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2015 J. Phys.: Conf. Ser. 635 092095

(http://iopscience.iop.org/1742-6596/635/9/092095)

Journal of Physics: Conference Series **635** (2015) 092095 doi:10.1088/1742-6596/635/9/092095

Relativistic calculations of atomic parameters in Ununoctium

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Synopsis K shell, and L and M subshells fluorescence and Coster-Kronig yields for the super-heavy element Uuo are calculated for the first time using the Dirac-Fock approach.

Ununoctium is the temporary IUPAC name for the transactinide element with $Z = 118$ to which corresponds the temporary element symbol Uuo. On the periodic table of the elements it is a group VIII element and the last one of the 7^{th} period. Uuo has the highest atomic number and the highest atomic mass of all the elements discovered so far. The first decay of Uuo atoms was observed in 2002 at the JINR in Dubna. In 2006, researchers from JINR and LLNL announced that they had indirectly detected a total of three (possibly four) nuclei of Uuo-294 produced via collisions of Cf-249 atoms and Ca-48 ions [1].

Transition probabilities needed to derive the atomic yields shown in Table 1 were calculated with the relativistic general purpose MCDF code (MCDFGME) developed by Desclaux [2] and Indelicato. The MCDFGME code has been adapted since 1986 to work with super-heavy elements [3]. The nuclear charge distribution is described by the Fermi model with a nuclear mean-square radius obtained from fits to the experimental data of Angeli [4]. Initial and final state wavefunctions were calculated taking into account quantum electrodynamics (QED) radiative corrections, namely the self-energy and vacuum polarization [5].

Radiative transition rates were calculated making use of wavefunctions obtained in a complete self-consistent process including relaxation. We used the so-called optimized levels to obtain the wavefunctions and energies of all levels involved. No orbital relaxation was allowed between the initial and final bound state wavefunctions during the calculation of the radiationless transitions in order to ensure orthogonality. However, these transitions were calculated using the correct energies obtained in previous independent calculations of initial and final state wavefunctions and eigenvalues [6].

Table 1. K-, L-, and M-shell yields of Uuo.

Fluorescence yield		Coster-Kronig yield	
ω_K	9.73E-01	$f_{L_{12}}$	9.94E-03
ω_{L_1}	4.33E-01	$f_{L_{13}}$	4.31E-01
ω_{L_2}	6.86E-01	$f_{L_{23}}$	1.60E-01
ω_{L_3}	6.42E-01	$f_{M_{12}}$	4.74E-02
ω_{M_1}	3.39E-02	$f_{M_{13}}$	5.65E-01
ω_{M_2}	3.63E-02	$f_{M_{14}}$	1.09E-01
ω_{M_3}	5.17E-02	$f_{M_{15}}$	1.30E-01
ω_{M_4}	1.23E-01	$f_{M_{23}}$	9.09E-02
ω_{M_5}	1.10E-01	$f_{M_{24}}$	6.16E-01
		$f_{M_{25}}$	1.14E-01
		$f_{M_{34}}$	2.83E-02
		$f_{M_{35}}$	5.45E-01
		$f_{M_{45}}$	4.39E-02

This work was supported by FCT project PEstOE/FIS/UI0303/2011, Portugal and the Allianz Program of the Helmholtz Association, contract EMMI HA-216 Extremes of Density and Temperature. BioISI is supported by the grant UID/MULTI/04046/2013 from FCT/MCTES/PIDDAC, Portugal. M.G. and T.I.M. acknowledges the FCT fellowships SFRH/BPD/92455/2013 and SFRH/BPD/69627/2010, respectively.

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