Yields of multiply charged ions in cascading decays of hollow argon and krypton with two initial vacancies in their K and/or L shells

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The yields of multiply charged ions produced by the cascading decay of doubly-inner-shell-ionized argon and krypton atoms are calculated *via* straightforward construction of de-excitation trees. The final-ion-charge spectra are found to be sensitive to the distribution of initial vacancies within K and L shells.

Keywords: vacancy cascade, de-excitation tree, ion yields, final-ion-charge spectra.

1. Introduction

Creation of a single inner shell vacancy in an atom produces a short-lived state liable to decay. A cascade of successive radiationless transitions (a vacancy cascade) produces multiply charged ions. The single-initial-vacancy cascade-produced final-ion-charge spectra have been being studied since sixties (Carlson and Krause, 1965) both theoretically and experimentally (see Kochur *et al.*, 1995 and references therein).

If a greater number of initial inner-shell vacancies is created then the decay cascades become much more complex, and much higher stages of ionization can be reached. Such hollow states are exotic ones, and the studies on their decays are scarce (Omar & Hahn, 1991). However, with coming fourth generation light sources the flux densities can be reached that could produce multiply inner-shell-ionized atoms with reasonable probabilities. Even with present day facilities the hollow states of heavy atoms can be obtained, for example, Kanter *et al*. (1999) reported on the observation of the molybdenum K^{-2} states produced by photoionization.

In this work we calculate the cascade-produced ion yield spectra of argon and krypton with two vacancies in their K- and/or L-shells

2. Method of calculation

The method of calculation we use in this work is described in detail elsewhere (Kochur *et al*., 1994, 1995), therefore, only its brief description is given in this section.

Branching ratios for each branching point (*i.e.* initial or intermediate configuration) of the de-excitation tree are calculated using radiative and non-radiative partial widths obtained in one-electron Hartree-Fock approximation. All energetically allowed radiative and non-radiative decay pathways are considered for every configuration of a cascade.

The processes of additional monopole ejection of electrons due to sudden change of the core potential during diagram transitions are included. Their probabilities are calculated in sudden limit. As discussed earlier by Kochur *et a.l.* (1995), this approximation, however simple, is good enough since most important shakes are due to high-energy transitions at first de-excitation steps.

For the low-energy transitions between the levels of the configurations whose multiplets overlap, the branching ratios were corrected to be proportional to the number of states for which the transitions are not forbidden by the energy conservation law. The energy spectra of initial and final states were simulated by Gaussian distributions centred on the configuration-average energies of respective configurations.

3. Results and discussion

Calculated probabilities for production of final multiply charged Ar^{q+} and Kr^{q+} ions via cascading decay of various inner-shell-ionized initial states are listed in Tables 1,2. Some of respective final-ion-charge spectra are shown in Figures 1,2.

Consider the argon final-ion charge spectra first. It is evident from Table 1 that the argon L^{-2} spectra are very simple: each of them gives almost pure final ion charge state. This is easily understandable. Consider the L_{23}^{-2} spectrum. Each of the two initial L_{23} vacancies decays via the $L_{23}MM$ Auger transitions, therefore, two Auger electrons are emitted and, with initial ionization of 2+, we reach the 4+ final states. If the L_1 vacancies are present in the initial state then we have a two-step decay: each L_1 vacancy decays via $L_1L_{23}M$ Coster-Kronig transition, then L_{23} vacancies decay via $L_{23}MM$. Thus we have the 5+ and 6+ dominant final states upon the decay of $L_1^{-1}L_{23}^{-1}$ and L_1^{-2} initial states.

The final-ion-charge spectra of argon produced by the decay of the states with at least one K vacancy are considerably more complex. They are shown in Figure 1. Calculated K^{-1} decay charge spectrum is compared with the ion yields measured by Hayaishi *et al.* (1995) upon photoionization right above the ArK threshold. Good agreement with the experiment shows that the theoretical model employed is adequate. Unfortunately, no experimental data on doubly ionized states are available. All the final-ion-charge spectra in Figure 1 have, roughly, similar double peak structures reflecting the concurrence of radiative and non-radiative decay branches for the decay of the K vacancy (Kochur *et al*, 1995). The argon final-ion-charge spectra for the initial states $K^{-1}L_{23}^{-1}$, $K^{-1}L_1^{-1}$, K^{-2} shift towards greater final charges as the additional initial vacancy becomes deeper. One is still able to predict roughly the dominant final charge state by counting possible non-radiative transitions. This is possible since, in the first place, in argon non-radiative decay pathways are dominant even for the K vacancies, then, for each branching point among several possible decay pathways only one normally dominates. For example, if we have the K^{-2} initial state, then each K vacancy will decay (most probably) into L_{23}^{-2}, after which two $L_{23}MM$ decays are possible. It follows then that we shall have the most probable final ion charge of 2(initial ionization) +2×3(number of Auger decays) = 8, which indeed is the case, see Figure 1.

No simple considerations like those above stand in the case of krypton charge spectra (see Table 2, Figure 2). The cascades in the case of krypton are much more complex, and it is unthinkable to analyse them qualitatively. For example, the number of considered branches in the case of the decay of the krypton K^{-2} initial state is about three million.

The charge spectra of the L^{-2} cascades in krypton are shown in the upper panel of Figure 1. They cover the ion charge region of +7 to +10. The spectra fit very nicely the Gaussian distributions (solid curves in upper panel of Figure 1). Positions of distributions maximums coincide with respective calculated mean final charges with the absolute accuracy of about 0.05 The L^{-2} final charge distributions shift towards higher charges almost linearly as the number of L_1 vacancies increases from 0 to 2. These shifts are less than those seen in the L^{-2} spectra of argon, namely, about 0.42.

Table 1
Probabilities for production of final Ar^{q+} ions upon decay of doubly ionized Ar^{2+} states

q	Initial state K^{-1}	L_{23}^{-2}	$L_1^{-1}L_{23}^{-1}$	L_1^{-2}	$K^{-1}L_{23}^{-1}$	$K^{-1}L_1^{-1}$	K^{-2}
1	0.007						
2	0.126						0.000
3	0.086	0.000	0.000	0.000	0.008	0.000	0.002
4	0.430	0.995	0.034	0.000	0.135	0.013	0.021
5	0.248	0.005	0.942	0.066	0.088	0.132	0.031
6	0.092	0.000	0.024	0.916	0.387	0.104	0.126
7	0.011		0.000	0.018	0.282	0.418	0.164
8	0.001			0.000	0.099	0.330	0.571
9	0.000				0.001	0.003	0.085
10					0.000	0.000	0.001
11							0.000
Mean q	4.107	4.005	4.990	5.953	6.099	6.929	7.483

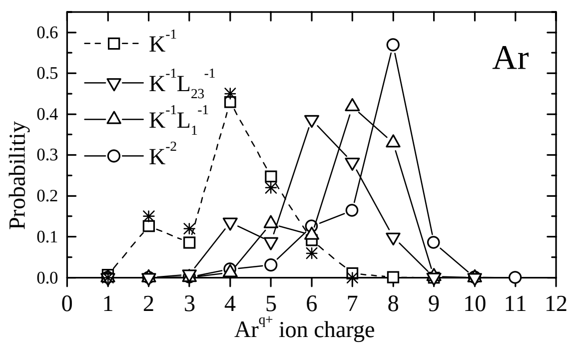

Figure 1
Final-ion-charge spectra produced by the decay of various Ar^{2+} states. Theory – symbols connected with straight lines; experiment for the K^{-1} decay (Hayaishi *et al.*,1995) - stars

The final-ion-charge spectra of krypton for initial states with K vacancies are presented in the lower panel of Figure 2. In contrast to the argon case, no regular pattern is seen here. The K^{-1}, $K^{-1}L^{-1}$ and K^{-2} final charge distributions differ from each other significantly. No regular overall shift upon deepening of initial vacancies is present. On the contrary, upon going from $K^{-1}L_1^{-1}$ to K^{-2} the mean final ion charge even decreases from 9.264 to 9.185 (see last line of Table 2).

Table 2
Probabilities for production of final Kr^{q+} ions upon decay of doubly ionized Kr^{2+} states

q	Initial state K^{-1}	L_{23}^{-2}	$L_1^{-1}L_{23}^{-1}$	L_1^{-2}	$K^{-1}L_{23}^{-1}$	$K^{-1}L_1^{-1}$	K^{-2}
1	0.006						
2	0.017						
3	0.086	0.000	0.000		0.000		0.000
4	0.237	0.001	0.000	0.000	0.001		0.001
5	0.172	0.001	0.001	0.000	0.006	0.001	0.006
6	0.117	0.021	0.005	0.001	0.018	0.004	0.019
7	0.088	0.110	0.052	0.020	0.115	0.0401	0.096
8	0.136	0.509	0.340	0.193	0.344	0.220	0.236
9	0.108	0.331	0.482	0.490	0.258	0.357	0.218
10	0.024	0.027	0.117	0.282	0.160	0.216	0.223
11	0.000	0.000	0.002	0.013	0.085	0.119	0.136
12			0.000	0.000	0.013	0.040	0.050
13					0.000	0.002	0.014
14						0.000	0.000
Mean q	5.779	8.227	8.658	9.069	8.715	9.264	9.185

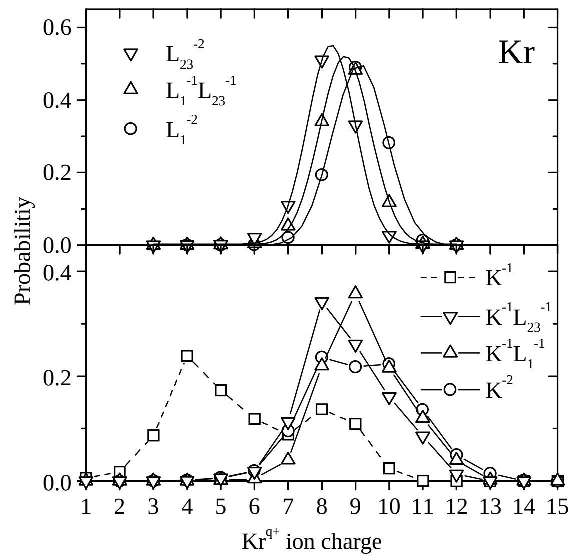

Figure 2
Final-ion-charge spectra produced by the decay of various Kr^{2+} states. Symbols connected with straight lines – calculated probabilities; solid curves in upper panel – Gaussian fits of calculated spectra.

Such a behaviour can be explained by the fact that in krypton the most probable decay channel for the K vacancy is radiative KL_{23} transition. Thus if the K vacancy is present in initial state, it just jumps to the L_{23} subshell. One then expects that there should be similarities in, say, $K^{-1}L_{23}^{-1}$ and L_{23}^{-2} final ion charge spectra. This is indeed so (see Figure 2). Similarity between K^{-1} and L_{23}^{-1} single-initial vacancy cascade-produced electron spectra caused by the same reason has been discussed earlier (Kochur & Sukhorukov, 1995).

4. Conclusions

The yields of multiply charged ions produced by the cascading decay of hollow initial ions with several vacancies in inner shells represent charge spectra which are sensitive both to the number of initial vacancies and to their distribution within electron shells. One may try to use the final-ion-charge spectra to identify and separate such states and to study the dynamics of their decay.

References

Carlson T.A. and Krause M.O. (1965). *Phys. Rev.* **137**, A1655- A1662.

Hayaishi T., Murakami E., Shigemasa E., Yagishita A., Koike F and Mirioka Y. (1995). *J.Phys.B At.Mol.Opt.Phys.*, **28**, 5261-5267.

Kanter E.P., Dunford R.W., Krässig B. and Southworth S.H. (1999). *Phys. Rev. Lett.* **83**(3) 508-511.

Kochur A.G., Dudenko A.I., Sukhorukov V.L. and Petrov I.D. (1994). *J.Phys.B At.Mol.Opt.Phys.*, **27**, 1709-1721.

Kochur A.G., Sukhorukov V.L., Dudenko A.I. and Demekhin Ph.V. (1995). *J. Phys. B: At. Mol. Opt. Phys.* **28**, 387-402.

Kochur A.G. and Sukhorukov V.L. (1995). *J. Electron Spectrosc. Relat. Phenom.* **76**, 325-328.

Omar G. and Hahn Y. (1991). *Phys. Rev. B.* **43**(1), 4695-4701.

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