SCALING OF CROSS SECTIONS FOR MULTIPLE ELECTRON TRANSFER TO HIGHLY CHARGED IONS COLLIDING WITH ATOMS AND MOLECULES *

Alfred MÜLLER and Erhard SALZBORN
Institut für Kernphysik, Justus-Leibig-Universität Giessen, 6300 Giessen, W. Germany

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For collision energies below 25 keV/amu cross sections for the transfer of up to 4 electrons in single collisions between multiply charged ions and neutral atoms and molecules are approximated by empirical scaling laws. Within a ±35% margin of error two third of altogether 268 measured cross sections coincide with the predicted values.

Aside from purely intrinsic interest, the importance of charge transfer collisions between multiply charged ions and atoms for several fields of application has been increasingly recognized [1, 2]. Especially from controlled nuclear fusion research urgent data needs aroused in connection with radiative energy loss, neutral beam injection as well as plasma properties and their diagnostics [3]. Even more recently, the conception of heavy ion induced fusion has stressed again the need of cross sections for charge transfer collisions [4].

During the last years research activities, both experimental and theoretical, were started towards studying charge changing collisions of multiply charged ions in the impact energy range below 25 keV/amu [5–7]. Up to now, however, one is still far from a detailed physical understanding of single electron capture not to speak at all of multiple electron transfer. In order to go round the complex theoretical difficulties it seemed to be useful therefore to look for empirical scaling laws describing measured cross sections for the capture of electrons in ion-atom collisions.

For this purpose we have systematically investigated the dependence of charge transfer cross sections, $\sigma_{i,i-k}$ on the initial charge state i of the projectiles, the number k of electrons transferred and the projectile energy. The projectiles used were rare gas ions Ne^{i+}, Ar^{i+}, Kr^{i+} and Xe^{i+} in charge states i between 2 and 8; the targets were the rare gases He, Ne, Ar, Kr, Xe and the molecular gases H_2, N_2, O_2, CH_4, CO_2. The number k of transferred electrons ranged from $k = 1$ up to $k = 4$. The laboratory impact energy varied from few keV to about 100 keV. The absolute experimental errors of the cross sections are estimated to be within ±30%.

Although not every possible projectile-target collision system has been investigated the following considerations are based on altogether 268 different cross section functions.

According to the theories of Olson and Salop [8] and of Presnyakov and Ulantsev [9] the one-electron capture cross sections $\sigma_{i,i-1}$ should not significantly depend on the impact energy in the range below 25 keV/amu. This has been approved in many experiments not only for single electron but also for multiple electron capture [10–15]. Furthermore, for $i \gtrsim 4$ the electron capture cross sections are nearly independent of the projectile ion species and should only depend on the initial charge state i [8, 9; 5, 11, 15].

With these basic features of the cross sections $\sigma_{i,i-\mathrm{k}}$ in mind, a scaling law for the energy range below 25 keV/amu should be a function only of the initial charge state i, the number of captured electrons k, and properties of the target particle. For initial projectile charges $i \gtrsim 10$ Presnyakov and coworkers [9, 16, 17] have given a very simple theoretical approximation for the one-electron capture cross sections $\sigma_{i,i-1}$:

$$\sigma_{i,i-1} = \pi a_0^2 \cdot i^2 \cdot (E_{\mathrm{Ry}}/I)^2 \qquad (1)$$

where $a_0 = 0.53$ Å is the Bohr radius, $E_{\mathrm{Ry}} = 13.6$ eV is the Rydberg energy, and I denotes the ionization potential of the target particle. Formula (1) which needs a minimum of information about the specific charge transfer process shows surprisingly good agreement with out experimental data and thus we were encouraged to fit all measured cross sections with a slightly modified but still most easy fit function

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Table 1
Least square adjusted fit parameters (together with their asymptotic standard deviations) for the cross section scaling laws

$\sigma_{i,i-k} = A_k \cdot i^{\alpha_k} \cdot (I_{[\mathrm{eV}]})^{\beta_k}\ \mathrm{cm}^2$; $k = 1, 2, 3, 4$

k	number n of cases	A_k	α_k	β_k
1	107	$(1.43 \pm 0.76) \times 10^{-12}$	1.17 ± 0.09	-2.76 ± 0.19
2	77	$(1.08 \pm 0.95) \times 10^{-12}$	0.71 ± 0.14	-2.80 ± 0.32
3	50	$(5.50 \pm 5.8) \times 10^{-14}$	2.10 ± 0.24	-2.89 ± 0.39
4	34	$(3.57 \pm 8.9) \times 10^{-16}$	4.20 ± 0.79	-3.03 ± 0.86

$$\sigma_{i,i-k} = A_k \cdot i^{\alpha_k} \cdot I^{\beta_k} \quad k = 1, ..., 4 \tag{2}$$

with A_k, α_k and β_k being free parameters.

In the beginning of the data analysis in eq. (2) the first ionization potential I of the target particle had been replaced by $I_{0,k}$, the energy needed to release k electrons from the target. This change however did not improve the fit results and therefore the quantity I which is well known for all target atoms and molecules was given preference to $I_{0,k}$.

The results of the regression analysis are given in table 1 showing the fit parameters A_k, α_k and β_k together with their asymptotic standard deviations. For an example of the fit quality figs. 1 and 2 compare cross sections computed from the scaling law (2) using the parameters from table 1 and measured cross sections for 30 keV Ar^{i+} ions incident on Xe and 30 keV Xe^{i+} ions incident on Kr, respectively. The agreement between experiment and empitical scaling law can be seen to be fairly good.

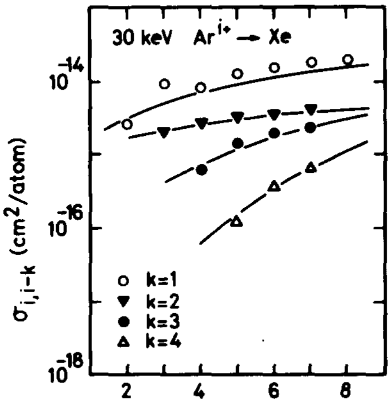

Fig. 1. Electron capture cross sections for 30 keV Ar^{i+} ions incident on Xe. The solid lines are computed with eq. (2) using the parameters of table 1 together with the ionization potential $I_{\mathrm{Xe}} = 12.13$ eV.

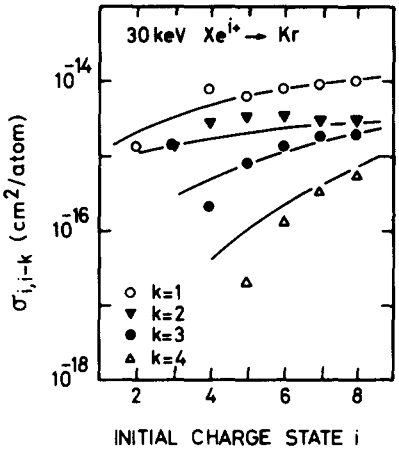

Fig. 2. Electron capture cross sections for 30 keV Xe^{i+} ions incident on Kr. The solid lines are computed with eq. (2) using the parameters of table 1 together with the ionization potential $I_{\mathrm{Kr}} = 14.0$ eV.

In order to get a more objective judgement of the applicability of formula (2) ratios

$$Q_k^{(\nu)} = \sigma^{\mathrm{exp}}_{i,i-k} / \sigma^{\mathrm{fit}}_{i,i-k}$$

of the experimental cross sections and the according scaling law values have been calculated. The index ν numbers the individual ratios. The frequency distribution of the values $Q_k^{(\nu)}$ in intervals $(x - 0.05, x + 0.05)$ with the middles $x = 0.0, 0.1, 0.2, ..., 2.1$ is shown in fig. 3. Obviously the values $Q_k^{(\nu)}$ are distributed with a single maximum around the ideal value $Q = 1.0$ where experiment and fit formula coincide.

The standard deviation s of the total frequency distribution (altogether $n = 268$ cases) is given by $s = 0.43$. The standard deviations s_k of those ratios $Q_k^{(\nu)}$ where the number of transferred electrons is fixed and

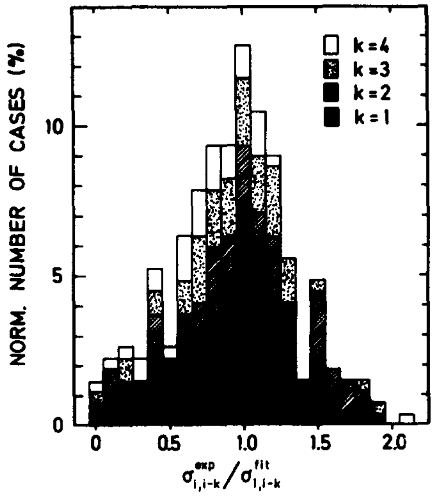

Fig. 3. Frequency distribution of ratios $\sigma_{i,i-k}^{\exp}/\sigma_{i,i-k}^{\mathrm{fit}}$ in intervals $(x - 0.05, x + 0.05)$ around $x = 0.0, 0.1, 0.2, \ldots 2.1$. The number of electrons transferred in a single ion-atom collision is denoted by k. The total number of cases is $n = 268$.

equals k are given by:

$$s_1 = 0.38\ (n = 107); \quad s_2 = 0.43\ (n = 77)$$

$$s_3 = 0.38\ (n = 50); \quad s_4 = 0.61\ (n = 34)$$

This implies that for each k about 2/3 of all experimental cross sections lie within a ±35% margin of error around the value predicted by the scaling law (2).

In the interval around $x = 0.0$ there are 4 cases of $Q_k^{(\nu)}$. All these belong to cross sections for endothermal charge exchange reactions. For such processes it is known that electron capture is much less likely than in exothermal reactions. Therefore formula (2) cannot be applied, in general, to endothermal electron transfer.

For exothermal electron capture ($n = 264$) the largest observed deviation between experiment and the scaling formula (2) is less than a factor of 10. Obviously, the simple approach presented here gives reasonable results for the most general trends of the exothermal capture cross sections. This holds in particular for many-electron collision systems where a vast variety of possible excited final states of projectile and target are involved in the charge transfer process. For initial charge states $i < 4$, however, discrepancies of the cross sections from the "normal" behaviour are found. A detailed paper on this problem is in preparation.

For practical use it is of great interest to know whether and how far formula (2) can be applied to initial charge states $i > 8$.

In the case $k = 1$ (one-electron capture) an extrapolation may be justified by the obtained rather close agreement between the extracted fit parameters $\alpha_1 = 1.17 \pm 0.09$, $\beta_1 = -(2.76 \pm 0.19)$ and the corresponding dependences obtained in theoretical approaches to the problem. While eq. (1) gives a i^2-dependence of $\sigma_{i,i-1}$, the theory of Olson and Salop [8] predicts a nearly linear dependence of $\sigma_{i,\mathrm{tot}} = \Sigma_k\, \sigma_{i,i-k}$ on i. The latter is in good agreement with α_1 as long as $\sigma_{i,i-1}$ represents the largest term in the sum. The I-dependence obtained empirically with β_1 is somewhat stronger than that in the theories of Olson and Salop ($\sigma_{i,\mathrm{tot}} \sim I^{-1}$) and of Presnyakov and Ulantsev ($\sigma_{i,i-1} \sim I^{-2}$).

In the cases with $k > 1$ (multiple electron capture) the question of extrapolation of eq. (2) is much more open since there is no general theoretical approach at all. In particular it would be interesting having $k = 2$ and $k = 3$ cross section data for initial charge states beyond the region presented here to see whether the curve crossing between $\sigma_{i,i-2}$ and $\sigma_{i,i-3}$ which is to be expected from figs. 1 and 2 for some higher value of i really comes true. It is known [18] that in few specific cases the capture of $k + 1$ electrons is at least as likely as the capture of k electrons (see also $\sigma_{3,2}$ and $\sigma_{3,1}$ in fig. 2), however, the general crossing of $\sigma_{i,i-2}$ and $\sigma_{i,i-3}$ inferred from eq. (2) for $i \simeq 9$ would be a novel feature of multiple electron capture cross sections.

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