization cross sections [8] as is often done. To date, most measurements [1] of RTE involving K-shell excitation followed by x-ray emission for ions with $9 \leq Z \leq 32$ have shown generally good agreement with calculations based on theoretical DR cross sections [2]. Additionally, measurements of RTE involving L-shell excitation [10] for Nb^{31+} ions show similar good agreement with theory.

An ion of particular importance in the study of DR is iron, largely because of its importance in the understanding of astrophysical plasmas [4]. Recently, detailed theoretical calculations [11] of DR cross sections for Fe^{15+}, Fe^{23+}, and Fe^{25+} have been reported, and the cross sections are found to decrease strongly with increasing projectile charge state. In addition to providing a test of the transition energies and magnitudes of the theoretical DR cross sections, RTE measurements can also establish and provide a test of the calculated charge-state dependence of DR. It is noteworthy that tests of the charge-state dependence of DR have not been forthcoming from direct DR measurements to date. Furthermore, such a test of theory is important since recent RTE measurements [12] of the charge-state dependence for Nb^{q+} ions involving L-shell excitation were in substantial disagreement with theoretical calculations [13,14], in contrast to earlier measurements [15] and calculations [2,16] for Ca^{q+} ions with K-shell excitation.

We report here measurements of RTE for Fe^{23+}, Fe^{24+}, and Fe^{25+} ions colliding with H_2. Measurements were made for each charge state by observing coincidences between single-electron capture events and Fe K x-ray emission resulting from decay of the intermediate doubly excited states formed in the RTE process, e.g.,

$$\begin{aligned} Fe^{23+}(1s^2 2s) + e^- &\rightarrow Fe^{22+}(1s2s2p^2) \\ &\rightarrow Fe^{22+}(1s^2 2s2p) + h\nu \; . \end{aligned}$$

For incident Fe^{25+} (hydrogenlike) ions, an additional method [17] of investigating RTE is afforded by detecting coincidences between the two Fe K x rays emitted, i.e.,

$$\begin{aligned} Fe^{25+}(1s) + e^- \rightarrow Fe^{24+}(2p^2) &\rightarrow Fe^{24+}(1s2p) + h\nu \\ &\rightarrow Fe^{24+}(1s^2) + h\nu' \; . \end{aligned}$$

Observation of coincidences between the two x rays emitted eliminates contributions from direct electron capture to excited states of Fe^{24+} ($n > 1$) which subsequently decay by x-ray emission when the initial K vacancy is filled. In x-ray–single-capture coincidence measurements, these competing events have the same signature as the RTE events of interest, and thus can contribute substantially to the measured coincidence yield. Furthermore, the x-ray–x-ray coincidence measurements provide information on the lifetimes of intermediate metastable states formed in the DR process.

II. EXPERIMENTAL PROCEDURE

The experimental measurements reported here were carried out at the Lawrence Berkeley Laboratory using the SuperHILAC Facility. The experimental technique consisted of measuring, for each incident charge state, Fe K x rays from the projectile coincident with single-electron-capture events, and, in the case of incident Fe^{25+} ions, measuring coincidences between two Fe K x rays as well. Iron ions in the charge state of interest were passed through a differentially pumped target cell containing H_2 gas. Iron K x rays emitted following projectile excitation were detected with two Si (Li) detectors each mounted at 90° to the beam axis in the target cell. After emerging from the gas cell the beam was magnetically analyzed into charge-state components, and ions undergoing electron capture in the target gas were detected with a solid-state detector. Ions not changing charge, i.e., those emerging in the incident charge state, were collected in a Faraday cup. Coincidences between K x rays and projectiles capturing an electron, as well as x-ray–x-ray coincidences, were measured with a time-to-amplitude converter. In all cases, the fraction of the beam leading to coincidence events was measured as a function of gas pressure in order to obtain the desired cross sections and to ensure that single-collision conditions prevailed. A capacitance manometer was used to measure the absolute pressure in the target gas cell. Systematic uncertainties are estimated to be 5% in the determination of the target gas pressure, 6% in the calculation of the effective gas-cell length, 5% due to beam fluctuations, 3% due to gas impurities, and 10% due to the solid angle and efficiency of the x-ray detector. When combined with the statistical uncertainties, the overall absolute uncertainty is less than ±20%.

III. THEORETICAL CALCULATIONS

The theoretical DR cross sections for Fe^{q+} ($q = 23-25$) were calculated in exactly the same way [16] as for the isoelectronic Ca^{q+} ($q = 17-19$) ions using the AUTOSTRUCTURE package [18–20]. This package is based on an isolated-resonance approximation using Thomas-Fermi-Dirac-Amaldi radial wave functions and the (Coulomb) Breit-Pauli Hamiltonian. The resulting KLL (i.e., $2s2p \rightarrow 1s + e^-$) Auger energies are less than 0.3% greater than those obtained by Chen *et al.* [21–23], which were calculated using Dirac-Fock wave functions and the Coulomb-Breit Hamiltonian. Additionally, the Fe^{25+} DR cross sections were calculated according to the method of Ref. [24] in order to compare with the RTE cross sections obtained from the x-ray–x-ray coincidence measurements. In all cases, the DR cross sections were converted to RTE cross sections by averaging [25] them over the Compton profile [26] of H_e, taking into account the binding energy of the target-gas electrons [see Ref. [16], Eq. (2)].

IV. RESULTS AND DISCUSSION

The experimental cross sections obtained from the x-ray–single-electron-capture coincidence measurements are shown in Figs. 1–3, and the cross sections obtained from the x-ray–x-ray coincidence measurements for the Fe^{25+} ions are shown in Fig. 4(a). The measurements ex-

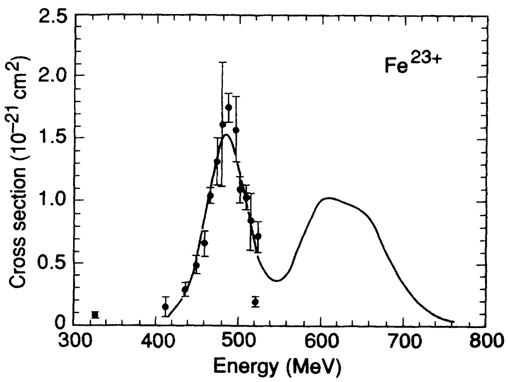

FIG. 1. Measured cross sections for Fe K x rays coincident with single-electron capture for Fe^{23+} ions colliding with H_2. Uncertainties shown are statistical and absolute uncertainties, which must be added in quadrature to those shown, are estimated to be less than ±20%. The smooth curve is the calculated RTE cross section for Fe^{23+} which was obtained from theoretical DR cross sections for Fe^{23+} averaged over the electron momentum distribution (Ref. [26]) of the target. The lower-energy maximum corresponds to resonant KLL transitions, while the higher-energy maximum is due to KLM, KLN, KLO, . . . transitions.

tend to 525 MeV (9.2 MeV/u), which is the maximum attainable energy for Fe ions using the SuperHILAC. Thus, these measurements cover the region corresponding to intermediate resonance states involving KLL transitions only. The absolute values of the measured cross sections were derived from the slopes of the coincidence yields measured as a function of gas pressure. In Figs. 1–3, the results obtained with each of the two detectors for a given projectile charge state were averaged to yield the cross-section values shown. For Fe^{25+} the large cross-section value near 325 MeV in Fig. 3 (x-ray–single-capture coincidences) is due to electron capture to $n \geq 2$ followed by K x-ray emission when this singly excited state decays. Relative statistical uncertainties in the averaged cross sections of Figs. 1–3 are found to

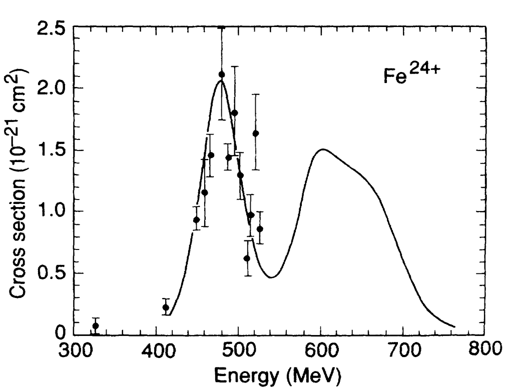

FIG. 2. Measured cross sections for Fe K x rays coincident with single-electron capture for Fe^{24+} ions colliding with H_2. See the caption to Fig. 1.

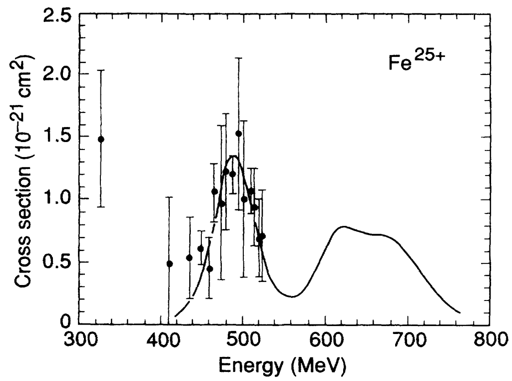

FIG. 3. Measured cross sections for Fe K x rays coincident with single-electron capture for Fe^{25+} ions colliding with H_2. See the caption to Fig. 1. The relatively large value near 325 MeV is due to electron capture to $n \geq 2$ with subsequent K x-ray decay.

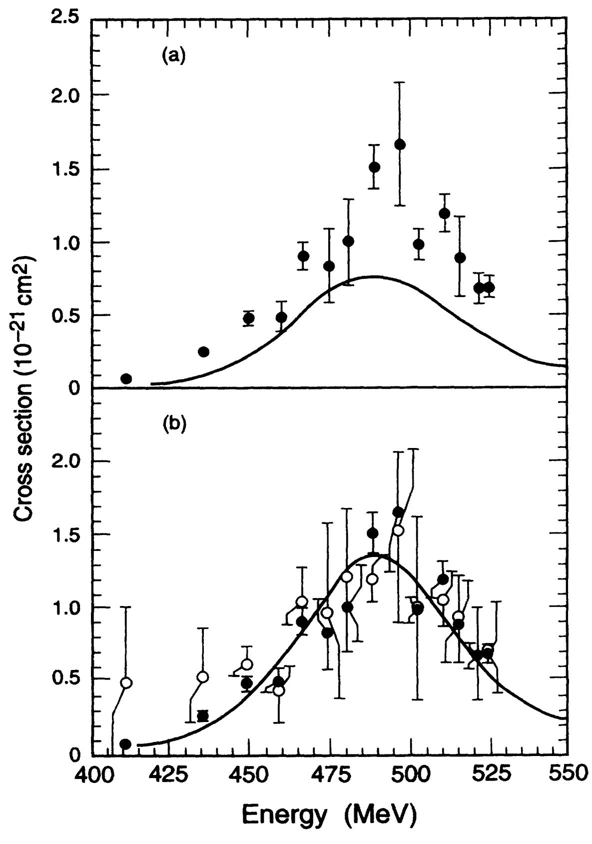

FIG. 4. (a) Measured cross sections for coincidences between two Fe K x rays for Fe^{25+} ions colliding with H_2. The uncertainties shown are statistical, and the absolute uncertainties (which must be added in quadrature) are estimated to be less than ±30%. The curve is the calculated RTE cross section corresponding to the detection of the two Fe K x rays resulting from the decay of the doubly excited intermediate states formed in the RTE process. Metastable states are taken into account (see text). (b) Comparison of cross sections [from Figs. 3 and 4(a)] obtained by x-ray–single-electron capture coincidences (○) with those obtained by x-ray–x-ray coincidences (●). The smooth curve is the calculated RTE cross section for Fe^{25+} (from Fig. 3) for x-ray–single-capture coincidences.

be about ±10%, ±10%, and ±15% for projectile charge states $q=23$, 24, and 25, respectively. In Fig. 4(a) the error bars show the statistical errors which are less than ±30%.

The smooth curves shown in Figs. 1–3 are absolute calculations of the magnitudes of the RTE cross sections and have not been normalized to the data. The maximum at higher energies in the theoretical RTE curves is due to KLn, $n \geq 3$ transitions. In general, the agreement between theory and experiment is very good, indicating that the cross sections for DR, upon which the RTE calculations are based, can be calculated with good accuracy for these highly charged iron ions. The curve in Fig. 4(a) is the calculated RTE cross section corresponding to measurements involving the detection of x-ray–x-ray coincidences, and, hence, metastable states are necessarily taken into account in the calculation. This curve is seen to underestimate the data by nearly a factor of 2.

Comparison of the x-ray–x-ray coincidence data of Fig. 4(a) with theory requires more careful consideration, however. Since observation of RTE events via x-ray–x-ray coincidences can involve the emission of a photon from a metastable state, the measured cross sections shown in Fig. 3 provide an upper limit to those shown in Fig. 4(a). For the gas cell used in the present experiment (about 4.0 cm long), the flight time of an ion through the cell is ~1 ns. Thus, any intermediate metastable states which are formed as a result of the RTE process need to decay in times less than this in order to be observed in the x-ray–x-ray coincidence measurements. The lifetimes of the metastable states which contribute most strongly to RTE for Fe^{25+} ions, namely, $2\,^1S_0$, $2\,^3S_1$, $2\,^3P_2$, 2^3P_0, are calculated in this work to be < 5 ns. Thus, it might be expected that not all of the RTE events resulting from metastable state formation will be viewed with the experimental setup used here. In the calculation of Fig. 4(a) all of the metastable states were arbitrarily assumed to be stable, thereby effectively eliminating their contributions to the curve shown.

However, we note from comparison of Figs. 3 and 4(a) that the magnitudes of the observed cross sections are nearly equal, indicating that, in fact, the metastable states formed by RTE are sufficiently short lived so as to be observable as x-ray–x-ray coincidence events for the present experimental arrangement. The data obtained by the two methods are compared directly in Fig. 4(b) and the theoretical curve from Fig. 3 for x-ray–single-capture coincidences is shown here as well. This comparison shows that either experimental technique gives essentially the same result, at least for Fe ions as studied here. In the case of lower Z ions for which metastable states are longer lived, x-ray–x-ray coincidence measurements can provide a direct test of theoretical calculations of DR involving metastable states (see Ref. [24]).

To display more clearly the nature of the projectile charge-state behavior of the RTE cross sections, we show in Fig. 5 the maximum value of the measured and calculated RTE cross sections as a function of the number of electrons on the incident Fe ions. Also shown are RTE maximum cross-section values obtained previously for Ca ions [15] and Nb ions [12]. The results for Ca involve K-

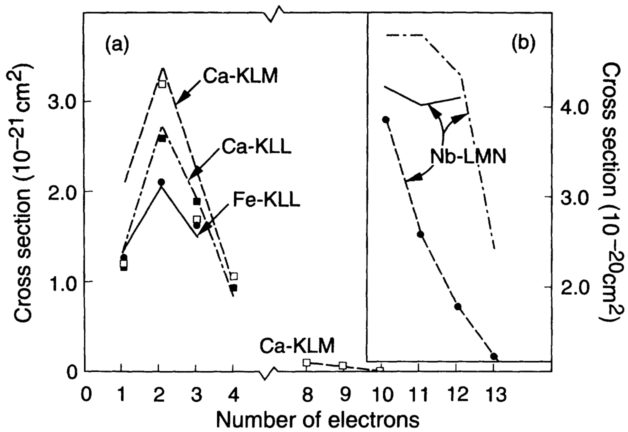

FIG. 5. Charge-state dependence of RTE cross-section maxima. (a) Experiment: ●, KLL transitions for Fe^{q+} (from Figs. 1–3); ■, KLL transitions for Ca^{q+} (Ref. [15]); □, KLM transitions for Ca^{q+} (Ref. [15]). Theory: ——, KLL for Fe^{q+} (present work); —·—·—·, KLL for Ca^{q+} (Ref. [2]); — — —, KLM for Ca^{q+} (Ref. [2]). (b) Experiment: ●, LMN transitions for Nb^{q+} (Ref. [12]). Theory: ——, LMN for Nb^{q+} (Ref. [13]); —·—·—·, LMN for Nb^{q+} (Ref. [14]).

shell excitation while those for Nb involve L-shell excitation. The near factor-of-2 decrease from two electrons to one electron in the incident ion reflects the fact that, in the former case, there are two K electrons which can participate in the RTE process, whereas for the latter there is only one.

The good agreement between theory and experiment for KLL and KLM transitions provides further evidence of the accuracy with which DR involving K-shell excitation may be calculated for these very highly charged ions. In view of these results, the large discrepancy between theory [13,14] and experiment for RTE involving L-shell excitation as reported in Ref. [12] and shown in Fig. 5 is difficult to understand.

V. CONCLUSIONS

Resonant transfer excitation has been studied for Li-like, He-like, and H-like Fe ions colliding with H_2. Absolute cross sections were obtained and compared with calculations based on theoretical cross sections for dielectronic recombination averaged over the target electron momentum distribution. The quantities of interest are the magnitudes of the cross sections and the resonant energies, and for each of these quantities the agreement between theory and experiment is very good. For incident Fe^{25+} ions, a comparison of the cross sections obtained from measurements of x-ray–single-electron capture coincidences with those obtained from x-ray–x-ray coincidences indicates that metastable states formed in the RTE process are sufficiently short lived so as to be observable.

The present results demonstrate that DR involving K-

shell excitation can be accurately predicted for these highly charged ions. Earlier RTE results [15] for *K*-shell excitation in Ne-like to H-like Ca ions also showed good agreement with theory [2,16]. However, this good agreement is contrary to results [12] obtained for RTE with *L*-shell excitation in Ne-, Na-, Mg-, and Al-like Nb ions for which it was found that theory [13,14] and experiment [12] disagreed by a factor of 2 or more (see Fig. 5).

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