



# One-electron capture with simultaneous ionization in $C^{q+}$ , $O^{q+}$ ( $q = 1-4$ )–Ar collisions

Baowei Ding<sup>a,\*</sup>, Ximeng Chen<sup>a,\*\*</sup>, Deyang Yu<sup>b</sup>, Bitao Hu<sup>a</sup>, Xiaohong Cai<sup>b</sup>, Zhaoyuan Liu<sup>a</sup>

<sup>a</sup> School of Nuclear Science and Technology, Lanzhou University, South Tianshui Road 222, Lanzhou 730000, PR China

<sup>b</sup> Institute of Modern Physics, Chinese Academy of Science, Lanzhou 730000, PR China

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## ABSTRACT

The ratios  $R_{k1}$  of  $k$ -fold to single ionization of the target atom with simultaneous one-electron capture by the projectile have been measured for 15–480 keV/u ( $v_p = 0.8-4.4$  a.u.) collisions of  $C^{q+}$ ,  $O^{q+}$  ( $q = 1-4$ ) with Ar, using time-of-flight techniques which allowed the simultaneous identification of the final charge state of both the low-velocity recoil ion and the high-velocity projectile for each collision event. The present ratios are similar to those for  $He^+$  and  $He^{2+}$  ion impact. The energy dependence of  $R_{k1}$  shows a maximum at a certain energy,  $E_{max}$ , which approximately conforms to the  $q^{1/2}$ -dependence scaling. For a fixed projectile state, the ratios  $R_{k1}$  also vary strongly with outgoing reaction channels. The general behavior of the measured data can be qualitatively analyzed by a simple impact-parameter, independent-electron model.

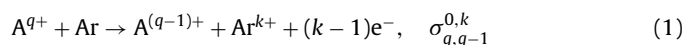
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## 1. Introduction

Ion–atom collisions with active electrons on the target have been of interest experimentally and theoretically, as they are of practical relevance in plasmas, planetary aurora and accelerator technology. The simplest system to study the multiple electron processes is the collisions of ions with a helium target, which has been extensively investigated up to now. However, the studies in low-to-intermediate collisions of ions with more than two active electrons on the target are relatively scarce. On the other hand, systematic studies of the energy dependence of cross sections for Ar targets are few and mainly limited to proton and helium ion impact [1–5]. For heavier projectiles in the intermediate-energy region, in which the multiple-ionization cross section will be up to its maximum at a certain energy, the available experimental data are much more lacking. When more electrons participate, the dynamics of multiple electron ionization and transfer is difficult from the theoretical point of view. The quantum-mechanical or even semi-classical treatment of collision systems with more than two active

electrons is generally a difficult task since a large number of reaction channels are involved. To calculate the capture probability for fast collisions, Brandt [6] firstly introduced an impact-parameter dependence into the Bohr–Lindhard model [7] to take into account the different times spent by the projectile having different impact parameters. Afterwards, the model is further developed by Ben-Iltzhak et al. [8]. At low and intermediate impact energies, the emission of the target electrons with the simultaneous electron capture by projectile is an important channel. Therefore, both ionization and capture probabilities have to be taken into account in calculations.

We previously reported the relative cross sections of multiple ionization accompanied by one-electron capture in 80–400 keV/u ( $v_p = 1.8-4$  a.u.)  $C^{q+}$ ,  $O^{q+}$  ( $q = 2, 3$ )–Ne collisions [9]. In the present work, we extend our previous method to study the production of recoil  $Ar^{k+}$  ions through one-electron capture by projectiles in  $C^{q+}$ ,  $O^{q+}$  ( $q = 1-4$ )–Ar collisions, in the energy range from 15 to 480 keV/u or  $v_p = 0.8-4.4$  a.u. The collisions associated with the cross sections studied can be described by



where  $A^{q+}$  and  $q$  are the projectile and its charge state, respectively, and  $k$  is the charge state of the recoil ion. The ratios  $R_{k1} = \sigma_{q,q-1}^{0,k} / \sigma_{q,q-1}^{0,1}$  have been determined. Comparison with the similar

\* Corresponding author. Tel.: +86 931 8913549; fax: +86 931 8913551.

\*\* Corresponding author. Tel.: +86 931 8913541.

E-mail addresses: [dingbw@lzu.edu.cn](mailto:dingbw@lzu.edu.cn), [dingbw2002@yahoo.com.cn](mailto:dingbw2002@yahoo.com.cn) (B. Ding), [chenxm@lzu.edu.cn](mailto:chenxm@lzu.edu.cn) (X. Chen).

experimental results for  $\text{He}^+$  and  $\text{He}^{2+}$ –Ar collisions by DuBois [3,4] is given. Within the independent-electron approximation (IEA), we have also carried out the calculations in terms of the work by Brandt [6] and Ben-Itzhak et al. [8]. The satisfactory agreement between calculations and experimental data is obtained. However, the calculations could not give a precise description due to the fact that it oversimplifies the processes of the electron emission and transfer. Throughout this paper, atomic units are used unless otherwise stated.

## 2. Experiment

The experiment was performed on the  $2 \times 1.7$  MV tandem accelerator at the Lanzhou University, China. A more detailed description of this experimental setup has been published elsewhere [9–11]. Negative carbon or oxygen ions extracted from a sputter ion source were accelerated, stripped in a gas stripper, and then accelerated again to the final energy. Ions with the desired energy and charge state were selected by a  $30^\circ$  analyzing magnet. Before entering the collision chamber, the beams were collimated to  $0.5 \text{ mm} \times 0.5 \text{ mm}$  by two groups of two-dimensional collimators, and then collided with an argon beam ejected from a gas jet in the collision chamber. The working pressure in the target cell was about 0.02 mTorr, whereas the background pressure in the beam line was maintained about  $1 \times 10^{-8}$  Torr in order to reduce the probability of charge transfer due to interactions between the projectiles and the residual gas atoms. After leaving the gas cell the scattered ions passed through the electrostatic deflection which acted as a charge-state separator and were finally detected with a position-sensitive microchannel plate (PS-MCP) detector. On the other hand,  $\text{Ar}^{k+}$  recoil ions with low energies, typically below 1 eV, were extracted and accelerated perpendicular to the direction of the beam in an electrostatic field (about  $50 \text{ V mm}^{-1}$ ). After have drifting in a field-free region, the recoil ions were detected by a microchannel plate recoil (R-MCP) detector ( $-2.2 \text{ kV}$ ) located at about 90 mm from the center of the target cell. The recoil-ion charge state was determined by a time-of-flight (TOF) measurement, since the recoil-ion time-of-flight from the center of the gas to the detector is proportional to the square root  $\sqrt{k}$  of its charge. The recoil-ion signal was used to start a time-to-amplitude converter (TAC), while a fast timing signal from PS-MCP was used to stop it. Fig. 1(a) shows a TOF spectrum obtained for 1.72 MeV  $\text{C}^{3+}$  colliding with the argon atom. It is seen that peaks of recoil  $\text{Ar}^{k+}$  ions ( $k=1-5$ ) are clearly identified. By means of position-sensitive detection and TOF coincident technique, the reaction channels were distinguished. The two-dimensional coincidence for 1.72 MeV  $\text{C}^{3+}$  + Ar collisions is shown in Fig. 1(b) in which the column labeled with  $\text{C}^{2+}$  denotes the results when projectiles  $\text{C}^{3+}$  capture one electron from the argon target. The relative cross sections  $R_{k1}$  was obtained by

$$R_{k1} = \frac{\varepsilon^1}{\varepsilon^k} \cdot \frac{N_{q,q-1}^{0,k}}{N_{q,q-1}^{0,1}} \quad (2)$$

where  $N_{q,q-1}^{0,1}$  and  $N_{q,q-1}^{0,k}$  are the number of detected  $\text{Ar}^+$  and  $\text{Ar}^{k+}$  events associated with one-electron capture by the projectile, respectively, and  $\varepsilon^1$  and  $\varepsilon^k$  are the detection efficiencies of  $\text{Ar}^+$  and  $\text{Ar}^{k+}$ , respectively. The main sources of uncertainties come from the efficiency of R-MCP detector (10%), multicollision (<3%), the uncertainty of determining the counting region in the two-dimensional spectrum (10%) and statistical errors which are within 10% for lower charge-state recoil ions. Full details of the error analysis have been given in our previous paper [9–11].

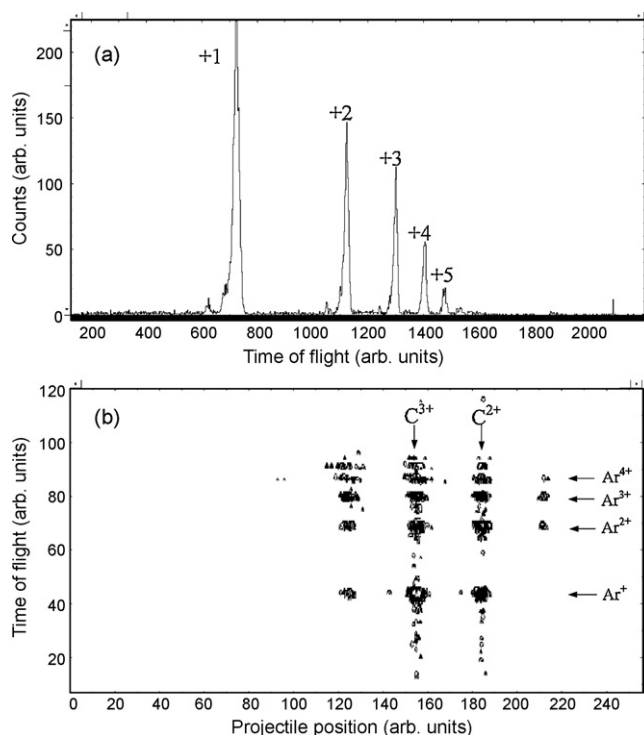


Fig. 1. (a) Time-of-flight (TOF) spectrum and (b) two-dimensional coincidence spectrum for  $\text{C}^{3+}$ –Ar collisions at 1.72 MeV.

## 3. Theory

A first classical description, which was employed to evaluate capture cross sections in ion–atom collisions, was proposed by Bohr and Lindhard [7]. Accordingly, one electron can be released from the target when the projectile is close enough that its attractive Coulomb force is equal to the binding force of this electron in the atom, i.e.,  $q/R_r^2 = v_e^2/a$ , in which  $q$  is the projectile charge state, and  $v_e$  and  $a$  are the electron velocity and its orbital radius, respectively. The release distance  $R_r$  is then given by  $R_r = (qa)^{1/2}/v_e$ . On the other hand, capture by the projectile can take place when the electron's potential energy in the projectile frame is larger than its kinetic energy. Hence, the capture distance  $R_c$  is determined by  $R_c = 2q/v_p^2$ , where  $v_p$  is the projectile velocity. For  $R_r < R_c$  the electron capture cross section is given by  $\sigma_c = \pi R_r^2$ , which means that the capture cross section is independent of the impact energy for lower energy collisions. For higher velocities,  $R_c$  is smaller than  $R_r$ , the released electron from the target can be captured or ionized. Release is a gradual process, which takes place with a probability per unit time of the order of  $v_e/a$ . The probability of electron release within a distance  $R_c$  is on the order of  $(R_c/v_p)(v_e/a)$ . In this case, the electron capture cross section is given as  $\sigma_c = 8\pi q^3(v_e/a) \cdot v_p^{-7}$ ; thus, for higher velocities, the electron capture cross section decreases rapidly with the increasing velocity as  $v_p^{-7}$  instead of the constant capture probability. Ionization occurs when the energy transferred exceeds the ionization potential. Therefore, the ionization cross section  $\sigma_i$  is obtained by the integration of the Rutherford cross section from the ionization potential  $I$  to the maximum transferable energy  $2v_p^2$ ,  $\sigma_i = 4\pi q^2 \cdot v_p^{-2} \cdot [(2I)^{-1} - (2v_p)^{-2}]$ . Following the Bohr–Lindhard model, Brandt [6] and Ben-Itzhak et al. [8] calculated the capture cross sections in fast collisions using the impact-parameter dependence by taking into account the different times spent by projectiles with different impact parameters. Differing from their studies, we attempt to make calculations involving capture as well as ionization cross sections for Ar atom by low-to-intermediate ions.

Let a target atom in the ground state rests at the origin and a projectile, which is considered as a structureless ion with charge state  $q$ , impact parameter  $\mathbf{b}$  and velocity  $\mathbf{v}_p$ , moves along a classical straightforward trajectory  $\mathbf{S} = \mathbf{b} + \mathbf{v}_p t$ . In terms of Bohr–Lindhard model, the release and capture conditions become, respectively

$$\frac{q}{|\mathbf{S} - \mathbf{r}|^2} = \frac{v_e^2}{|\mathbf{r}|^2} \quad (3)$$

and

$$\frac{q}{|\mathbf{S} - \mathbf{r}|} = \frac{1}{2} v_p^2 \quad (4)$$

where  $\mathbf{r}$  is the location of the electron with respect to the target nucleus.

If  $\rho$  is the impact parameter of the projectile with respect to the target electron, the release of a target electron becomes possible when  $\rho < R_r$ . In this case, one-electron release probability  $f_r(\rho, q, v_p, r)$  is expressed by

$$f_r(\rho, q, v_p, r) = \frac{2\sqrt{R_r^2 - \rho^2}}{v_p} \cdot \frac{1}{\tau} \quad (5)$$

with  $1/\tau$  being the release rate. One released electron may be captured if it is in the capture sphere. The capture probability is given as

$$f_c(\rho, q, v_p, r) = \frac{2\sqrt{R^2 - \rho^2}}{v_p} \cdot \frac{1}{\tau} \quad (6)$$

where  $R$  satisfies that  $R = R_r$  when  $R_c > R_r$  and otherwise  $R = R_c$ . The ionization probability  $f_i(\rho, q, v_p, r)$  is given by

$$f_i(\rho, q, v_p, r) = f_r(\rho, q, v_p, r) - f_c(\rho, q, v_p, r) \quad (7)$$

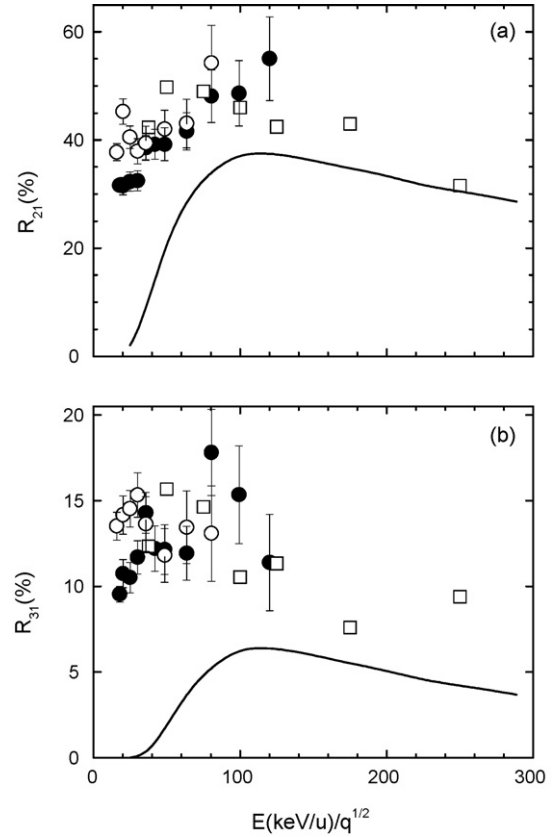
The probability that the electron is in  $d^3\mathbf{r}$  at  $\mathbf{r}$  is  $|\psi(\mathbf{r})|^2 d^3\mathbf{r}$ . Thus the release, capture and ionization probabilities are expressed as

$$P_{r,i,c}(b, q, v_p) = \int f_{r,i,c}(\rho, q, v_p, r) |\psi(\mathbf{r})|^2 d^3\mathbf{r} \quad (8)$$

#### 4. Results, discussion and conclusions

In Figs. 2–5, the experimental ratios  $R_{k1}$  are shown as a function of  $E/q^{1/2}$  ( $E$  is the projectile energy in keV/u). The present results are consistent with those for  $\text{He}^+$ ,  $\text{He}^{2+}$ –Ar collisions by DuBois [3,4]. The general shapes of the experimental curves are independent of outgoing channels. And when  $q$  is not changed,  $R_{k1}$  strongly depends on the projectile energy. In our previous studies [9] for Ne targets, the maximum of  $R_{k1}$  distribution has been found to be located at  $E_{\max} \approx 160q^{1/2}$  keV/u. Similarly, the present data for Ar targets also show that  $E_{\max}$  is approximately in proportion to  $q^{1/2}$ , but, due to lower binding of outer electrons,  $E_{\max}$  is around  $130q^{1/2}$  keV/u smaller than that of Ne targets. Because of the limited energy range, the  $E_{\max}$  value for  $q=4$  is not very evident.  $R_{k1}$  is also dependent on projectile charge state,  $q$ . The maximum value of  $R_{k1}$  increases with the increasing projectile charge state, which indicates that the multiple ionization becomes more important channel associated with one-electron transfer relative to purely single-electron capture by the projectile due to the stronger potential for higher  $q$ . For instance, the maximum value for  $q=2$  is around unity and for  $q=3$  or 4, they both are larger than unity.

Since the average binding energy of Ar M-shell electrons is more than one order of magnitude lower than that of Ar L-shell electrons, M-shell ionization of the target would play a main part compared with L-shell ionization. Therefore, for simplicity, we assume that only the M-shell electrons are active. Suppose the M-shell electron density of the target atom is an exponentially decaying function of



**Fig. 2.** Ratios  $R_{k1}$  of  $k$ -fold to single ionization accompanied by single capture of Ar by projectiles with charge state  $q = 1$  against the projectile energy  $E$  (keV/u). Experiment: full circles,  $\text{C}^+$ ; open circles,  $\text{O}^+$ ; open squares,  $\text{He}^+$ , Ref. [3]. Calculation: solid line.

the distance:

$$|\psi(\mathbf{r})|^2 = A e^{-2\sqrt{2I}r} \quad (9)$$

where  $I$  is the binding energy of M-shell, and the parameter  $A$  is determined by the normalization condition of the density

$$\int_0^\infty |\psi(r)|^2 \cdot 4\pi r^2 dr = 1 \quad (10)$$

The capture and ionization probabilities can be obtained by the integral in Eq. (8), which can be done in cylinder coordinate

$$P_{r,i,c}(b, q, v_p) = \int_0^{R_r} \rho d\rho \int_0^{2\pi} d\varphi \int_{-\infty}^{+\infty} f_{r,i,c}(\rho, q, v_p, r(b, \rho, \varphi, z)) \cdot A e^{-2\sqrt{2I}r(b, \rho, \varphi, z)} dz \quad (11)$$

Since the probabilities  $P_{r,i,c}(b, v_p, r)$  may be larger than unity, the unitarized probabilities [12] can be written as

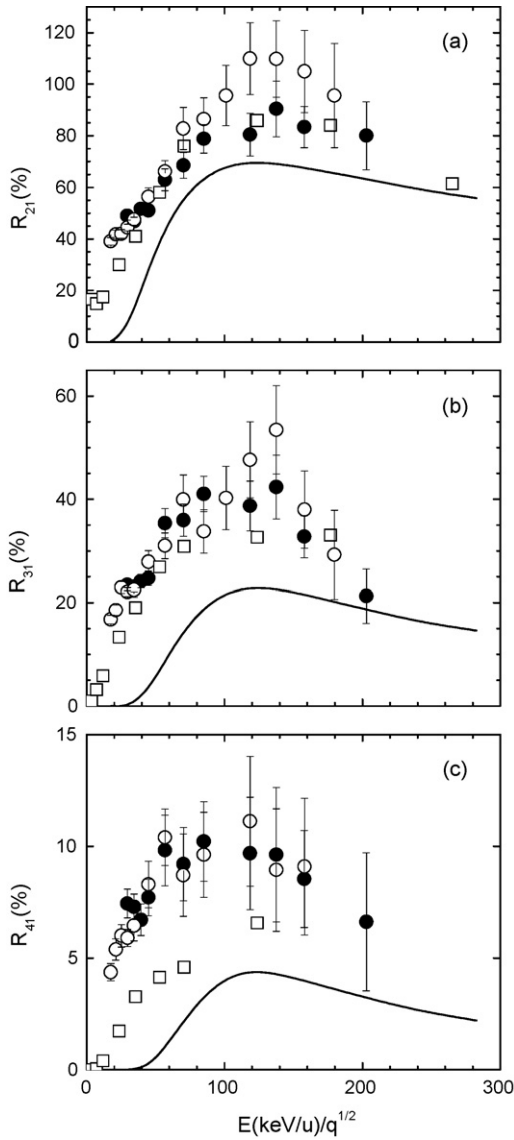
$$P_{ur}(b, q, v_p) = 1 - \exp[-P_r(b, q, v_p)] \quad (12)$$

$$P_{uc}(b, q, v_p) = \frac{P_c(b, q, v_p)}{P_r(b, q, v_p)} \cdot P_{ur}(b, q, v_p) \quad (13)$$

$$P_{ui}(b, q, v_p) = P_{ur}(b, q, v_p) - P_{uc}(b, q, v_p) \quad (14)$$

where the subscript ‘u’ denotes the corresponding unitarized probability.

Within the IEA, the probability of  $k$ -fold ionization accompanied by one-electron capture to a projectile can be calculated by the following equation [13]:



**Fig. 3.** Ratios  $R_{k1}$  of  $k$ -fold to single ionization accompanied by single capture of Ar by projectiles with charge state  $q=2$  against the projectile energy  $E$  (keV/u). Experiment: full circles,  $C^{2+}$ ; open circles,  $O^{2+}$ ; open squares,  $He^{2+}$ , Ref. [4]. Calculation: solid line.

$$P_{q,q-1}^{0,k}(b, q, v_p) = \begin{bmatrix} 8 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ k-1 \end{bmatrix} \cdot P_{uc}(b, q, v_p) \cdot P_{ui}(b, q, v_p)^{k-1} \cdot [1 - P_{uc}(b, q, v_p) - P_{ui}(b, q, v_p)]^{8-k} \quad (15)$$

Then ionization and capture cross sections are obtained by integrating the corresponding probabilities over the impact parameter:

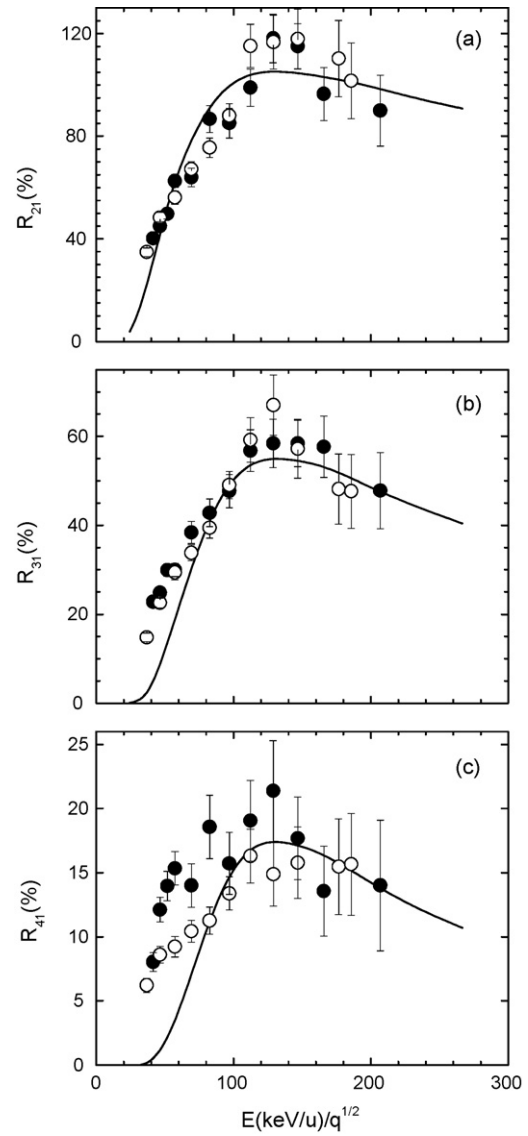
$$\sigma_{q,q-1}^{0,k}(q, v_p) = 2\pi \int_0^\infty P_{q,q-1}^{0,k}(b, q, v_p) b \, db \quad (16)$$

The ratio  $R_{k1}$  is then calculated from

$$R_{k1} = \frac{\sigma_{q,q-1}^{0,k}}{\sigma_{q,q-1}^{0,1}} \quad (17)$$

In the present calculations, the release rate  $1/\tau(r)$  is chosen through  $E(r) \cdot \tau(r) \sim 1$  ( $E(r)$  is the local electron energy). As a result, a simple release rate of the form is given as

$$\frac{1}{\tau(r)} \sim E(r) = \frac{Z_{\text{eff}}}{2r} \quad (18)$$



**Fig. 4.** Ratios  $R_{k1}$  of  $k$ -fold to single ionization accompanied by single capture of Ar by projectiles with charge state  $q=3$  against the projectile energy  $E$  (keV/u). Experiment: full circles,  $C^{3+}$ ; open circles,  $O^{3+}$ . Calculation: solid line.

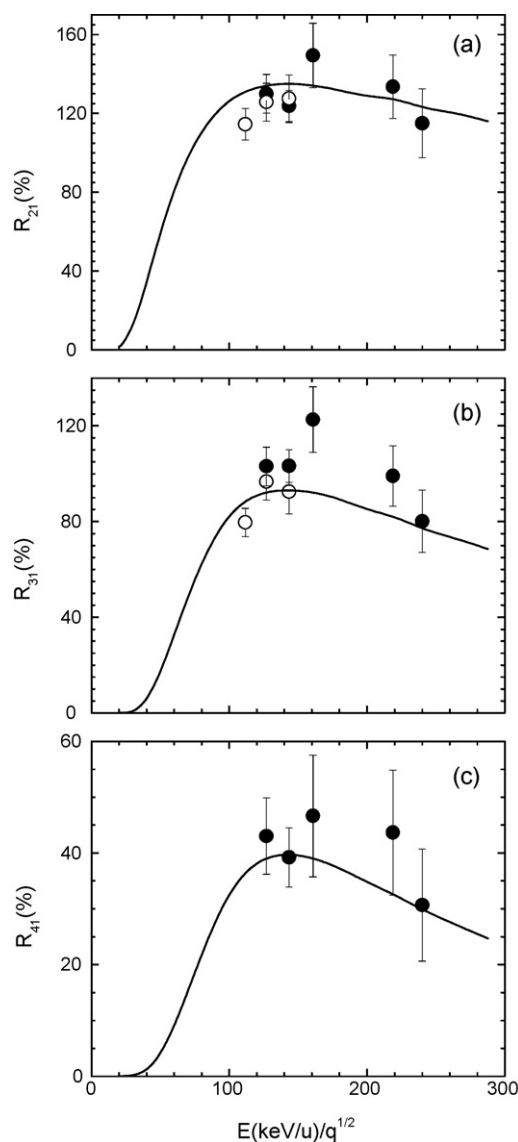
where  $Z_{\text{eff}}$  is the effective charge of the target nuclear. Calculations are also shown in Figs. 2–5 where they are compared with the experimental data. In general, the calculations described in this paper give correct qualitative behavior of the relative cross sections as functions of projectile energy and charge state, which satisfies with our original intention. It is well known that the single capture cross section,  $\sigma_{q,q-1}^{0,1}$ , monotonously decreases with increasing energy at intermediate velocities, while the cross section of  $k$ -fold ionization accompanied by one-electron capture,  $\sigma_{q,q-1}^{0,k}$ , has a maximum at certain energy  $E_{\text{max}}$ . As an approximation,  $\sigma_{q,q-1}^{0,k}$  will reach a maximum when  $P_i = P_c$ , i.e.,

$$f_r = 2f_c \quad (19)$$

For simplicity, when  $\rho = 0$ , according to Eqs. (5), (6) and (19) we have the simple formula

$$E_{\text{max}} = \frac{1}{2} v_p^2 = 2v_e r^{-1/2} q^{1/2} \quad (20)$$

which is helpful to understand the  $q^{1/2}$ -dependence scaling of  $E_{\text{max}}$  to a certain extent.



**Fig. 5.** Ratios  $R_{k1}$  of  $k$ -fold to single ionization accompanied by single capture of Ar by projectiles with charge state  $q=4$  against the projectile energy  $E$  (keV/u). Experiment: full circles,  $C^{4+}$ ; open circles,  $O^{4+}$ . Calculation: solid line.

In conclusions, we have measured the ratios  $R_{k1}$  of  $k$ -fold to single ionization of the target atom with simultaneous one-electron capture of the projectile for 15–480 keV/u ( $v_p = 0.8$ –4.4 a.u.) collisions of  $C^{q+}$ ,  $O^{q+}$  ( $q = 1$ –4) with Ar. The present results are similar with our previous investigations for the Ne target and in good agreement with those by DuBois for  $He^{1,2+}$ –Ar collisions. The ratios depend upon both the projectile energy and charge state. The corresponding projectile energy of the maximum ratio,  $E_{max}$ , is found about  $130q^{1/2}$  keV/u. The general behavior can be qualitatively analyzed by a simple impact-parameter, independent-electron model.

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