# Charge transfer leading to multiple ionization of neon, sodium, and magnesium

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Absolute cross sections for proton and helium-ion impact on neon, sodium, and magnesium are presented. By using coincidence techniques cross sections for pure single- or double-electron capture are separated from those events where one or more ionizations accompany the capture process. In addition, information about the direct-ionization channel is presented. The present data are combined with previous experimental information to identify specific channels which contribute to the cross sections presented here.

## I. INTRODUCTION

Ion-atom collisions produce target ions as a result of either electron capture or direct Coulomb ionization. When the projectile velocity is comparable to, or smaller than, the bound target-electron velocity, capture of that electron by the projectile is the most probable process. Quite often, additional target ionization accompanies the electron-capture process, leaving the target multiply ionized.

There are several different methods by which electron capture can lead to multiple ionization of an atom. For large impact energies where the projectile velocity is comparable to, or larger than, that of an inner-shell electron, that electron may be captured, and the subsequent Auger cascades can produce relatively high degrees of ionization. In this case, it has been shown that multiple target ionization is more probable than single target ionization.<sup>1</sup> For very low impact energies, inner-shell electron capture is negligibly small with respect to outer-shell capture. In this case, multiple ionization occurs predominantly via the "transfer ionization" process. Here, in some cases, the charge-transfer process is excergic. This excess energy, which can be calculated by the difference of the ionization potentials before and after the collision, is available to ionize additional target electrons. In the case of slow highly-charged ion impact, large ionization potentials are involved, and the transfer ionization process is an effective method for producing high degrees of target ionization. However, even for  $He^{2+}$  impact, it has been shown<sup>2</sup> that the transfer ionization channel (single-electron capture plus ionization channel) can exceed the pure singleelectron-capture channel.

For intermediate energies, inner-shell electron capture is still relatively unimportant with respect to outer-shell capture, but now the projectile has sufficient kinetic energy to produce additional outer-shell ionization through direct Coulomb excitation. This "capture-plus-ionization" (C + I) process has been experimentally investigated for single-electron capture in H<sup>+</sup> and He<sup>+</sup> collisions with rare-gas atoms.<sup>1,3-7</sup> For these collision systems C + I can be quite important, but pure electron capture still dominates. However, for He<sup>2+</sup> impact it was recently shown<sup>8</sup> that C + I can exceed pure electron capture in both the single and double capture channels.

It is the purpose of the present paper to investigate charge-transfer interactions for  $H^+$ ,  $He^+$ , and  $He^{2+}$  impact on neon, sodium, and magnesium. The total chargetransfer cross sections are broken into their constituents, namely, pure charge transfer and charge transfer plus one or more additional ionizations. The targets presented here have outer-shell electronic configurations consisting of a filled *L* shell (Ne), one *M* shell (Na) and two *M*-shell electrons (Mg). Data are presented and discussed for multiple ionization of these targets associated with single-electron capture by  $H^+$  and  $He^+$  and for single- and doubleelectron capture by  $He^{2+}$  ions. In addition, since the C + I channels liberate electrons to the continuum, total electron-production cross sections are included to provide an indication of the contribution of the C + I channels to the total electron production.

A specific goal of this paper is to identify, whenever possible, and present absolute cross sections for channels leading to pure single and double capture channels, to single capture-plus-ionization channels, and to double capture-plus-ionization channels. This will be done by using new data as well as previously published cross sections to determine the relative importance of various possible channels. In cases where cross sections are not available for some of the possible channels being considered, data for other projectiles and/or targets will be used to provide indications as to which channels may be the most important.

### **II. EXPERIMENTAL PROCEDURE**

The apparatus and procedures used in this work have been described previously<sup>3,8,9</sup> and will be discussed only briefly here. A collimated, momentum-analyzed ion beam was passed through a diffuse atomic beam and was then electrostatically charge-state analyzed and detected by channel electron multipliers. Slow target ions were extracted perpendicular to the projectile and target beams. The target-ion charge states were identified by their flight times between the interaction region and the target-ion detector. Coincidences between these slow ions and the postcollision projectile beams provided identification and separation of the pure electron-capture channels from the

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capture-plus-ionization channels.

The following capture, capture-plus-ionization and ionization reactions were studied: for single capture

$$\begin{vmatrix} \mathbf{H}^{+} \\ \mathbf{H}\mathbf{e}^{+} \\ \mathbf{H}\mathbf{e}^{2+} \end{vmatrix} + T \rightarrow \begin{vmatrix} \mathbf{H}^{0} \\ \mathbf{H}\mathbf{e}^{0} \\ \mathbf{H}\mathbf{e}^{+} \end{vmatrix} + T^{+} ,$$

.

double capture

$$\operatorname{He}^{2+} + T \rightarrow \operatorname{He}^{0} + T^{2+}$$

single capture plus ionization

$$\begin{pmatrix} \mathbf{H}^+ \\ \mathbf{H}\mathbf{e}^+ \\ \mathbf{H}\mathbf{e}^{2+} \end{pmatrix} + T \rightarrow \begin{pmatrix} \mathbf{H}^0 \\ \mathbf{H}\mathbf{e}^0 \\ \mathbf{H}\mathbf{e}^+ \end{pmatrix} + T^{q+} + (q-1)e , \quad q > 1 ,$$

double capture plus ionization

$$He^{2+} + T \rightarrow He^{0} + T^{q+} + (q-2)e$$
,  $q > 2$ ,

and ionization

$$\begin{vmatrix} \mathbf{H}^+ \\ \mathbf{H}\mathbf{e}^+ \\ \mathbf{H}\mathbf{e}^{2+} \end{vmatrix} + T \rightarrow \begin{vmatrix} \mathbf{H}^+ \\ \mathbf{H}\mathbf{e}^+ \\ \mathbf{H}\mathbf{e}^{2+} \end{vmatrix} + T^{q+} + qe ,$$

where T represents the targets Ne, Na, or Mg. The coincidence signal  $S_q^{if}$  (where q is the final charge state of the target; i and f are the initial and final charge states of the ion beam) was measured for each of the reactions indicated above. The measured coincidence signal  $S_a^{if}$  is proportional to the cross section,  $\sigma_q^{if}$ , the beam intensity, I; the target density, N; the slow-ion-detection solid angle,  $\Delta\Omega(q)$ ; and the detection efficiency for both slow,  $\eta_s(q)$ , and fast,  $\eta_f(f)$ , ions. Note that both the detection solid angle and detection efficiency may depend on the slow ion charge state. Thus we have

$$S_q^{if} = K \sigma_q^{if} NI \Delta \Omega(q) \eta_s(q) \eta_f(f) , \qquad (1)$$

where K is a proportionality constant. In this notation, f = i, i - 1, and i - 2 for pure ionization, single, and double capture, respectively. Tests were run to demonstrate that for the experimental parameters used, the slow ion detection was independent of the slow ion charge state. In addition, the beam detection efficiency was measured as unity for 100-200-keV neutral, singly, and doubly charged ions (see Ref. 10 for details). Thus,

$$S_a^{if} = K \sigma_a^{if} N I \Delta \Omega \eta_s . \tag{2}$$

By simultaneously recording the coincidence signals for single and double charge transfer we note that the total single-charge-transfer cross section is given by

$$\sigma^{i,i-1} = \sum_{q} \sigma_q^{i,i-1} , \qquad (3)$$

or, from Eq. (2),

$$\sigma^{i,i-1} = \sum_{q} S_{q}^{i,i-1} / (KNI\Delta\Omega\eta_{s}) .$$
<sup>(4)</sup>

Equations (2) and (4) combine to give

$$\sigma_q^{10} = \frac{\sigma^{10}}{\sum S_q^{10}} S_q^{10} , \qquad (5)$$

$$\sigma_{q}^{2l} = \frac{\sigma^{2l}}{\sum_{q} S_{q}^{2l}} S_{q}^{2l} \,. \tag{6}$$

This places the single-electron-capture yields on an absolute scale, by using known single-electron-capture cross sections. The same normalization can be applied to the double capture yields since they were recorded simultaneously. Thus, double-electron-capture cross sections are given by

$$\sigma_{q'}^{20} = \frac{\sigma^{2l}}{\sum_{q} S_{q'}^{2l}} S_{q'}^{20} . \tag{7}$$

Note that in the case of double capture,  $q' \ge 2$  unless multiple collisions occur, in which case the ion may be neutralized in a two-step process:

$$\frac{\mathrm{He}^{2+} + T \rightarrow \mathrm{He}^{+} + T^{+}}{+ T \rightarrow \mathrm{He}^{0} + T^{+}}$$

Thus double-collision processes are distinguishable, since a singly charged target ion will then be measured in coincidence with a projectile that has captured two electrons. This can be an important feature of the coincidence technique for low-energy collisions where multiple collisions may make interpretation of charge-transfer measurements extremely difficult or unfeasible.

For the present work, absolute cross sections  $\sigma^{10}$  and  $\sigma^{21}$  were taken from Refs. 10 and 11. Using these cross sections and the procedure outlined, the coincidence cross sections  $\sigma_q^{if}$  are believed to be accurate to approximately 20% for the pure single capture channel, with larger uncertainties ( $\sim 50\%$  or larger) for the highest charge states and smallest cross sections measured. These values include statistical as well as normalization uncertainties. Previous work<sup>8,9</sup> has indicated that this method of normalization may tend to overestimate the double capture cross sections for some unexplainable reason (see Ref. 8 for details). However, since no experimental uncertainties could be identified that would affect only the double capture cross sections, and since the total double capture cross sections have inherently larger uncertainties than do the total single capture cross sections, it was decided to use the normalization procedure as a best estimate of their absolute values.

Total electron-production cross sections  $\sigma_{-}$  can be derived from these data by

$$\sigma_{-} = \sum_{q} q \sigma_{q}^{ii} + \sum_{q>1} (q-1)\sigma_{q}^{i,i-1} + \sum_{q>2} (q-2)\sigma_{q}^{i,i-2} .$$
(8)

In the case of neon, the individual cross sections  $\sigma_{-}$ ,  $\sigma_{q}^{ii}$ ,  $\sigma_{q}^{i,i-1}$ ,  $\sigma_{q}^{i,i-2}$  have all been measured.<sup>3,9</sup> However, for sodium and magnesium, the target densities were too small to measure the direct ionization cross sections  $\sigma_a^{ii}$ , therefore the following procedure was used to obtain ionization information. The total number of slow target ions (n) (noncoincidence) was measured simultaneously with the coincidence signals  $(S_q^{i,i-1}, S_q^{i,i-2})$  which are the number of target ions created by electron transfer to the projectile. Since the beam-particle-detection efficiencies were measured to be unity, and the slow-ion-detection efficiency was assumed to be independent of the interaction process, e.g., direct ionization, single or double charge transfer, the following equation applies:

$$n = k \sum_{q} (S_{q}^{ii} + S_{q}^{i,i-1} + S_{q}^{i,i-2}) .$$
(9)

This can be used to determine the *number* of ions due to direct target ionization  $(\sum_q S_q^{ii})$  from the measured total slow-ion signal (n) and the coincidence  $S_q^{ii}$  cross sections.

These relative numbers were then converted to absolute cross sections by again normalizing to the total singlecharge-transfer cross sections:

$$\sum_{q} \sigma_{q}^{ii} = \frac{\sigma^{i,i-1}}{\sum S_{q}^{i,i-1}} \sum_{q} S_{q}^{ii} .$$
(10)

These ionization cross sections represent the sum of the cross sections for direct ionization to all target charge states which differ from the total electron production cross section  $\sigma_{-}$  by the contributions from direct multiple ionization and charge transfer-plus-ionization channels. In cases where direct multiple ionization can be neglected, in particular for very-low- $\hat{Z}$  target atoms  $\sum_{q} \sigma_{q}^{ii} \approx \sigma_{l}^{ii}$ , and can therefore be compared with theoretical calculations that do not include multiple ionization events. The method described above was used previously to obtain ionization cross sections for lithium<sup>9</sup> where good agree-

#### **III. RESULTS**

Figures 1-3 present charge transfer and ionization cross sections for  $H^+$ ,  $He^+$ , and  $He^{2+}$  impact on Ne, Na, and Mg. The total single- and double-charge-transfer cross sections ( $\sigma^{10}, \sigma^{21}, \sigma^{20}$ ), are broken down into their pure single- and double-charge-transfer cross sections  $(\sigma_1^{10}, \sigma_1^{21}, \sigma_2^{20})$  and their charge-transfer-plus-ionization cross sections  $(\sigma_{q>1}^{10}, \sigma_{q>1}^{21}, \sigma_{q>2}^{20})$  that comprise them. Also included are cross sections for total electron production,  $\sigma_{-}$ , for direct single target ionization,  $\sigma_{1}^{11}$ , and  $\sigma_{1}^{22}$ , as well as cross sections for the sum of the direct target ionization channels,  $\sum_q \sigma_q^{11}$  and  $\sum_q \sigma_q^{22}$ , for Na and Mg targets. The cross sections are shown graphically versus the impact energy divided by projectile mass in order to more easily make comparisons of different projectiles. Where the projectile velocity matches that of the various bound target electrons are indicated by arrows at the abscissa, since this is energy in which capture of those particular electrons is expected to maximize.

Before discussing the various systems in detail, some general features of the cross sections are worth mentioning. For impact velocities less than the velocity of the



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FIG. 1. Ionization and charge transfer cross sections for H<sup>+</sup>, He<sup>+</sup>, and He<sup>2+</sup> impact on neon. Ionization: total electron production,  $\sigma_-$ ; H<sup>+</sup>,..., Ref. 13; He<sup>+</sup>, ----, Ref. 14; He<sup>2+</sup>, ----, Ref. 11. Single direct ionization  $\Theta$ ;  $\sigma_1^{11}$ , H<sup>+</sup>, He<sup>+</sup>, Ref. 3;  $\sigma_1^{22}$ , He<sup>2+</sup>, Ref. 8. Charge transfer: total - -;  $\sigma^{10}$ , H<sup>+</sup>, He<sup>+</sup>, Ref. 3;  $\sigma^{21}$ ,  $\sigma^{20}$ , Ref. 11;  $\sigma^{20}$ ,  $\times$ , Ref. 8. Pure charge transfer  $\sigma_1^{10}$  and  $\sigma_1^{21}$ ,  $\bullet$ ;  $\sigma_2^{20}$ ,  $\blacksquare$ ; H<sup>+</sup>; He<sup>2+</sup>, Ref. 8. Charge transfer-plus-ionization:  $\sigma_q^{10}$  and  $\sigma_q^{21}$ , q > 1 and  $\sigma_q^{20}$ , q > 2; H<sup>+</sup>, He<sup>+</sup>, Ref. 3; He<sup>+</sup>, Ref. 3; He<sup>2+</sup>, Ref. 8. Total 2s and 2s 2p vacancy production  $\sigma(2s^{-1})$  and  $\sigma(2s^{-1}2p^{-1})$ ; Refs. 15, 16, and 18. Equivalent velocities of bound 2s and 2p target electrons indicated by arrows.

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FIG. 2. Ionization and charge transfer cross sections for H<sup>+</sup>, He<sup>+</sup>, and He<sup>2+</sup> impact on atomic sodium. Ionization:  $\sum_{q} \sigma_{q}^{ii}$  (see text for explanation);  $\Theta$ , present results;  $\nabla$ , Ref. 22;  $\sigma_{-}$  electron impact,..., Refs. 19 and 20; He<sup>+</sup>-..., Ref. 21. Charge transfer: total - -;  $\sigma^{10}, \sigma^{21}, \sigma^{20}$ , Ref. 10;  $\sigma^{20}$ ,  $\times$ , present results; pure charge transfer  $\bullet$ , and charge transfer plus ionization  $\blacksquare$ ;  $\blacktriangle$ , present results. Equivalent velocities of bound 3s, 2p, and 2s electrons are indicated by arrows.

outermost bound electron, charge transfer is more probable than is direct ionization. (See Fig. 1; note that the ionization cross sections have been multiplied by 10.) For impact velocities larger than the outermost electron velocity, the opposite is true. A change in slope occurs in the cross section curves for pure single capture ( $\sigma_1^{10}$  and  $\sigma_1^{21}$ ) and to some extent in pure double capture  $\sigma_2^{20}$  in sodium, but not in magnesium, targets. However, it is observable in the capture-plus-ionization channels ( $\sigma_2^{10}$ ,  $\sigma_2^{21}$ , and  $\sigma_3^{20}$ ) for both Na and Mg targets. Since this change in slope occurs for projectile velocity nearly matching the *L*-shell bound-electron velocities it is an indication than an inner-



FIG. 3. Ionization and charge transfer cross sections for H<sup>+</sup>, He<sup>+</sup>, and He<sup>2+</sup> impact on atomic magnesium. Ionization:  $\sum_{q} \sigma_{q}^{ii}$  (see text for explanation);  $\Theta$ , present results;  $\sigma_{-}$ , for electron impact, ..., Ref. 20; 2p ionization,  $\sigma(2p)_{i}, \dots, \dots$ , from Ref. 28 divided by 3.5 as explained in text. Charge transfer: total  $- - ; \sigma^{10}\sigma^{21}, \sigma^{20}$ , Ref. 10;  $\sigma^{20}$ ,  $\times$ , present results; 2p capture,  $\dots, \dots$ , Ref. 28 divided by  $\sim 3.5$  as explained in text. Pure charge transfer  $\sigma^{10}, \sigma^{21}, \Theta$ , and  $\sigma^{20}, \blacksquare$ , Ref. 10;  $\sigma^{20}, \times$ , present results. Charge transfer plus ionization  $\sigma_{2}^{10}, \sigma_{3}^{10}, \sigma_{q>1}^{21}, \sigma_{q>2}^{20}$ , present results. Equivalent velocities of bound 3s and 2p electrons are indicated by arrows.

shell contribution to the capture cross section is becoming important. The reason that it is not seen for the Mg  $\sigma_1^{10}$ ,  $\sigma_1^{21}$ , and  $\sigma_2^{20}$  cross sections will be explained in detail later.

At the higher energies, comparison of pure singlecharge-transfer cross sections for the individual targets shows that equivalent velocity  $H^+$  and  $He^+$  impact cross sections are approximately identical and are a factor of 2-4 times smaller than for  $He^{2+}$  impact. Comparing data for different targets shows that the importance of the charge transfer-plus-ionization channels increases with respect to pure charge transfer as the target becomes heavier. In fact, for the higher energy Na and Mg data charge transfer-plus-ionization exceeds pure charge transfer.

#### A. Neon

The cross sections shown for neon in Fig. 1 are taken from previously published data.<sup>3,8,11</sup> Observe that direct single ionization  $\sigma_1^{11}$  and  $\sigma_1^{22}$  (Refs. 3 and 8) is considerably smaller than the total electron production cross sections  $\sigma_{-}$  (Refs. 11, 13, and 14) even though it has been previously shown that the direct-multiple-ionization cross sections are less than 20-30% of the direct-singleionization cross sections.<sup>3,8</sup> This is because higher-order charge-transfer channels also contribute free electrons. These higher-order charge-transfer channels are considerably more important for  $He^{2+}$  impact than for  $H^+$  or He<sup>+</sup> impact. The present double capture cross sections  $\sigma^{20}$  tend to be 30–50 % larger than those measured using a growth-curve technique.<sup>11</sup> As was previously stated, this has been observed for other systems, and thus far, no experimental reason for this discrepancy has been identified.

It is possible to identify which target electrons and processes contribute to cross sections for direct ionization, pure charge transfer and charge transfer plus one additional ionization for neon. Neon has a  $1s^22s^22p^6$  electronic configuration, but only L-shell electrons (n=2)can contribute to the cross sections shown in Fig. 1 since the K-shell (n = 1) electrons are too tightly bound to be ionized by the projectile energies being considered here. Channels that may contribute to pure single and double capture, to single and double capture plus one additional ionization, and to direct ionization are as follows. The general notation used is  $nl \mid_x$  where x may be either c or i for capture or ionization and l designates either s or pelectrons for the targets being discussed here. Note that the values of n and l will be explicitly stated in certain cases to avoid confusion; otherwise a more general nl notation will be used.

Pure single capture Single capture plus ionization	$\sigma_1^{10}, \sigma_1^{21}, \sigma_2^{10}, \sigma_2^{21}$	21   <sub>c</sub> 21   <sub>c</sub> 21   <sub>i</sub>
Pure double capture	$\sigma_2^{20}$	$2l^2  _{c}$
Double capture plus ionization	$\sigma_3^{20}$	$2p 2s  _{c}$ $2p^{2} _{c} 2l  _{i}$ $2p 2s  _{c} 2l  _{i}$
Ionization	$\sigma_1^{11}, \sigma_1^{22}$	$\frac{2s^2}{c^2p}\Big _i$ $\frac{2l}{i}$

For the range of impact energies discussed here it is possible to determine which of these channels are dominant by comparing the cross sections presented here with previously published data. For example, pure single capture  $\sigma_1^{10}$  for H<sup>+</sup> and He<sup>+</sup> impact occurs via 2p capture. 2s capture can be neglected since the *total* 2s vacancy production cross sections<sup>15,16</sup> shown in Fig. 1 are, at most, only 25% of  $\sigma_1^{10}$ . It is known that direct ionization dominates the charge-transfer mechanism for Ne<sup>+</sup> production

in this energy range;<sup>3</sup> thus 2s capture is only a small portion of this 25% and can be ignored. This conclusion is supported by theoretical calculations of 2p and 2s capture.<sup>17</sup> The same arguments are assumed to also hold for equivalent velocity  $He^{2+}$  impact as well.

In the case of single capture plus ionization, all channels except  $2p \mid_c 2p \mid_i$  can be eliminated since the *total* 2s2p vacancy production cross sections<sup>15,18</sup> are smaller than 20% of the  $\sigma_2^{10}$  cross section, and the *total*  $2s^2$  vacancy production is even less likely.<sup>15,17,18</sup> In both cases, the charge-transfer portion of these channels should represent only a portion of these total cross sections and are thus negligible with respect to  $\sigma_2^{10}$ . This is rigorously true only for the H<sup>+</sup> and He<sup>+</sup> impact energies shown but is assumed to be true for equivalent velocity He<sup>2+</sup> impact also.

Pure double charge transfer  $\sigma_2^{20}$  can occur via double 2p capture, 2p2s capture, or double 2s capture. Although not directly verifiable with existing experimental or theoretical data, the arguments presented above imply that only the double 2p capture channel is important. Likewise, the most probable double capture-plusionization channel is the  $2p^2 |_c 2p |_i$ .

In the case of direct ionization of neon by proton impact, the measured<sup>3</sup> direct-single-ionization cross sections are attributed to 2p ionization, since the 2s ionization cross sections are known to be considerably smaller.<sup>15,17</sup> Again, it is assumed that this also holds true for He<sup>+</sup> and He<sup>2+</sup> impact.

#### B. Sodium

Cross sections for pure capture, capture plus ionization, and pure ionization or H<sup>+</sup>-,He<sup>+</sup>-, and He<sup>2+</sup>-Na collisions are shown in Fig. 2. The influence of inner-shell contribution to the capture cross sections is indicated by a change in slope of the cross sections for impact velocities near the velocity of the sodium *L*-shell electrons. This is most evident for pure single capture  $\sigma_1^{10}$  and  $\sigma_1^{21}$  by H<sup>+</sup> and He<sup>2+</sup> and, to a lesser extent, in the pure double capture  $\sigma_2^{20}$  and the capture-plus-ionization cross sections  $\sigma_2^{10}$ ,  $\sigma_2^{21}$  and  $\sigma_3^{20}$ . In the case of high-energy He<sup>2+</sup> impact, the charge transfer-plus-ionization cross section exceeds the pure charge-transfer cross section, both in the single and double capture channels. This has been previously observed for He<sup>2+</sup>-Ar, -Kr collisions.<sup>8</sup> Again we note that the present total double capture cross sections (*x*) are 30-100% larger than those measured using the growthcurve method (dashed line<sup>10</sup>).

The proton-impact ionization cross sections shown in Fig. 2 agree reasonably well with electron-impact data<sup>19,20</sup> at higher energies and with the He<sup>+</sup> impact ionization

calculations of Tiwary and Rai.<sup>21</sup> However, comparison of these data for  $H^+$  and  $He^+$  ionization of sodium with cross sections deduced from the data of O'Hare *et al.*<sup>22</sup> shows that these data are smaller by approximately a factor of 2. This is similar to results we previously reported<sup>10</sup> for total single-charge-transfer cross sections where the data of O'Hare *et al.* were approximately two times larger than our measurements as well as those of others. This could indicate that their target density measurements were inaccurate.

In order to interpret the cross sections presented in Fig. 2 we note that sodium has an electronic configuration of a neonlike core plus an additional outer-shell electron, i.e., a  $1s^22s^22p^63s$  configuration. Since the K-shell electrons are so tightly bound that they can be ignored in the interactions reported here, and since the neon data showed that it is probably safe to also ignore the 2s contributions with respect to the 2p influence, the channels that might contribute to the cross sections shown in Fig. 2 are

Pure single capture	$\sigma_{1}^{10}, \sigma_{1}^{21}$	$3s \mid c$
•		$2p \mid_c$ leading to $3s \rightarrow 2p$ photon deexcitation
Single capture plus ionization	$\sigma_2^{10}, \sigma_2^{21}$	$3s  _{c}2p  _{i}$ $2p  _{c}3s  _{i}$ $2p  _{c}2p  _{i} \text{ with } 3s \rightarrow 2p$ photon deexcitation. autoionization channels $2p  _{c}2p \text{ excitation}$ $2s  _{c}$ $2s  _{c}3s \text{ excitation}$
Pure double		
capture	$\sigma_2^{20}$	$\begin{array}{c} 2p \ 3s \mid c \\ 2p^2 \mid c \end{array}$
Double capture plus ionization	$\sigma_3^{20}$	$\begin{array}{c c} 2p \ 3s \   \ _{c} 2p \   \ _{i} \\ 2p^{2} \   \ _{c} \ 3s \   \ _{i} \end{array}$
Ionization	$\sigma_{1}^{11}, \sigma_{1}^{22}$	$3s \mid_i \\ 2p \mid_i$

As pointed out earlier, both the 3s and the 2p capture channels contribute to the pure single-electron-capture cross section. The contribution from 2p capture is observed as a change in slope in the projectile velocity dependence for projectile velocities that nearly match the bound *L*-shell electron velocities. At lower energies, 3s capture should dominate, with 2p capture becoming important above approximately 30 keV/amu. Note that following 2p capture, a  $3s \rightarrow 2p$  photon transition will occur.

In the case of ionization, previous data<sup>22</sup> have shown that direct double ionization is small with respect to single ionization. However, insufficient information is available to determine the relative importance of 3s and 2pionization—both of which probably contribute, as in the pure single capture case. For single capture plus ionization several channels could contribute to the measured cross sections. Of the channels listed, some information about those leading to autoionization is known. For example, many autoionizing transitions have been identified,<sup>23-25</sup> and relative autoionization intensities have been measured for H<sup>+</sup> and He<sup>+</sup> (Ref. 26) impact. In the case of H<sup>+</sup> impact, it is possible to place the relative intensities for transitions leading to double ionization of sodium on an absolute scale (subject to uncertainties of a factor of 2 or 3) by normalizing to the total absolute  $2p^{5}3s^{2}(^{2}P) \rightarrow 2p^{6}(^{1}S_{0})$  intensity, which has recently been measured.<sup>27</sup> Doing so yields a total autoionization contribution to double ionization of sodium of approximately  $5 \times 10^{-18}$  cm<sup>2</sup> for proton energies between 50 and 300 keV.

This value is not totally inconsistent with the measured  $\sigma_2^{10}$  value of approximately  $1 \times 10^{-17}$  cm<sup>2</sup>. However, the autoionization intensity of approximately  $5 \times 10^{-18}$  cm<sup>2</sup> results from both capture and ionization processes, whereas the present  $\sigma_2^{10}$  value of  $1 \times 10^{-17}$  cm<sup>2</sup> is due only to capture events. It will be shown in the next section, for H<sup>+</sup>-Mg collisions, that the 2p ionization cross section is approximately twice the 2p capture cross section for velocities equal to the bound 2p electron velocity. Assuming this to be approximately the same for H<sup>+</sup>-Na collisions, the autoionization channels probably account for less than 25% of the measured  $\sigma_2^{10}$  cross section for H<sup>+</sup> impact on sodium.

This would leave the  $3s |_c 2p |_i$ ,  $2p |_c 3s |_i$ , and  $2p |_c 2p |_i$  channels to be primarily responsible for the observed  $\sigma_2^{10}$  and  $\sigma_2^{21}$  cross sections. However, one would expect that the removal of two electrons is much less probable than the removal of either electron alone, e.g.,  $3s |_c 2p |_i \ll 3s |_c$ ,  $2p |_c 3s |_i$ , and  $2p |_c 2p |_i \ll 2p |_c$ . Thus, we would expect that  $\sigma_2^{10} \ll \sigma_1^{10}$  and  $\sigma_2^{21} \ll \sigma_1^{21}$ . Since the higher-energy He<sup>2+</sup> results show that  $\sigma_2^{21} \ll \sigma_1^{21}$ , either autoionization plays a larger role than estimated, or some of our assumptions are invalid, or the combined effect of the capture-plus-ionization channels for He<sup>2+</sup> impact is larger than that of the pure capture channels. Additional experimental or theoretical analysis is required to resolve this question.

In the case of double capture,  $\sigma_3^{20} > \sigma_2^{20}$  at higher energies. The pure double capture channels are 3s 2p capture and double 2p capture, both of which will be associated with a  $3s \rightarrow 2p$  photon relaxation. As was the case for proton impact, both channels are probably important, since the cross section changes slope at higher energies. For double capture-plus-ionization, both the  $2p 3s |_c 2p |_i$  and  $2p^2|_c 3s |_i$  are expected to be smaller than the pure double capture channels,  $2p 3s |_c$  and  $2p^2|_c$ . Thus, in order that  $\sigma_3^{20} > \sigma_2^{20}$  at higher impact energies, there may be important unidentified autoionization transitions contributing to  $\sigma_3^{20}$  or, possibly, channels such as 2s capture that need to be considered.

#### C. Magnesium

Cross sections for magnesium are shown in Fig. 3. For the case of ionization, the data for electron impact<sup>28</sup> appear to merge smoothly with the  $H^+$  results at higher energies. Note that the  $2p \mid_i$  and  $2p \mid_c$  cross sections shown in Fig. 3. have been reduced by a factor of approximately 3.5 from those presented in Ref. 29 in order to make the 2p capture cross sections consistent with the  $\sigma_2^{10}$  cross sections presented here and because 2p capture cannot exceed the total single-electron-capture cross section  $\sigma^{10}$ , taken from Ref. 10. It is assumed that the 2p cross sections presented in Ref. 29 are overestimated in absolute value because of the normalization process that was used.

As was observed for sodium, the ionization cross sections are considerably larger than the charge-transfer cross sections. Also, the dominance of capture-plusionization over pure capture at higher energies is quite obvious.

In order to identify the specific channels leading to ionization, capture, and capture-plus-ionization, we note that magnesium has a  $1s^22s^2p^63s^2$  electronic configuration. For the energy range presented here, only the 2p and 3selectrons are expected to contribute to the cross sections. Thus, the various available channels ionization are

Pure single capture	$3s \mid c$
Single capture plus ionization	$3s  _{c} 3s  _{i}$ $3s  _{c} 2p  _{i}$ $2p  _{c} 3s  _{i}$ $2p  _{c} + \text{Auger relaxation}$
Pure double capture	$3s^{2} _{c}$ 2p 3s   <sub>c</sub> with 3s-2p photon
Double capture plus ionization	$3s^{2} _{c}2p _{i}$ $2p 3s _{c}3s _{i}$ $2p 3s _{c}2p _{i}$ $2p^{2} _{c}3s _{i}$ $2p^{2} _{c} + Auger relaxation$
Ionization, single double	$3s  _i$ $3s^2  _i$ $2p  _i + \text{Auger relaxation}$

Note that pure single electron capture from magnesium can occur only via the  $3s \mid_c$  channel, since 2p capture would lead to double target ionization via Auger relaxation. Hence, the  $\sigma_1^{10}, \sigma_1^{21}$  cross sections show a rapid decrease for impact velocities considerably larger than the 3s binding energy.

The ionization cross sections shown for magnesium most likely result from single 3s ionization, since double 3s ionization is considered to be much less likely, and 2p ionization is shown to be small with respect to the measured ionization cross sections. As noted previously in this paper, this is rigorously true only for H<sup>+</sup> impact but is assumed to be valid for the He<sup>+</sup> and He<sup>2+</sup> collision systems also.

Single capture-plus-ionization can occur via several different channels. At lower impact energies only the  $3s \mid_c 3s \mid_i$  channel contributes, since all other channels have contributions from 2p electrons, and the 2p cross sections are shown to be relatively small for lower impact energies. At higher energies, it is shown that  $3s |_i$ , i.e.,  $\sum_q \sigma_q^{11}$ , is much larger than  $2p |_i$ . Thus  $3s |_c 3s |_i >> 3s |_c 2p |_i$ . Also at higher energies, since it is also assumed that  $2p |_c 3s |_i$  is less probable than  $2p |_c$ alone, and since  $3s |_c$  (i.e.,  $\sigma_1^{10}$ ) is small with respect to  $2p |_c$  (see Fig. 3), this leaves only the  $2p |_c$  channel to account for the higher energy  $\sigma_2^{10}$  cross section. It is the inclusion of this inner-shell capture channel that causes  $\sigma_2^{10}$  to exceed  $\sigma_1^{10}$ , as seen in Fig. 3. Again, these arguments and conclusions are for H<sup>+</sup>-Mg collisions but it is expected that cross sections for equal velocity He<sup>+</sup> and He<sup>2+</sup> impact will behave in the same manner.

In the double capture channels we again have the situation, as was seen for the sodium target, that the captureplus-ionization cross section is larger than the pure double capture cross section at higher energies. The only pure double capture channels are  $3s^2|_c$  and  $2p3s|_c$ , both of which may contribute. However,  $3s^2|_c2p|_i$ ,  $2p 3s |_{c} 3s |_{i}, 2p 3s |_{c} 2p |_{i}, 2p^{2} |_{c} 3s |_{i}, 2p^{2} |_{c}$  followed by Auger relaxation are possible double captureplus-ionization channels. Of these,  $2p 3s \mid c 2p \mid i$  $\ll 2p 3s \mid_c 3s \mid_i$  since  $2p \mid_i \ll 3s \mid_i$ . Also, it is expected that  $2p^2|_c 3s|_i \ll 2p^2|_c$ . At lower impact energies,  $2p^2|_c$  is expected to be negligible with respect to  $3s^2 \mid c^2p \mid a$  and  $2p 3s \mid c^3s \mid a$ , but it is not possible to determine the relative importance of these latter two terms. At higher energies it has been shown that means  $3s \mid_c \ll 2p \mid_c;$  this that  $2p 3s \mid_c 3s \mid_i$  $\ll 2p^2 |_c 3s |_i$ , which is small with respect to  $2p^2 |_c$ . Also, it is expected that  $3s^2 |_c 2p |_i \ll 2p^2 |_c$  since  $3s \mid_c \ll 2p \mid_c$ . Hence, the most likely channels leading to double capture-plus-ionization are  $3s^2 |_c 2p |_i$  and  $2p 3s \mid_c 3s \mid_i$  at lower energies and, at higher energies, double 2p capture followed by Auger relaxation. Again, it is likely that the inclusion of inner-shell capture followed by Auger relaxation causes  $\sigma_3^{20}$  to be larger than  $\sigma_2^{20}$  at higher energies. However, such transitions have not been identified thus far.

#### **IV. CONCLUSIONS**

Cross sections for pure single and double capture, single and double capture-plus-additional-ionization of one or two electrons, and information about direct ionization for  $H^+$ ,  $He^+$ , and  $He^{2+}$  ions impacting on neon, sodium, and magnesium have been presented. It was observed that, for lower-energy  $H^+$  and  $He^+$  impact, the total single capture cross section is almost entirely due to pure single capture. But for higher impact energies, charge transfer plus ionization becomes more important and, in some cases, dominates.

In many cases it was possible to identify specific channels contributing to these cross sections. These cross sections provide the opportunity to test theoretical calculations of charge transfer in great detail.

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