Dirac-Fock calculations of K-, L-, and M-shell fluorescence and Coster-Kronig yields for Ne, Ar, Kr, Xe, Rn, and Uuo

J. M. Sampaio,[1,*] T. I. Madeira,[1] M. Guerra,[2] F. Parente,[2] J. P. Santos,[2] P. Indelicato,[3] and J. P. Marques[1]

[1]*BioISI–Biosystems & Integrative Sciences Institute, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, C8, 1749-016 Lisboa, Portugal*

[2]*Laboratório de Instrumentação, Engenharia Biomédica e Física da Radiação (LIBPhys-UNL), Departamento de Física, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte da Caparica, 2892-516 Caparica, Portugal*

[3]*Laboratoire Kastler Brossel, École Normale Supérieure, CNRS, Sorbonne Universités, UPMC Univ. Paris 06, Case 74; 4, place Jussieu, 75252 Paris CEDEX 05, France*

(Received 27 March 2015; published 28 May 2015)

In this work, we calculated the fluorescence and Coster-Kronig yields for the K shell and the L and M subshells of Ne, Ar, Kr, Xe, Rn, and Uuo ($Z = 118$), using a Dirac-Fock model which provides a better description of the electron-electron interaction than previous approaches, and is suitable to handle superheavy elements. The results are compared with available data from other authors. In what concerns Ne, Ar, Kr, Xe, and Rn K shells, the obtained results are in very good agreement with the adopted values of Krause [25] and with experiment when available. For the L subshells, our results are in line with existing ones. For the M subshells and for all shells of Uuo there are no previous experimental and theoretical results to compare to our calculations.

DOI: 10.1103/PhysRevA.91.052507 PACS number(s): 31.15.−p, 32.10.−f, 32.50.+d, 32.80.Hd

I. INTRODUCTION

The knowledge of accurate values of atomic parameters is essential in many branches of physics and technology such as spectroscopy, plasma physics, astrophysics, materials science, and so on [1]. Among these parameters, fluorescence, Coster-Kronig, and Auger yields are extremely relevant, because they are needed for the quantitative analysis of materials, as well as the determination of quantities such as ionization and excitation cross sections from the detected spectra.

Atomic parameters have been objects of intense research, both theoretically and experimentally, since the second half of the 20th century. A review and compilation of the values known until then was published in 1972 [2] as well as several books on the subject [3–5].

From the theoretical point of view, calculation of radiative and radiationless yields for a one-hole configuration implies the calculation of transition probabilities from one or several initial levels to, in general, many final levels, depending on the number of electrons in partially filled outer shells. In extreme cases, where the multiplicity of the initial and final states is large, the number of transition probabilities to be calculated may approach one million. An example is the case of Fe, where about 350 000 radiative and radiationless transitions can contribute just for the calculation of the K-shell fluorescence yield. In the past, when computation tools were slow and computer memory was scarce, some authors avoided this issue by neglecting the interaction of inner holes with electrons in partially filled outer shells [6].

In the rare gases, having only closed shells except the one in which the initial hole is created, the number of transitions to be dealt with is relatively small. Thus the calculation of the required transition probabilities is faster, allowing for easier tests of the theoretical models by comparison with experiment.

The Bambynek *et al.* [2] compilation includes virtually all the work published on this subject up to 1972. In what concerns theoretical calculations, it lists the results of McGuire [7], using nonrelativistic Hartree-Fock-Slater (HFS) wave functions, Kostroun *et al.* [8], which made use of Slater-screened bound-state hydrogenic wave functions, and Walters *et al.* [9], also using HFS wave functions. The Slater approach to the Hartree-Fock method makes use of an average potential for the exchange contribution of the electron-electron interaction, to simplify the calculation.

Total and partial atomic-level widths for the K up to the N shells covering values of Z up to 120 for K and L shells were presented in graphic form by Keski-Rahkonen and Krause [10] (1974). For the K-shell radiative widths, the published values were based on relativistic Dirac-Hartree-Slater (DHS) calculations [11,12], and Auger widths were taken from [7,8,13,14]. For the L shell, the values are from [15–19]. The widths and yields calculations for M subshells were taken from [17,20–24]. The DHS approach is the relativistic version of the HFS method.

In 1979, Krause [25] published extensive calculations of atomic radiative and radiationless yields for the K shell and the L subshells for elements with Z up to 110, from the existing information on fluorescence, Auger, and Coster-Kronig yields, radiative and radiationless transition rates, level widths, x-ray and Auger linewidths, x-ray and Auger spectra, and Coster-Kronig energies. The theoretical values used in that work for the radiative transition rates were from the relativistic Hartree-Fock calculations by Scofield [26,27], Anholt *et al.* [28], and the DHS values of Scofield [11]. Theoretical radiationless transition probabilities were taken from the works of McGuire [7], Kostroun *et al.* [8], Bhalla *et al.* [13], and Bhalla *et al.* [14].

Puri *et al.* [29] calculated L-subshell fluorescence yields and Coster-Kronig transition probabilities using radiative and nonradiative transition rates based also on the DHS model for all the elements in the atomic number range $25 < Z < 96$.

*jmsampaio@fc.ul.pt

Hubbel and co-workers published in 1994 [30] a review including bibliography, and tabulation of *K*-, *L*-, and higher atomic shell x-ray fluorescence yields, covering most of the existing experimental results relative to the period 1978–1993. In this work, reference is made to the calculations by Chen *et al.* [18], Crasemann *et al.* [15], Chen *et al.* [31], and Puri *et al.* [29], which used a DHS approach.

In 2001, Campbell and Papp [32] published a compilation of widths of the atomic *K*-*N*7 levels, including experimental measurements and theoretical widths derived from the Evaluated Atomic Data Library (EADL) of Lawrence Livermore National Laboratory. The EADL values were based upon DHS calculations [11,33–37], Dirac-Fock calculations [26], and, in a small number of cases, on many-body theory predictions [38–40].

Later on, Campbell [41] presented a compilation of fluorescence yields and Coster-Kronig probabilities for the atomic *L* subshells, obtained from experimental measurements, including recommended values for these quantities. The values are still compared with the DHS theoretical calculations of Chen *et al.* [35], and Scofield [11]. These rather old calculations are still used widely for comparison with experiment, as can be found in the very recent work of Llovet *et al.* [42].

In this work, we used the relativistic general purpose multiconfiguration Dirac-Fock (MCDF) computer code *mcdfgme* of Desclaux and Indelicato [43,44] to calculate the fluorescence, and Coster-Kronig yields for the *K* shell, and *L*, and *M* subshells of Ne, Ar, Kr, Xe, Rn, and Uuo. The Auger yields for the same shells and subshells are obtained by subtracting, in each case, the sum of these yields from unity. The MCDF allows for a better description of the electron-electron interaction when compared with previous HFS and DHS calculations. In the present calculation, that interaction is described by the Coulomb-Breit operator, which includes magnetic and retardation terms. The *mcdfgme* code can work with superheavy elements [45], allowing for the extension of our calculation to the Uuo case.

The *mcdfgme* code was used by Santos *et al.* [46,47] to compute relativistic L_1 atomic subshell decay rates and fluorescence yield for Yb and Hg. Casteleiro *et al.* [48] used the same code to obtain relativistic *K*-shell decay rates and fluorescence yields for Zn, Cd, and Hg. More recently, *M*-shell decay rates and yields for the same elements were calculated by Sampaio *et al.* [49,50]. *K*-shell decay rates and fluorescence yields of Ge were also calculated by Sampaio *et al.* [1].

II. FLUORESCENCE AND COSTER-KRONIG YIELDS

When an atom is ionized through the creation of a hole in an inner shell, it becomes highly unstable and may decay to a lower-energy state through a radiative or a radiationless transition. In the first case, energy is carried away through the emission of a photon and, in the latter case, the atom becomes doubly ionized due to the emission of a secondary electron. Fluorescence, Coster-Kronig, and Auger yields, which give the relative probabilities of decay of the ionized atom through radiative, in the first case, or radiationless, in the latter two cases, respectively, are defined below.

As pointed out by the authors in Ref. [49], the definitions of fluorescence, Auger, and CK yields require great precaution because quite often authors use slightly different definitions that create difficult comparisons between theoretical and experimental results. We refer the reader to that article for the definitions used in the present work and the more complete description of the calculation methods.

A. Definitions

The fluorescence yield of an atomic subshell is defined as

$$\omega_i = \frac{\Gamma_i^{\mathrm{R}}}{\Gamma_i} = \frac{\Gamma_i^{\mathrm{R}}}{\Gamma_i^{\mathrm{R}} + \Gamma_i^{\mathrm{NR}}}, \tag{1}$$

where Γ_i^{R} and Γ_i^{NR} are, respectively, the radiative and the radiationless widths of a one-hole state in subshell i, and Γ_i is the corresponding total width.

The radiative width of a subshell i is obtained by summing the partial widths, Γ_{ij}^{R}, of a hole in this subshell decaying to higher subshells $j > i$,

$$\Gamma_i^{\mathrm{R}} = \sum_{j(>i)} \Gamma_{ij}^{\mathrm{R}}. \tag{2}$$

In the same way, the radiationless width of a subshell i is obtained by summing the partial widths, $\Gamma_{ij}^{\mathrm{NR}}$, of a hole in this subshell being filled with an electron from a subshell j of the same (Coster-Kronig transitions) or a higher shell (Auger transitions),

$$\Gamma_i^{\mathrm{NR}} = \sum_{j(>i)} \Gamma_{ij}^{\mathrm{NR}}. \tag{3}$$

Here,

$$\Gamma_{ij}^{\mathrm{NR}} = \sum_{k(\geqslant j)} \Gamma_{ij;k}^{\mathrm{NR}}, \tag{4}$$

where $\Gamma_{ij;k}^{\mathrm{R}}$ is the radiationless probability of a hole created in the subshell i being filled with an electron from a subshell j of a higher shell, and simultaneously a second hole being created in another subshell $k > i$ of the same or a higher shell, with the emission of an electron to the continuum.

Similar to the fluorescence yield, Coster-Kronig and Auger yields are defined, respectively, as the probability that a vacancy in a subshell is filled through a transition of an electron from the same shell together with the ejection of a second electron from a higher shell, and as the probability that a vacancy in a subshell is filled through a transition of an electron from a higher shell together with the ejection of a second electron also from a higher shell. Thus the Coster-Kronig yield for subshell X_i in a shell X is the probability that a vacancy in this subshell is filled by an electron making a transition from a higher subshell X_j in the same shell, while the ejected electron may come from the same or a higher shell [2],

$$f_{X_{ij}} = \frac{\Gamma_{ij}^{\mathrm{NR}}}{\Gamma_i^{\mathrm{R}} + \Gamma_i^{\mathrm{R}}}. \tag{5}$$

Here i assumes values from 1 to $n - 1$, and j assumes values from 2 to n, where n is the number of subshells, and $i < j$.

B. Relativistic calculations

Radiative transitions are calculated, in a single-configuration approach, using the multipole expansion of the

matrix element between one-hole initial and final states and the emission of a photon with energy $E_i - E_f$, where E_i and E_f are the energies of the initial and final states, respectively,

$$\Gamma^{\mathrm{R}}_{if} = \frac{4\pi}{\hbar} \sum_{M_i M_f} \left| \sum_{JM} \langle J_f M_f | T^{\Pi}_{JM} | J_i M_i \rangle \right|^2 . \tag{6}$$

The multipole operators T^{Π}_{JM} are irreducible tensors of rank J and parity Π and are divided into two types—electric and magnetic operators. The explicit form of the tensor operators can be found, for example, in [51]. Radiative transition rates were calculated making use of wave functions obtained in a complete self-consistent process including relaxation. We used the so-called optimized levels (OL) to obtain the wave functions and energies of all levels involved. Löwdin's method [52] was employed to account for the nonorthogonality of the initial and final fully relaxed wave functions.

Nuclear size effects were taken into account by using a uniformly charged sphere model for Ne, Ar, and Kr, and the Fermi model for Xe, Rn, and Uuo, instead of a point nucleus. For the atomic masses and the nuclear radii values were taken from the tables by Audi *et al.* [53], and Angeli [54], respectively. Initial- and final-state wave functions were calculated taking into account quantum electrodynamics (QED) radiative corrections, namely the self-energy and vacuum polarization. The one-electron self-energy was evaluated using the one-electron values of Mohr and co-workers [55–58] and corrected for finite nuclear size [58]. The self-energy screening and vacuum polarization were included using the methods developed by Indelicato and co-workers [44,59–61].

In what concerns the radiationless transitions, we do not account for the interaction between the electron ejected in the process of creation of the initial hole and the Auger electron, and we will assume that the creation of the inner-shell hole is independent of the decay process. These transitions are treated in the calculations as transitions between an initial state, defined as a hole in a subshell and a second hole in the continuum, and a final state, defined as two holes in subshells and an electron in the continuum. The total radiationless probability transition per unit time between two states i and f can be written as [2]

$$\Gamma^{\mathrm{NR}}_{if} = \frac{2\pi}{\hbar} \sum_{M_i M_f} |D(J_i M_i \to J_f M_f) - E(J_i M_i \to J_f M_f)|^2 \rho(E_f), \tag{7}$$

where D and E are the direct and exchange matrix elements, respectively,

$$\begin{aligned} &D(J_i M_i \to J_f M_f) \\ &\quad = \left\langle l^c_j(1) l^d_j(2); J_f M_f \middle| V_{12} \middle| l^a_j(1) l^b_j(2); J_i M_i \right\rangle, \\ &E(J_i M_i \to J_f M_f) \\ &\quad = \left\langle l^c_j(1) l^d_j(2); J_f M_f \middle| V_{12} \middle| l^a_j(2) l^b_j(1); J_i M_i \right\rangle, \end{aligned} \tag{8}$$

and $\rho(E_f)$ is the density of the final states for an electron in the continuum with energy E_f.

The two-electron operator V_{12} is the Coulomb-Breit operator, including the magnetic and retardation terms,

$$V_{12} = \frac{e}{r_{12}} + \frac{e}{2r_{12}} \left[\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + \frac{(\boldsymbol{\alpha}_1 \cdot \boldsymbol{r}_{12})(\boldsymbol{\alpha}_2 \cdot \boldsymbol{r}_{12})}{r^2_{12}} \right], \tag{9}$$

where $\boldsymbol{\alpha}_{1,2}$ are the Dirac matrices, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the distance between the positions of the electrons.

The Dirac-Fock equations were solved with the same atomic potential as that of the initial state to obtain the continuum wave functions, normalized to represent one ejected electron per unit energy. No orbital relaxation was allowed between the initial and final bound-state wave functions during the calculation of the radiationless transitions in order to ensure orthogonality. However, these rates were calculated using the correct transition energies obtained in previous independent calculations of initial- and final-state wave functions and eigenvalues.

The accuracy of transition energies calculated with the method used in this work was investigated by Indelicato and co-workers [62] who found a very good agreement with experiments. This was confirmed by Deslattes *et al.* [63]. For example, calculations of K- and L-shell transitions in Xe showed an agreement less than 0.1 eV with experiment [64]. The latter work demonstrated also the importance of treating the core-core effects relativistically. Especially when both intermediate-core holes lie above the initial hole, the result is sensitive to small changes in the orbital energy.

Uncertainties in the calculations of transition rates depend on the atomic number and on the shell considered. As a general rule uncertainties increase for low Z atoms and for higher shells. We estimated the uncertainty in the radiative transition rates from the relative difference between the values obtained in the length and velocity gauges. These are of the order of ~1% for the dominant K-shell transitions, ~4% for the L-shell transitions, and ~15% for the M-shell transitions. Assuming

TABLE I. Radiative transition probabilities (in a.u.) for a system with an initial hole in K, L, and M subshells.

	Ne	Ar	Kr	Xe	Rn	Uuo
K	1.72×10^{-04}	3.02×10^{-03}	6.54×10^{-02}	3.74×10^{-01}	$2.58 \times 10^{+00}$	$8.82 \times 10^{+00}$
$L1$	4.88×10^{-07}	1.31×10^{-05}	6.85×10^{-04}	6.30×10^{-03}	6.42×10^{-02}	3.81×10^{-01}
$L2$	9.16×10^{-20}	6.11×10^{-07}	5.13×10^{-04}	5.35×10^{-03}	5.73×10^{-02}	2.79×10^{-01}
$L3$		1.24×10^{-06}	1.01×10^{-03}	1.01×10^{-02}	9.82×10^{-02}	4.27×10^{-01}
$M1$		3.44×10^{-07}	8.17×10^{-06}	1.72×10^{-04}	2.76×10^{-03}	2.63×10^{-02}
$M2$		1.28×10^{-18}	1.21×10^{-05}	1.75×10^{-04}	3.17×10^{-03}	2.29×10^{-02}
$M3$			1.09×10^{-05}	1.73×10^{-04}	3.44×10^{-03}	2.36×10^{-02}
$M4$			2.80×10^{-07}	1.21×10^{-05}	4.40×10^{-03}	3.39×10^{-02}
$M5$			2.66×10^{-07}	1.05×10^{-05}	4.12×10^{-03}	2.99×10^{-02}

TABLE II. Radiationless transition probabilities (in a.u.) for a system with an initial hole in K, L, and M subshells.

	Ne	Ar	Kr	Xe	Rn	Uuo
K	1.07×10^{-02}	2.27×10^{-02}	3.53×10^{-02}	4.63×10^{-02}	7.88×10^{-02}	2.44×10^{-01}
$L1$		1.13×10^{-01}	2.22×10^{-01}	1.17×10^{-01}	4.75×10^{-01}	5.00×10^{-01}
$L2$		3.19×10^{-03}	2.23×10^{-02}	5.01×10^{-02}	6.94×10^{-02}	1.28×10^{-01}
$L3$		6.73×10^{-03}	4.75×10^{-02}	9.94×10^{-02}	1.58×10^{-01}	2.38×10^{-01}
$M1$			1.81×10^{-01}	4.74×10^{-01}	6.58×10^{-01}	7.50×10^{-01}
$M2$			9.92×10^{-02}	1.85×10^{-01}	4.78×10^{-01}	6.09×10^{-01}
$M3$			9.69×10^{-02}	1.98×10^{-01}	3.68×10^{-01}	4.33×10^{-01}
$M4$			2.73×10^{-03}	2.46×10^{-02}	1.11×10^{-01}	2.42×10^{-01}
$M5$			2.68×10^{-03}	2.16×10^{-02}	1.17×10^{-01}	2.43×10^{-01}

that radiationless transitions have uncertainties of the same order, the resulting fluorescence yields for the K, L, and M shell are affected by uncertainties up to ∼2%, ∼6%, and ∼20%, respectively.

III. RESULTS AND DISCUSSION

Using the method outlined in Sec. II B, we calculated all possible radiative and radiationless transitions corresponding to the deexcitation of the atoms with an initial hole in K, L, and M shells.

TABLE III. Fluorescence yields for Ne, Ar, Kr, Xe, Rn, and Uuo calculated in this work (TW) compared with literature. Experimental values are indicated with error bars (in parentheses).

Ref.	ω_K	ω_{L_1}	ω_{L_2}	ω_{L_3}	ω_{M_1}	ω_{M_2}	ω_{M_3}	ω_{M_4}	ω_{M_5}
					Ne				
TW	1.59×10^{-02}	$1.00 \times 10^{+00}$	$1.00 \times 10^{+00}$						
[8]	2.04×10^{-02}								
[9]	1.64×10^{-02}								
[25]	1.60×10^{-02}								
[66]	$1.8(2) \times 10^{-02}$								
[67]	$1.55(22) \times 10^{-02}$								
					Ar				
TW	1.17×10^{-01}	1.16×10^{-04}	1.92×10^{-04}	1.84×10^{-04}	$1.00 \times 10^{+00}$	$1.00 \times 10^{+00}$			
[8]	1.11×10^{-01}								
[9]	1.22×10^{-01}								
[67]	$1.22(21) \times 10^{-01}$								
[25]	1.18×10^{-01}	1.80×10^{-04}	2.20×10^{-04}	2.20×10^{-04}					
[35]		1.08×10^{-04}		1.82×10^{-04}					
					Kr				
TW	6.49×10^{-01}	3.08×10^{-03}	2.25×10^{-02}	2.08×10^{-02}	4.51×10^{-05}	1.22×10^{-04}	1.12×10^{-04}	1.03×10^{-04}	9.96×10^{-05}
[8]	6.55×10^{-01}								
[9]	6.75×10^{-01}								
[25]	6.43×10^{-01}	4.10×10^{-03}	2.00×10^{-02}	2.20×10^{-02}					
[20,21]					4.95×10^{-05}	6.00×10^{-05}	6.00×10^{-05}	1.49×10^{-04}	
[35]		2.21×10^{-03}	2.11×10^{-02}	2.16×10^{-02}					
[68]	$6.55(30) \times 10^{-01}$								
					Xe				
TW	8.90×10^{-01}	5.10×10^{-02}	9.64×10^{-02}	9.22×10^{-02}	3.63×10^{-04}	9.48×10^{-04}	8.73×10^{-04}	4.94×10^{-04}	4.86×10^{-04}
[8]	9.04×10^{-01}								
[9]	9.18×10^{-01}								
[20,21]					4.70×10^{-04}	9.04×10^{-04}	6.80×10^{-04}	4.40×10^{-04}	
[69]	$8.89(10) \times 10^{-01}$								
[34]	8.87×10^{-01}								
[35]		4.75×10^{-02}	9.30×10^{-02}	9.42×10^{-02}					
[25]	8.91×10^{-01}	4.60×10^{-02}	8.30×10^{-02}	8.50×10^{-02}					
					Rn				
TW	9.70×10^{-01}	1.19×10^{-01}	4.52×10^{-01}	3.84×10^{-01}	4.18×10^{-03}	6.58×10^{-03}	9.26×10^{-03}	3.82×10^{-02}	3.40×10^{-02}
[20,21]					3.95×10^{-03}	9.75×10^{-03}	6.30×10^{-03}	3.55×10^{-02}	3.62×10^{-02}
[25]	9.69×10^{-01}	1.34×10^{-01}	4.29×10^{-01}	4.11×10^{-01}					
					Uuo				
TW	9.73×10^{-01}	4.33×10^{-01}	6.86×10^{-01}	6.42×10^{-01}	3.39×10^{-02}	3.63×10^{-02}	5.17×10^{-02}	1.23×10^{-01}	1.10×10^{-01}

For the radiative transitions the results are shown in Table I. The first column of this table indicates the subshell where the initial hole is located. This table lists the total decay rates, which is a sum over all possible radiative deexcitation mechanisms. Transition probabilities were calculated using the multipole expansion, as mentioned above, and include all electric and magnetic transitions of any order allowed by the selection rules.

The total radiationless rate for a system with an initial K-, L-, or M-shell hole is the weighted sum over all subsequent allowed radiationless transitions. The results of these rates for Ne, Ar, Kr, Xe, Rn, and Uuo are listed in Table II.

The fluorescence yields ω_i for the considered elements, obtained according to the definitions given in Sec. II, are summarized in Table III and compared with selected results from other authors. In what concerns ω_K, we note that the present results agree within 1% with the recommended values of Krause [25] for all elements considered in this work. Furthermore, the values are within the error bars of the most reliable experimental values. For the L subshells, available data are more scarce than for the K shell. Our values are close to the ones from Krause [25] and Chen *et al.* [35] for the $L2$ and $L3$ subshells in all three elements, the relative differences being less than 15%. In what concerns the $L1$ subshell, our values lie between the values of these authors for Ar and Kr and slightly above both of them for Xe. We did not find any experimental values for these quantities in the literature. For the M subshells, the only results available are the nonrelativistic calculations published in 1971 by McGuire [20,21]. Our values are higher than the ones of McGuire except for the $M1$ subshell in Kr and Xe, and for the $M4$ subshell in Kr. McGuire does not present results for the $M5$ subshell for these elements.

Coster-Kronig yields of Ar, Kr, and Xe and Rn, computed in this work for the L and M subshells, are listed in Table IV and are compared in Table V with selected values from other authors for the L subshells. No values exist, to our knowledge, for the M subshells. In what concerns the L subshells, our values are very close to the calculated ones from other authors (a relative difference less than 20%, with the exception of the $f_{L_{23}}$ value for Kr and the $f_{L_{12}}$ value for Rn) and to the experimental result of Jitschin *et al.* [65], the relative difference being less than 25%. For Uuo there are no experimental or theoretical data available with which to compare our results but we note that our yields are consistent with the values obtained for the natural rare gases.

TABLE V. Coster-Kronig yields for the L shell of Ar, Kr, Xe, and Rn calculated in this work (TW) compared with literature. Experimental values are indicated with error bars (in parentheses).

Ref	$f_{L_{12}}$	$f_{L_{13}}$	$f_{L_{23}}$
		Ar	
TW	4.73×10^{-01}	4.83×10^{-01}	
[35]	3.27×10^{-01}	6.28×10^{-01}	
		Kr	
TW	2.44×10^{-01}	6.13×10^{-01}	6.71×10^{-03}
[41]	1.98×10^{-01}	7.04×10^{-01}	9.50×10^{-02}
[25]	2.70×10^{-01}	5.20×10^{-01}	1.00×10^{-01}
[35]	1.98×10^{-01}	7.04×10^{-01}	9.50×10^{-02}
		Xe	
TW	1.69×10^{-01}	3.04×10^{-01}	1.23×10^{-01}
[25]	1.90×10^{-01}	2.80×10^{-01}	1.54×10^{-01}
[35]	1.96×10^{-01}	3.28×10^{-01}	1.74×10^{-01}
[69]	$5(3) \times 10^{-02}$	$8.9(8) \times 10^{-02}$	$1.00(3) \times 10^{-01}$
[65]	$1.2(3) \times 10^{-01}$	$2.3(4) \times 10^{-01}$	$1.4(2) \times 10^{-01}$
		Rn	
TW	5.11×10^{-02}	6.76×10^{-01}	1.06×10^{-01}
[25]	1.00×10^{-01}	5.90×10^{-01}	1.10×10^{-01}

IV. CONCLUSIONS

Fluorescence and Coster-Kronig yields for the K shell and the L and M subshells of Ne, Ar, Kr, Xe, Rn, and Uuo were computed in this work, in single configuration mode, using the multiconfiguration Dirac-Fock code of Desclaux and Indelicato. The results for the K shell are in very good agreement with the adopted values of Krause [25] and with experiment. For the L shells, our results are close to the existing ones from other authors. For the M subshells and for all shells in Uuo there are no previous experimental and theoretical values to compare to our results.

TABLE IV. Coster-Kronig yields for Ar, Kr, Xe, Rn, and Uuo.

	Ar	Kr	Xe	Rn	Uuo
$f_{L_{12}}$	4.73×10^{-01}	2.44×10^{-01}	1.69×10^{-01}	5.11×10^{-02}	9.94×10^{-03}
$f_{L_{13}}$	4.83×10^{-01}	6.13×10^{-01}	3.04×10^{-01}	6.76×10^{-01}	4.31×10^{-01}
$f_{L_{23}}$		6.71×10^{-03}	1.23×10^{-01}	1.06×10^{-01}	1.60×10^{-01}
$f_{M_{12}}$		2.29×10^{-01}	3.24×10^{-01}	8.31×10^{-02}	4.74×10^{-02}
$f_{M_{13}}$		4.94×10^{-01}	4.59×10^{-01}	6.01×10^{-01}	5.65×10^{-01}
$f_{M_{14}}$		1.52×10^{-01}	7.89×10^{-02}	9.56×10^{-02}	1.09×10^{-01}
$f_{M_{15}}$		1.11×10^{-01}	9.79×10^{-02}	1.31×10^{-01}	1.30×10^{-01}
$f_{M_{23}}$			3.35×10^{-03}	8.70×10^{-02}	9.09×10^{-02}
$f_{M_{24}}$		9.09×10^{-01}	5.52×10^{-01}	6.78×10^{-01}	6.16×10^{-01}
$f_{M_{25}}$		6.40×10^{-02}	3.31×10^{-01}	1.02×10^{-01}	1.14×10^{-01}
$f_{M_{34}}$		4.70×10^{-01}	1.52×10^{-01}	6.67×10^{-02}	2.83×10^{-02}
$f_{M_{35}}$		5.00×10^{-01}	7.36×10^{-01}	7.03×10^{-01}	5.45×10^{-01}
$f_{M_{45}}$				1.18×10^{-02}	4.39×10^{-02}

ACKNOWLEDGMENTS

This work was supported, in part, by center grant (to BioISI, Centre Reference: UID/MULTI/04046/2013), from FCT/MCTES/PIDDAC, Portugal and by FCT Project No. PEstOE/FIS/UI0303/2011. We also thank the Allianz Program of the Helmholtz Association, Contract No. EMMI HA-216 Extremes of Density and Temperature: Cosmic Matter in the Laboratory. M.G. and T.I.M. acknowledge the support of the FCT, under Contracts No. SFRH/BPD/92455/2013 and No. SFRH/BPD/69627/2010, respectively. Laboratoire Kastler Brossel is Unité Mixte de Recherche du CNRS, de l' ENS et de l'UPMC No. 8552.

[1] J. M. Sampaio, T. I. Madeira, J. P. Marques, F. Parente, A. M. Costa, P. Indelicato, J. P. Santos, M.-C. Lépy, and Y. Ménesguen, Phys. Rev. A **89**, 012512 (2014).

[2] W. Bambynek, B. Crasemann, R. W. Fink, H. U. Freund, H. Mark, C. D. Swift, R. E. Price, and P. V. Rao, Rev. Mod. Phys. **44**, 716 (1972).

[3] *Atomic Inner-Shell Processes*, edited by B. Crasemman (Academic Press, New York, 1975), Vol. I.

[4] *Atomic Inner-Shell Processes*, edited by B. Crasemman (Academic Press, New York, 1975), Vol. II.

[5] *Atomic Inner-Shell Physics*, edited by B. Crasemman (Plenum Press, New York, 1985).

[6] M. H. Chen, E. Laiman, B. Crasemann, M. Aoyagi, and H. Mark, Phys. Rev. A **19**, 2253 (1979).

[7] E. J. McGuire, Phys. Rev. A **2**, 273 (1970).

[8] V. O. Kostroun, M. H. Chen, and B. Crasemann, Phys. Rev. A **3**, 533 (1971).

[9] D. L. Walters and C. P. Bhalla, Phys. Rev. A **3**, 1919 (1971).

[10] O. Keski-Rahkonen and M. O. Krause, At. Data Nucl. Data Tables **14**, 139 (1974).

[11] J. Scofield, At. Data Nucl. Data Tables **14**, 121 (1974).

[12] H. R. Rosner and C. P. Bhalla, Z. Phys. **231**, 347 (1970).

[13] C. P. Bhalla and D. J. Ramsdale, Z. Phys. **239**, 95 (1970).

[14] C. P. Bhalla, H. R. Rosner, and D. J. Ramsdale, J. Phys. B **3**, 1232 (1970).

[15] B. Crasemann, M. H. Chen, and V. O. Kostroun, Phys. Rev. A **4**, 2161 (1971).

[16] E. J. McGuire, Phys. Rev. A **3**, 587 (1971).

[17] E. J. McGuire, in *Inner Shell Ionization Phenomena and Future Applications*, edited by R. W. Fink, S. T. Manson, J. M. Palms, and P. V. Rao (USAEC CONF-720404, Oak Ridge, Tennessee, 1973), p. 662.

[18] M. H. Chen, B. Crasemann, and V. O. Kostroun, Phys. Rev. A **4**, 1 (1971).

[19] L. I. Yin and I. Adler, Phys. Rev. A **7**, 897 (1973).

[20] E. J. McGuire, Phys. Rev. A **5**, 1043 (1972).

[21] E. J. McGuire, Phys. Rev. A **6**, 851 (1972).

[22] C. P. Bhalla, J. Phys. B **3**, 916 (1970).

[23] S. T. Manson and D. J. Kennedy, At. Data Nucl. Data Tables **14**, 111 (1974).

[24] L. I. Yin, I. Adler, T. Tsang, M. H. Chen, D. A. Ringers, and B. Crasemann, Phys. Rev. A **9**, 1070 (1974).

[25] M. O. Krause, J. Phys. Chem. Ref. Data **8**, 307 (1979).

[26] J. H. Scofield, Phys. Rev. A **9**, 1041 (1974).

[27] J. H. Scofield, Phys. Rev. A **10**, 1507 (1974).

[28] R. Anholt and J. O. Rasmussen, Phys. Rev. A **9**, 585 (1974).

[29] S. Puri, D. Mehta, B. Chand, N. Singh, and P. N. Trehan, X-Ray Spectrom. **22**, 358 (1993).

[30] J. H. Hubbell, P. N. trehan, N. Singh, B. Chand, D. Mehta, M. R. Garg, S. Singh, and S. Puri, J. Phys. Chem. Ref. Data **23**, 339 (1994).

[31] M. H. Chen, B. Crasemann, and K.-N. Huang, At. Data Nucl. Data Tables **19**, 97 (1977).

[32] J. Campbell and T. Papp, At. Data Nucl. Data Tables **77**, 1 (2001).

[33] J. H. Scofield, Phys. Rev. **179**, 9 (1969).

[34] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **21**, 436 (1980).

[35] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **24**, 177 (1981).

[36] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **21**, 449 (1980).

[37] M. H. Chen, B. Crasemann, and H. Mark, Phys. Rev. A **27**, 2989 (1983).

[38] M. Ohno, J. Phys. B **17**, 195 (1984).

[39] M. Ohno, Phys. Rev. B **29**, 3127 (1984).

[40] M. Ohno and G. Wendin, Phys. Rev. A **31**, 2318 (1985).

[41] J. L. Campbell, At. Data Nucl. Data Tables **85**, 291 (2003).

[42] X. Llovet, C. J. Powell, F. Salvat, and A. Jablonski, J. Phys. Chem. Ref. Data **43**, 013102 (2014).

[43] J. P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).

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

[45] P. Indelicato, J. Bieroń, and P. Jönsson, Theor. Chem. Acc. **129**, 495 (2011).

[46] J. P. Santos, J. P. Marques, F. Parente, E. Lindroth, P. Indelicato, and J. P. Desclaux, J. Phys. B **32**, 2089 (1999).

[47] J. P. Santos, J. P. Marques, F. Parente, P. Indelicato, and J. P. Desclaux, At. Data Nucl. Data Tables **76**, 49 (2000).

[48] C. Casteleiro, F. Parente, P. Indelicato, and P. Marques, Eur. Phys. J. D **56**, 1 (2010).

[49] J. M. Sampaio, F. Parente, P. Indelicato, and J. P. Marques, J. Phys. B **46**, 065001 (2013).

[50] J. Sampaio, F. Parente, P. Indelicato, and J. Marques, At. Data Nucl. Data Tables **100**, 1277 (2014).

[51] W. Johnson, *Atomic Structure Theory* (Springer, Berlin, 2007).

[52] P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955).

[53] G. Audi, A. Wapstra, and C. Thibault, Nucl. Phys. A **729**, 337 (2003).

[54] I. Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).

[55] P. J. Mohr and Y.-K. Kim, Phys. Rev. A **45**, 2727 (1992).

[56] P. J. Mohr, Phys. Rev. A **46**, 4421 (1992).

[57] P. Indelicato and P. J. Mohr, Phys. Rev. A **46**, 172 (1992).

[58] P. J. Mohr and G. Soff, Phys. Rev. Lett. **70**, 158 (1993).

[59] P. Indelicato, O. Gorceix, and J. P. Desclaux, J. Phys. B **20**, 651 (1987).

[60] P. Indelicato and E. Lindroth, Phys. Rev. A **46**, 2426 (1992).

[61] P. Indelicato and P. J. Mohr, Hyperfine Interact. **114**, 147 (1998).

[62] P. Indelicato, S. Boucard, and E. Lindroth, Eur. Phys. J. D **3**, 29 (1998).

[63] R. D. Deslattes, E. G. Kessler, P. Indelicato, L. de Billy, E. Lindroth, and J. Anton, Rev. Mod. Phys. **75**, 35 (2003).

[64] T. Mooney, E. Lindroth, P. Indelicato, E. G. Kessler, and R. D. Deslattes, Phys. Rev. A **45**, 1531 (1992).

[65] W. Jitschin, R. Stötzel, T. Papp, M. Sarkar, and G. D. Doolen, Phys. Rev. A **52**, 977 (1995).

[66] A. Langenberg and J. van Eck, J. Phys. B **9**, 2421 (1976).

[67] H. Tawara, K. Harrison, and F. J. D. Heer, Physica **63**, 351 (1973).

[68] V. Gehrling, J. W. Hammer, and K. W. Hoffmann, Z. Phys. **246**, 376 (1971).

[69] M. Hribar, A. Kodre, and J. Pahor, Z. Phys. A **280**, 227 (1977).