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Research Note

K-photoionisation of atomic carbon: shake up processes

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Abstract. We evaluate the shake up process in the K–photoionisation of atomic carbon, i.e. the 2s $\rightarrow$ 2p and 3s, and 2p $\rightarrow$ 3p shake up excitations, within the photon energy range 25 to 45 Ry. As in the atomic boron case, the 2s $\rightarrow$ 3s excitation is still relatively strong and due to configuration interaction effects dominates the 2p subshell excitation to 3p. The conjugate shake up 2s $\rightarrow$ 2p is 3% near 45 Ry, decreasing slowly as expected. This infers that the shake off process would lead mostly to terms related to the configurations $1s2s2p^2$ with a percentage of about 20%.

Key words: atomic data – atomic processes – line: formation

The importance of the two–step process, K–photoionisation followed by Auger decay in X–ray photoionized gas, has been demonstrated a number of years ago (McAlpine 1974). Through this process the target, if its atomic mass is low, has a good chance of losing 2 or 3 electrons since the probability of radiationless (Auger) decay exceeds radiative decay by about a factor of 100, (see Bambynek et al. 1972). Many authors (Weisheit and Dalgarno 1972, Weisheit 1974, Davidson & Netzer 1979) have shown that this two step process affects the ionisation structure and energy balance of the gaseous nebula in which it occurs. In the aforementioned work, some features of innershell photoionisation, such as shake up and shake off processes, have been ignored, although they are particularly strong for light atoms and ions. Morever KLL Auger decay of light cosmic elements populates the excited configurations preferentially; therefore UV and optical lines are produced from these with specific relative intensities (Petrini & da Silva 1996), as long as the electron collisional excitation from the ground states is dominated by the above double process (a condition generally fulfilled for the upper configuration states). Such situations occur in the UV line spectra of quasars and Seyfert galaxies; as well as those of Galactic compact X–ray sources (Shapiro & Bahcall 1981) or ionized regions surrounding supersoft X–ray sources (Rappaport et al. 1994).

The initial step (K–photoionisation) creates $1s2s^22p^n$ 1s–hole terms (single photoionisation) and the terms mainly produced are those with L value equal to the one targetted. Simultaneously the outer subshells, in this example 2s and 2p, can then either be excited (shake up) or ionized (shake off) with the latter dominating. Åberg (1969) has used the Sudden Approximation for the shake processes in order to estimate its effectiveness in the high energy photon limit and for targets with atomic number Z greater than 9. The general trend is a rapid increase of the whole shake process with decreasing Z values; and for fluor the relative production of KL double-hole states is about 30%. Detailed experiments on these processes are scarce and incomplete. For beryllium the 2s $\rightarrow$ 3s excitation is about 20% of single photoionisation and just above the 1s threshold the relative 2s $\rightarrow$ 2p excitation is about 40% and drops off rapidly with photon energy (Krause & Caldwell 1987a,b). For atomic neon, the shake up and the shake off

processes promote one electron in 21% of all the events with about 2/3 going to the continuum and 1/3 into discrete bound states (Krause 1971). We have recently shown that the shake up process of atomic boron is strong, some tenths of the single photoionisation (Badnell et al. 1997) and dominated by the 2s $\rightarrow$ 3s excitation. Therefore, these last results suggested that the shake off process produces both $1s2s^2$ and 1s2s2p terms. If experiments did not show any substantial 2s $\rightarrow$ 3s excitation for atomic neon (Krause 1971), the question still arises of the importance of 2s and 2p excitations for the light cosmic elements such as C, N, O and their ions.

Our aim in this paper is to obtain an estimate of the relative importance of the shake up excitations compared to the single K–photoionisation for atomic carbon. For this purpose, we follow the method and approximations presented in our previous paper on boron (Badnell et al. 1997). We use the R–matrix codes (Berrington et al. 1987) and SUPERSTRUCTURE (Eissner et al. 1974). Once described the terms of the C^+ residual ion, the initial neutral target $1s^22s^22p^2\ ^3P$ term and the multiple diffusion of the 1s–ejected electron, are approximated using the R–matrix codes. This method takes account of configuration effects both in the target and the residual ion, and of the channel coupling for the $C^+ + e^-$ free system.

We consider two sets of 5–electron configurations: i) the lower ones $1s^22s^22p$, 3s, 3p, 3d, $1s^22s2p^2$, $1s^22p^3$, $1s^22s2p3d$, $1s^22p^23s$, 3p, 3d; ii) the 1s–hole ones $1s2s^22p^2$, $1s2s2p^3$,

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$1s2s^22p3p$, $1s2s2p^23s$, $1s2p^4$, $1s2s^22p3s$. The i) set gives 46 terms and the 11 lower ones are included in the close–coupling (CC) expansion. The intermediate terms do not influence significantly the results and are removed from the CC expansion.

The orbitals 1s, 2s, 3s, 2p, 3p, 3d have respective scaling parameters of 1.4330, 1.3059, 1.2020, 1.5955, 1.3997 and the 3d scaling parameter is chosen equal to 2.5. The gf_L values related to the ground term compare fairly with the Opacity Project results (Cunto et al. 1993), however the comparison of length/velocity values is not satisfactory for some of these transitions. The 1s–hole terms are situed 1 to 3% above their experimental values (Jannitti et al. 1993).

In a first series of calculations we consider successively only two 1s–hole configurations (plus the selected 11 i) terms), for example $1s2s^22p^2$ and $1s2s^22p3p$ for estimating the $2p \rightarrow 3p$ shake up excitation. Then we consider the whole set of configurations and corresponding terms previously mentioned. A relative shake up excitation is defined by the ratio of the cross section considered divided by the single cross section ($1s2s^22p^2$).

$2p \rightarrow 3p$ excitation. With two $1s^{-1}$ configurations, we get a high–energy limit relative excitation of 4.72%, a value to be compared with 6% of boron. The two ^2P and one ^4P terms give the main contribution as expected from the sudden–approximation. The value 0.8298 Ry is achieved for the first ionisation potential, a value less than 0.5% of the experimental one (Moore 1966).

$2s \rightarrow 3s$ excitation. The high–energy limit relative excitation cross section is 7.49%. This percentage has to be compared with 22% in the boron case where the 2p subshell screening is weak. We verify that the three ^2P and three ^4P terms give the main contribution (the sextuplet is not involved since the initial ground term is a triplet).

If we add the 3p shake up configuration, we note that the 3s excitation increases to 11.8% which is unfavorable to the 3p one, now about 1%. The collapse of the 3p excitation is due mainly to configuration interaction effect ($1s2s^22p^2$–$1s2s^22p3p$) on ^4P terms.

$2s \rightarrow 2p$ excitation. The *conjugate* excitation, which is due to the collisional effect induced by the ejected electron (dipole excitation), decreases slowly on the 25–45 energy range but still competes with 3s and 3p excitations.

All configurations model. All configurations are present except $1s2s^22p3s$, the $2p \rightarrow 3s$ excitation is minimal. Intermediate terms have been removed from the CC expansion as been said above, 49 terms are therefore included in the C.C. expansion. The high energy limit for the relative 3s excitation is now 10.65% (Fig. 1), and about 3% for the conjugate excitation (Fig. 2). The 3p shake up excitation is less than 1% (Fig. 2). The single cross section is shown in Fig. 3.

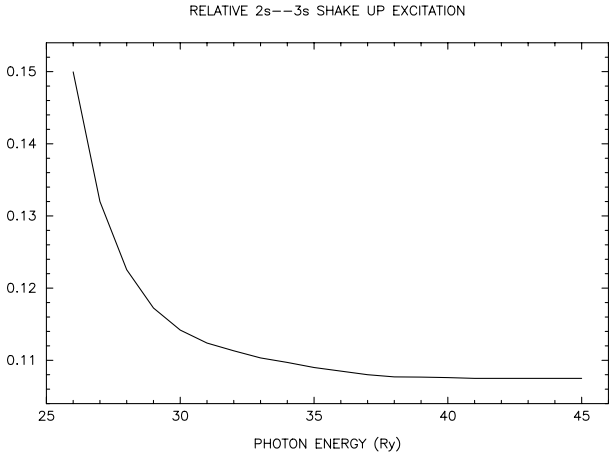

Fig. 1. relative excitation $2s \rightarrow 3s$ versus photon energy (Ry)

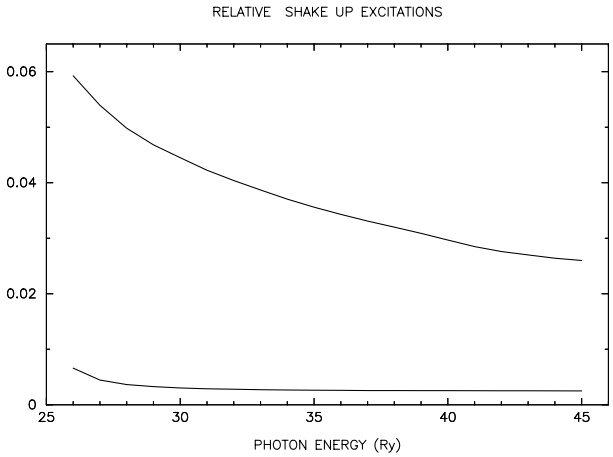

Fig. 2. relative shake up excitations versus photon energy (Ry). The upper curve is $2s \rightarrow 3s$ excitation, the lower one is $2p \rightarrow 3p$ excitation.

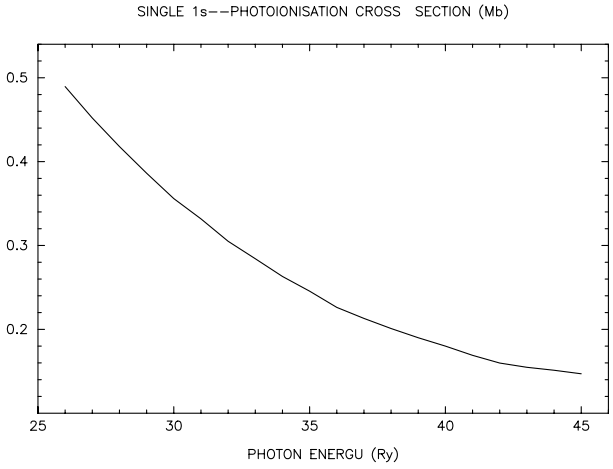

Fig. 3. single photoionisation cross section versus photon energy.

For carbon the $2s \rightarrow 3s$ excitation is still dominating the shake up processes but we note a decrease factor of 2 when compared with boron. The $2p \rightarrow 3p$ relative excitation undergoes configuration interaction effects on P terms which reduce

its effectiveness. However, when isolating this configuration the result obtained infers that the 2p shake off process, although not so large as the 2s one, is important. 2s shake off process leads to C^{++} 1s–hole P terms which Auger decay only on C^{3+} $1s^2 2p$. This statement does not modify the conclusion of a previous work on carbon (Petrini & da Silva 1997). Note that the $1s2s2p^2 3s$ P terms will Auger decay mainly to C^{++} $1s^2 2p3s$ terms. From this last configuration are issued the lines 322.57 and 585.4 Å.

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