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Letter to the Editor

Shake-up processes following K-shell photoionization in the Boron isoelectronic sequence

S. Stoica*, **D. Petrini, and F. Bely-Dubau**

Observatoire de la Côte d'Azur, Department G. D. Cassini, BP 4229, F-06304 Nice Cedex 4, France (e-mail: petrini@obs-nice.fr)

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Abstract. The direct and conjugate shake-up cross sections for the 2p → 3p, 3s and 2s → 2p, 3s transitions are calculated for CII, NIII, OIV, FV and NeVI in a close-coupling approximation using the R-matrix method. We find that the total shake-up cross section relative to that for single photoionization decreases with increasing Z. The decrease is about a factor 10 when going from BI to NeVI. When the full shake-up regime is reached, i.e. for about twice the 1s threshold energy, the cross section ratio ranges from about 15% for CII to about 3.5% for NeVI, of the single 1s inner-shell photoionization cross section. The 2s → 3s transition gives the dominant contribution for all ions. The 2p → 3p and 2s → 2p excitation contributions are broadly comparable in this energy range, while the 2p → 3s transition is negligible. Our results suggest that the importance of shake off excitation is significant for low Z ions.

Key words: atomic physics: K–photoionization: shake-up process

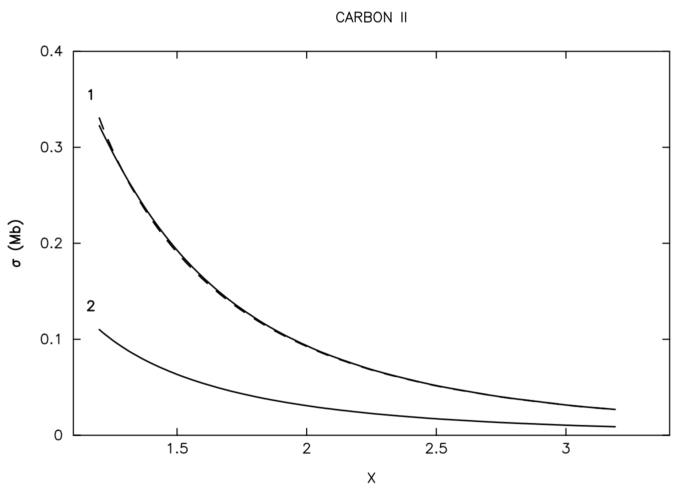

Fig. 1. Single inner-shell photoionization cross sections (in Mb) versus $X = E_{h\nu}/E_{1s}$ for CII. $E_{h\nu}$ and E_{1s} represent the photon and 1s ionization energies, respectively. With full lines are drawn ($^3P^o$) (1) and ($^1P^o$) (2) symmetries. With dashed line is drawn the ($^1P^o$) symmetry multiplied by a spin statistical weight of 3

1. Introduction

Once 1s-hole ions are created by single photoionization, with simultaneous shake-up and shake-off processes, Auger decay populates directly *excited* states of the residual ions. These produce UV lines (Petrini and Da Silva 1996 and Petrini and Araújo 1997). Knowledge of the importance of the secondary processes which accompany single inner-shell photoionization is an useful information for a detailed analysis of both laboratory and astrophysical plasmas. The growing availability of synchrotron-radiation sources and the discovery of soft X-ray sources in the Universe have stimulated the interest in a quantitative understanding of these processes. However, despite their importance (Åberg 1969), results are at present rather scarce. For instance, in the case of Ne, Krause and his collaborators found in the early seventies (Krause 1971, Krause et al. 1971, Carlson et al. 1971) that the direct shake-up and the KL shake-off processes represented about 8% and 13.8% of the total 1s photoionization processes, respectively. The shake-up processes in this case are dominated by 2p → 3p excitation, the 2p → 3s and the 2s → 3s ones being weak. For Be, Krause and Caldwell (1987a,b) reported cross sections above the K-edge where the 2s → 3s and the 2s → 2p transitions represent about 19% and 10.5% of the total 1s photoionization cross section respectively.

Recently, Badnell et al. (1997) performed for boron a complex calculation of the direct and conjugate shake-up cross sections for transitions 2p → 3p, 3s and 2s → 2p, 3s, in the photon energy interval 17-45 Ry, in a close-coupling approximation using the R-matrix method and found that the total cross section for these secondary processes represents about 30% of the single 1s photoionization cross section. Furthermore, they highlighted the importance of the 2s → 3s shake-up excitation which dominates 2p → 3p and found a conjugate shake-up 2s → 2p transition broadly comparable with the 2p → 3p one.

Send offprint requests to: S. Stoica
* *Permanent address*: Department of Theoretical Physics, Institute of Physics and Nuclear Engineering, P.O. Box MG-6, 76 900-Bucharest, Romania (e-mail: stoica@theor1.ifa.ro)

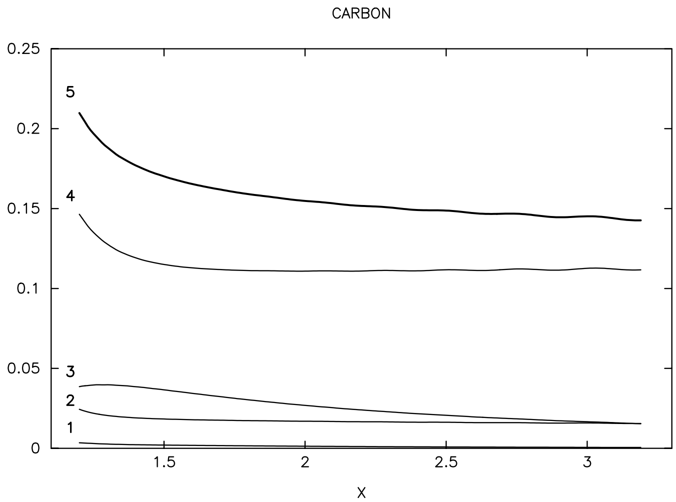

Fig. 2. Shake-up cross sections, relative to the 1s photoionization cross section, versus X, for CII. Curve (5) represents the total relative shake-up cross section. The other curves represent the relative shake-up cross sections for the transitions: 2s $\rightarrow$ 3s (curve 4), 2s $\rightarrow$ 2p (curve 3), 2p $\rightarrow$ 3p (curve 2) and 2p $\rightarrow$ 3s (curve 1). The curve (1) was obtained by multiplying the actual values for the 2p $\rightarrow$ 3s cross section by a factor of 10. Curve (3) refers to the excitations to terms of the $1s2s^23p$ and $1s2p^3$ configurations

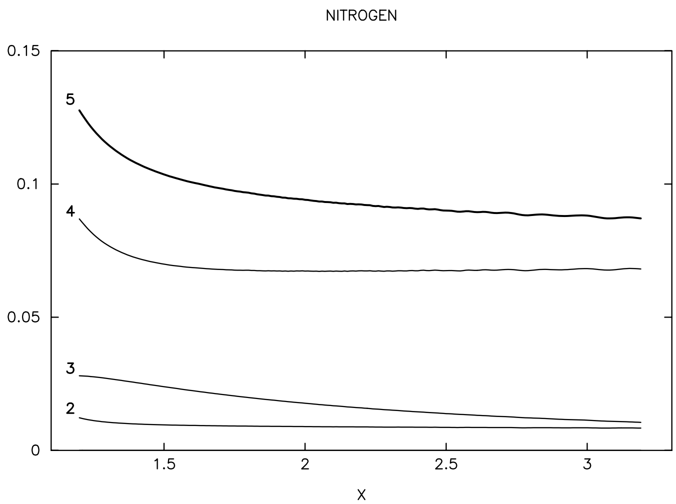

Fig. 3. Shake-up cross sections, relative to the 1s photoionization cross section, versus X, for NIII

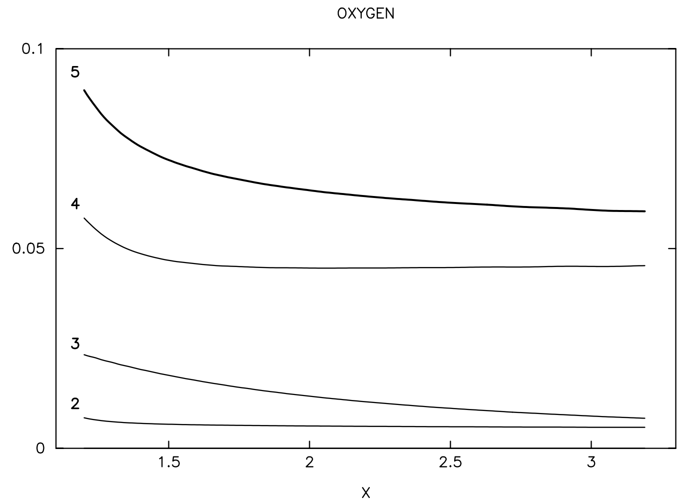

Fig. 4. Shake-up cross sections, relative to the 1s photoionization cross section, versus X, for OIV

In this note we report the results of a similar calculation to that of Badnell et al. (1997) but extended to the case of CII, NIII, OIV, FV and NeVI ions. We were particularly interested on the behavior of the total shake-up cross section as function of Z and on the contribution of direct and conjugate shake-up excitations.

2. Results

For the calculation we used the R-matrix method (Berrington et al. 1987 and Berrington et al. 1995) and covered the photon energy interval X= [1.2-3.2] (in K-edge energy units), where all channels are open. To describe the residual ion we used the SUPERSTRUCTURE code developed by Eissner et al. (1974). We chose the following two categories of configurations: i) K-shell closed: $1s^22s^2$, $1s^22s2p$, $1s^22p^2(^1S)$ and $1s^22s3s$ and ii) K-shell open: $1s2s^22p$, $1s2s2p^2$, $1s2s^23s$, $1s2s^23p$, $1s2p^3$ ($^3P^o$, $^1P^o$) and 1s2s2p3s. The latter case gives rise to 20 terms since neither the quintet nor the $^3S^o$, $^3D^o$, $^1D^o$ terms are required. The values of the λ_{nl} scaling parameters occurring in the Thomas Fermi potential that we used to produce the 1s, 2s, 2p, 3s, and 3p orbitals are 1.3972, 1.2055, 1.1520, 2.4040 and 1.9149, respectively i.e. the values used for boron. A correlation configuration $1s^22p3d$ was also introduced with λ_{3d} = 9.5 to improve the description of the residual ion. We obtained fair agreement between the length and velocity forms of the 2s–2p weighted oscillator strength. The agreement between our calculated energies and the experimental ones was within 1% for the lowest terms and 2% for the 1s-hole terms for which data is available. Note that the 1s-hole terms are described by a few configurations using the nl orbitals of the K-shell closed configurations. For the $^2P^o$ symmetry (target ground state) 41 closed channels occur. For the ^2S, ^2P and ^2D symmetries, representing the diffusion of the ejected electron by the residual ion, we have 23, 21 and 43 channels, respectively. From the R-matrix calculation, we obtained ionization energies which are in close agreement to the experimental ones (see Table 1 where experimental energies IP(exp) are taken from Moore,1966). These results have been obtained using the same set of scaling parameters for the series. In Fig. 1, we present the cross sections for the 1s photoionization versus energy in threshold units X: $X = E_{h\nu}/E_{1s}$, where $E_{h\nu}$ and E_{1s} are the photon and 1s ionization energies, respectively, in the case of CII. We see that the ratio of cross sections for the transitions $1s^22s^22p\ ^2P^o \rightarrow 1s2s^22p\ ^3P^o$ and $1s^22s^22p^2P^o \rightarrow 1s2s^22p^1P^o$ is very close to statistical (3:1) for values of $X > 1.25$. In Figs. 2, 3 and 4 we display total and partial shake-up cross sections for ions of astrophysical inter-

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Table 1. Relative shake-up cross sections and ionization potentials

	BI	CII	NIII	OIV	FV	NeVI
σ_{tot}	30%	15%	10%	6%	4.5%	3.5%
σ(2s–3s)	22.3%	11.2%	6.8%	4.6%	3.3%	2.5%
IP (th) Ry.	0.608	1.792	3.486	5.690	8.398	11.611
IP(exp) Ry.	0.610	1.783	3.473	5.671	8.373	11.578
K-edge (eV)	204	318	460	630	827 1	1051

est: CII, NIII and OIV, respectively. Curve 5 represents the total shake-up cross section. Partial shake-up cross sections corresponding to the transitions 2s $\rightarrow$ 3s (curve 4), 2p $\rightarrow$ 3p (curve 2), 2s $\rightarrow$ 2p (curve 3) and 2p $\rightarrow$ 3s (curve 1), all relative to the 1s single photoionization cross section, are also displayed. This shows that the conjugate shake-up process corresponding to the 2p $\rightarrow$ 3s transition is negligible and for this reason that curve is not drawn on Figs. 3 and 4. One sees that the importance of the shake-up processes (curves 5 on each figure) decreases with the increase of Z, ranging from about 15%, in the case of CII, to about 3.5% in the case of Ne. Comparing these values with 30% obtained in our previous calculation in the case of BI (Badnell et al. 1997) we have an image of the importance of these shake-up processes for the entire boron isoelectronic series (Table 1). Furthermore, one can see that the direct shake-up 2s $\rightarrow$ 3s transition (curve 4) gives the dominant contribution, while the conjugate shake-up 2s $\rightarrow$ 2p (curves 3) and direct shake-up 2p $\rightarrow$ 3p (curves 2) transitions are broadly comparable. These features found in the case of boron are also present for all the other ions of the sequence.

In Table 1 are displayed relative shake-up cross sections and ionization potentials for the first 6 members of the sequence. The first row has percentage values representing the magnitude of the total shake-up cross section relative to the K-shell single photoionization cross section for each ion. One observes a rapid decrease of importance of these shake-up processes as Z increases, but one also remarks that for the low-Z ions the effect of them is significant. This result suggests that the ionization equilibrium of multiply charged B, C, N, O, in a low-density soft-X ray photoionized plasma will be perturbed strongly by such processes (including shake–off). Consequently, for a detailed analysis of such plasmas one should take them into account. In the second row we give values of the dominant shake-up transitions relative to the single 1s photoionization cross section, while the third and forth rows contain the calculated (th) and experimental (exp) ionization potentials (in Ry). In the last row the K-edge potentials in eV are shown.

3. Conclusion

In conclusion, we have calculated cross sections for the shake-up processes accompanying the K-shell photoionization of CII, NIII, OIV, FV and NeVI, in a close-coupling approximation using the R-matrix method. We have covered the photon energy interval X= [1.2-3.2] and find that the total cross section for these processes ranges from about 15% to about 3.5% of the single inner-shell photoionization cross section, when going from CII to NeVI. The full shake-up regime is reached for $X > 2$ due to the strong 2s $\rightarrow$ 2p conjugate shake-up transition. We find that the 2s $\rightarrow$ 3s excitation gives the dominant contribution since the 2p screening is weak and this favours the 2s excitation. This feature is not limited to the case of BI but it is present, for all ions studied. This result also suggests a strong shake-off process leading mostly to the 1s2s2p adjacent ion terms for the entire boron isoelectronic series. These features, strong 2s and 2p excitations, are of interest in astrophysical plasmas undergoing soft–X ray irradiation (Petrini and Da Silva 1996).

More experimental and theoretical work is needed, especially to confirm the strong 2s $\rightarrow$ 3s excitation and to obtain accurate relative shake-up probabilities for the $1s^2 2s^2 2p^n$ second row atoms and ions. For carbon and nitrogen, the 2s $\rightarrow$ 3s excitation is expected to weaken substantially when compared to the 2p $\rightarrow$ 3p one. These processes (including shake-off and double Auger process) are of great importance in low-density astrophysical plasmas since highly-ionized species are produced perturbing the ionization equilibrium and giving rise directly to excited states. This will be critical for diagnosing spectra from the next generation high-resolution X-ray satellites XMM and AXAF, for example.

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