Relativistic calculations of M-shell yields in Zn, Cd and Hg

J. M. Sampaio[1], F. Parente[2] P. Indelicato[3], J. P. Marques[1]

[1]Centro de Física Atómica, CFA, Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, FCUL, Campo Grande, Ed. C8, 1749-016 Lisboa, Portugal
[2]Centro de Física Atómica, CFA, Departamento de Física, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal
[3]Laboratoire Kastler Brossel, École Normale Supérieure, CNRS, Université P. et M. Curie, Paris, Case 74; 4 place Jussieu, 75252 Paris CEDEX 05, France
jmsampaio@fc.ul.pt

Experimental and theoretical data in M-shell atomic rates and yields are scarce due to the complexity resulting from the high number of possible transitions, when compared with the K- and L-shells cases. M-shell yields calculations by Chen *et al.* in the early 1980s show that relativistic effects in individual transitions probabilities amount to 10% - 50% compared to non-relativistic results. These studies also stressed the importance of going beyond the independent particle model. More recently, total M-shell x-ray production cross-sections and average fluorescence yields were measured with high precision, showing an agreement with the available data between 0.3% and 28% [1].

In this work, we present a relativistic calculation of M-shell transition rates and fluorescence yields of three elements with similar electronic configurations: Zn, Cd and Hg. The last M-shell calculations found in the literature for Zn and Cd are those on reference [2], using a non-relativistic HFS. For Hg there is the relativistic calculation in reference [3], based on the DHS approach. In our calculations, we use the MCDF code of Desclaux and Indelicato [4,5] in the single-configuration approach, with the Breit interaction and the vacuum polarization terms included in the self-consistent field calculation. Other QED effects are included as perturbations. Great care is given in the definitions of fluorescence, Auger and Coster-Kronig yields, since quite often authors use slightly different definitions, making it difficult to perform comparisons between theoretical and experimental results. This is particularly true when dealing with the complex rearrangements that can occur in the M-shell transitions.

M-subshell fluorescense, Auger and Coster-Kronig yields will be presented and compared with the available theoretical, semi-empirical and experimental results for Zn, Cd and Hg [6].

References:

[1] G. Apaydin *et al.*, Radia. Phys. Rev. Chem. 74, 549 (2005).

[2] E. J. McGuire, Phys. Rev. A 5, 1043 (1973).

[3] M. H. Chen *et al,* Phys. Rev. A 21, 449 (1980) and Phys. Rev. A 27, 2989 (1983).

[4] J. Descalux, Comput. Phys. Commun. 9, 31 (1975).

[5] P. Indelicato, J. P. Desclaux, Phys. Rev. A 42, 5139 (1990).

[6] J. M. Sampaio *et al.*, J. Phys. B 46, 065001 (2013).