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Overview and calculation of X-ray K-shell transition yields for comprehensive data libraries

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The simulation of atomic relaxation relies on data libraries with tabulated partial fluorescence yield values of radiative transitions, commonly derived from the Evaluated Atomic Data Library (EADL). However, recent studies support that the data library EADL could be improved by adopting Scofield's Hartree-Fock calculations instead of current Scofield's Hartree-Slater calculations. This work presents a bibliography overview of relevant atomic parameter values in order to verify the partial fluorescence yields presented in EADL. The references include libraries and articles, in which the atomic parameter values were theoretically calculated, experimentally measured, or obtained with semi-empirical and empirical fitting formulas. We present a comparison of total K-shell fluorescence yields and partial K-L_2, K-L_3, K-M_2, K-M_3 fluorescence yields that are either obtained directly from its references, or are derived from atomic parameters presented in these references. Additionally, we obtain comprehensive partial fluorescence yield values from the combination of semi-empirical and empirical fitting functions from different references. The comparisons performed in this work confirm that total K-shell, partial K-L_2, and partial K-L_3 fluorescence yield values, obtained from Scofield's Dirac-Slater calculations have better agreement with the most recent empirical values. Partial K-M_2, and partial K-M_3 fluorescence yield values obtained from Scofield's Dirac-Fock calculation have better agreement with the most recent empirical values. Therefore, further studies should be performed before changing the EADL data library.

1 | INTRODUCTION

Several references can be found in literature containing values related to atomic transitions, such as: transition rates (also commonly referred as transition probability per time unit, or transition probability), ratios of emission rates (where the values may be the ratio of single or several transitions), shell fluorescence yields, fluorescence

widths, Auger yields, Auger widths, etc. These values were obtained through experimental measurements, theoretical calculations, or semi-empirical fittings to the available data. Although total shell fluorescence yield and partial fluorescence yield values can generally be derived from these data, there is no comparison of comprehensive libraries with partial fluorescence yield values in the literature, possibly due to the different nomenclatures used in the literature.

Many codes and software of elemental analysis and Monte Carlo simulation of atomic relaxation (softwares based on the AXIL package,[1,2] PENELOPE,[3–5] PyMCA,[6] among many others) rely on the data available in literature regarding atomic relaxation, such as transition probabilities, fluorescence yields, partial fluorescence yields and radiationless transition yields. The accuracy of these codes and softwares are strongly related to the accuracy of the data used.

GEometry ANd Tracking (Geant4) toolkit[7,8] is widely employed for the simulation of the passage of the interaction of particles with matter. It includes a variety of packages for the simulation of the electromagnetic interactions of particles with matter using Monte Carlo methods. The Geant4 Low Energy Electromagnetic package[9,10] handles physics in energy ranges that extend down to 100 eV, with a detailed description of particle interaction by taking into account the atomic structure of matter.[11] To extend the use of the Geant4 to the simulation of experiments regarding X-ray, or Auger emission, the Low Energy Electromagnetic package incorporates a cascade model that handles atomic relaxation.[11] In the simulation of the atomic relaxation cascade, secondary photons or electrons are generated through radiative and radiationless transitions. The selection of the transitions is based on the respective partial transition yields and the energy of the emitted particles is calculated taking into account the atomic electron's binding energies. The transition yields and binding energies are tabulated in Geant4's library G4EMLOW and the values are derived from the Evaluated Atomic Data Library (EADL).[12]

Several studies from Pia *et al.*[13–15] present comparisons between partial fluorescence yield values of the radiative transitions from EADL tabulations with the values obtained from different references, namely Scofield's Dirac-Hartree-Slater calculations,[16,17] Scofield's Dirac-Hartree-Fock calculations,[18,19] and experimental values obtained from Salem *et al.* fit to experimental data.[20] The result of these evaluations highlight that the radiative transition partial fluorescence yields obtained from Scofield's Dirac-Hartree-Fock calculations are globally in better agreement with the experimental values than the ones obtained using Scofield's Dirac-Hartree-Slater calculations. Pia *et al.* concluded[15] that EADL library do not provide the state-of-the-art radiative transition partial fluorescence yield values. Since Geant4 uses data from EADL, its revision would improve the accuracy of its simulation whenever processes with X-ray fluorescence are essential. These studies from Pia *et al.*[13–15] present a very complete comparison with detailed description of how the partial fluorescence yield values are derived for the different transitions. However, the partial fluorescence yields in these comparisons were normalized without taking into account the radiationless (or Auger) transition probabilities of the respective shell. These radiationless probabilities must be included because the partial transition yields presented in EADL library are normalized with these probabilities. Furthermore, codes and software where the simulation of radiationless transitions is relevant, use partial fluorescence yield values normalized taking into account the radiationless transitions. For these reasons, a comparison of comprehensive values of partial fluorescence yields obtained from different references is of significant importance for the context of improving data libraries. Such comparison can also complement the studies of Pia *et al.*[13–15]

We thus present an overview of the existing references that contain comprehensive values related to atomic transitions. Furthermore, we calculate and compare K-shell fluorescence yield, and partial fluorescence yield values using the data presented in those references.

2 | THEORETICAL BACKGROUND

An atom in an excited atomic state may decay to a lower energy level through spontaneous emission. In this process, an atomic electron spontaneously transits from an energy level E_2 to a lower energy level E_1. The probability A of this spontaneous transition has units of s^{-1}. This quantity is also usually designated as "transition rate" or just "transition probability per unit of time". To avoid terminology confusion, we will refer to this quantity as "transition probability". Since the energy width Γ and the mean life τ of the excited atomic state are related through Heisenberg uncertainty principle $\Gamma \times \tau = \hbar$, the transition probability of the state is therefore given as $A = 1/\tau = \Gamma/\hbar$.[21] The system may transit from an excited state to lower energy states through a radiative transition, or radiationless transition. In both cases a vacancy in an atomic shell is filled by an atomic electron coming from a higher energy shell or subshell. While in radiative transitions this results in the emission of an X-ray photon, in radiationless transitions, another atomic electron of an higher energy shell or subshell is emitted instead. If the electron filling the vacancy comes from a higher shell, the radiationless transition is commonly denominated as Auger transition, and the emmited electron is the Auger electron. Specific cases of radiationless transitions include the Coster-Kronig transition, in which the electron transition is intra-shell, and

super Coster-Kronig transition, where, in addition to the previous case, the Auger electron is emitted from the same shell.

For an atomic state with an initial hole in the *i* sub-shell, the total radiative width $\Gamma_i^{(\mathrm{TR})}$ is the energy width associated with all radiative transitions, and the total radiationless width $\Gamma_i^{(\mathrm{TA})}$ is the energy width associated with all radiationless transitions (including Auger, Coster-Kronig, and super Coster-Kronig transitions). The total state width is given as: $\Gamma_i^{(\mathrm{T})} = \Gamma_i^{(\mathrm{TR})} + \Gamma_i^{(\mathrm{TA})}$. Likewise, the total transition probability of the state is given as $A_i^{(\mathrm{T})} = A_i^{(\mathrm{TR})} + A_i^{(\mathrm{TA})}$, where $A_i^{(\mathrm{TR})}$ is the total radiative transition probability, and $A_i^{(\mathrm{TA})}$ is the total radiationless transition probability. Both $A_i^{(\mathrm{TR})}$ and $A_i^{(\mathrm{TA})}$ are given as,

$$A_i^{(\mathrm{TR})} = \sum_{j(>i)} A_{ij}^{(\mathrm{R})}, \tag{1a}$$

$$A_i^{(\mathrm{TA})} = \sum_{j(>i)} \sum_{k(\geq j)} A_{\mathrm{ijk}}^{(\mathrm{A})}, \tag{1b}$$

where $A_{ij}^{(\mathrm{R})}$ is the transition probability of the radiative transition where the hole in *i* sub-shell is filled with an electron from the *j* sub-shell, and $A_{ijk}^{(\mathrm{A})}$ is the transition probability of the radiationless transition where the hole in *i* sub-shell is filled with an electron from the *j* and an Auger electron is emitted from the *k* sub-shell. The fluorescence yield of an atomic state, ω, is the probability that it deexcites through radiative transition. For an atomic state with a hole in the *i* sub-shell it is given by:

$$\omega_i = \frac{\Gamma_i^{(\mathrm{TR})}}{\Gamma_i^{(\mathrm{T})}} = \frac{\Gamma_i^{(\mathrm{TR})}}{\Gamma_i^{(\mathrm{TR})} + \Gamma_i^{(\mathrm{TA})}}. \tag{2}$$

or,

$$\omega_i = \frac{A_i^{(\mathrm{TR})}}{A_i^{(\mathrm{T})}} = \frac{A_i^{(\mathrm{TR})}}{A_i^{(\mathrm{TR})} + A_i^{(\mathrm{TA})}} = \frac{\sum_{j(>i)} A_{ij}^{(\mathrm{R})}}{\sum_{j(>i)} A_{ij}^{(\mathrm{R})} + \sum_{j(>i)} \sum_{k(\geq j)} A_{\mathrm{ijk}}^{(\mathrm{A})}}. \tag{3}$$

The partial fluorescence yield of a specific radiative transition (or set of transitions) can be calculated in a similar way. The partial radiative transition fluorescence yield ω_{ij} of a the transition *ij*, in which the hole in a *i* sub-shell is filled with an electron from the *j* sub-shell, with respective transition probability $A_{ij}^{(\mathrm{R})}$, is written as:

$$\omega_{ij} = \frac{A_{ij}^{(\mathrm{R})}}{A_i^{(\mathrm{T})}} = \frac{A_{ij}^{(\mathrm{R})}}{A_i^{(\mathrm{TR})} + A_i^{(\mathrm{TA})}} = \frac{A_{ij}^{(\mathrm{R})}}{\sum_{j(>i)} A_{ij}^{(\mathrm{R})} + \sum_{j(>i)} \sum_{k(\geq j)} A_{\mathrm{ijk}}^{(\mathrm{A})}}, \tag{4}$$

representing the probability that the atom will deexcite through the specific transition *ij* instead of all other possible radiative and radiationless transitions. As expected, for any excited state, the sum of all partial radiative transition fluorescence yields equals the fluorescence yield of the shell:

$$\sum_j \omega_{ij} = \omega_i. \tag{5}$$

Frequently, in literature,[13–15] the radiationless transition rates $A_{\mathrm{ijk}}^{(\mathrm{A})}$ are not included in Equation (4), as it was previously mentioned. The values calculated in this way have varying designations among the literature.

In Pia *et al.* work[13–15] the designation "transition probability" was used. In the present work we use the designation "partial fluorescence yield (normalized without accounting radiationless transitions)" and use the symbol "$\omega_{ij}^{(\mathrm{NA})}$" (where NA stands for "No Auger") to represent it. Thus, the radiative transition partial fluorescence yield (normalized without accounting radiationless transitions) "$\omega_t^{(\mathrm{NA})}$", for the radiative transition *ij*, is given as:

$$\omega_{ij}^{(\mathrm{NA})} = \frac{A_{ij}^{(\mathrm{R})}}{A_i^{(\mathrm{TR})}} = \frac{A_{ij}^{(\mathrm{R})}}{\sum_{j(>i)} A_{ij}^{(\mathrm{R})}}, \tag{6}$$

representing the probability that the atom will deexcite through a specific radiative transition *ij* instead of all other possible radiative transitions. The sum of all partial fluorescence yields (normalized without accounting radiationless transitions) is unity:

$$\sum_j \omega_{ij}^{(\mathrm{NA})} = 1. \tag{7}$$

For any radiative transition *ij*, the respective partial fluorescence yield ω_{ij}, and the respective partial fluorescence yield (normalized without accounting radiationless transitions) $\omega_{ij}^{(\mathrm{NA})}$, follow the relation:

$$\omega_{ij} = \omega_i \times \omega_{ij}^{(\mathrm{NA})}, \tag{8}$$

where ω_i is the fluorescence yield of the respective sub-shell.

Usually in literature, the fluorescence yield of a shell is defined in a way related to its experimental measurement. The fluorescence yield for the K shell is defined by the ratio: $w_{\mathrm{K}} = I_{\mathrm{K}}/n_{\mathrm{K}}$, where I_{K} is the average number of characteristic K- shell X-rays emitted from the sample as result of radiative transition to fill the n_{K} number of primary K-shell vacancies created in the sample. The definition of fluorescence yield for higher atomic shells is more complicated since vacancies can now be distributed in different subshells. In these cases an average or mean fluorescence yield $\bar{w}$ is defined, the relative numbers of primary vacancies in each subshell must be taken into account. Bambynek *et al.*[22] proposed an unambiguous definition of the average fluorescence yield $\bar{w}_{\ \mathrm{i}}$ for an i shell expressed as a linear combination of the relative numbers of primary vacancies in the subshells. The quantities presented in this section have various designations in literature. In fact, the

various references that are presented in Section 3 often use different designations and symbols than the ones used in the present work. To help readability, in Tables 1, 2 and 3, we compare the different designations and symbols used in the present work, with the ones used in the references presented in Section 3. To simplify, the variable subscripts corresponding to the shells and sub-shells are omitted. Also to simplify, the transition probability A, presented in the first column of Table 1, can refer to either the transition probability $A_{ij}^{(\mathrm{R})}$ of a radiative transition ij, or the transition probability $A_{ijk}^{(\mathrm{A})}$ of a radaitionless transition ijk (both quantities are presented in Equation (1)). We choose to make this simplification because most of the works that are listed in Table 1 do not use different symbols or nomenclature to differ a single radiative transition probability from a single radiationless transition probability.

2.1 | Atomic structure calculations

Before we present the atomic parameters from different works, it is worthwhile to present the basic description of the calculation of such parameters. All state of the art atomic structure calculations aim to solve the multi-electronic atomic Hamiltonian, where the the electron-electron interactions must be taken into account. The relativistic Hamiltonian for N-electron atomic systems can be written by:

$$H = \sum_{i=1}^{N} H_{\mathrm{D}}(\boldsymbol{r}_i) + \sum_{i<j=1}^{N} G(i,j), \tag{9}$$

where $G(i,j)$ is the operator for the relativist interaction between the electron i and the electron j, and $H_{\mathrm{D}}(\boldsymbol{r}_i)$ is the one-electron Dirac's Hamiltonian. $H_{\mathrm{D}}(\boldsymbol{r}_i)$ is given as:

$$H_{\mathrm{D}} = mc^2\beta + c\alpha.\boldsymbol{p} + V(r), \tag{10}$$

where r is the electron position, m the electron rest mass, $\boldsymbol{p}$ the momentum operator, $\boldsymbol{\alpha}$ e β the Dirac matrices and $V(r)$ the nuclear potencial. The operator G partially accounts for the relativist interaction between electrons, and it is written as:

$$G(i,j) = \frac{1}{r_{ij}} + \frac{1}{2r_{ij}}\left[\alpha_1 \cdot \alpha_2 \frac{(\alpha_1 \cdot \boldsymbol{r}_{ij})(\alpha_2 \cdot \boldsymbol{r}_{ij})}{r_{ij}^2}\right] \tag{11}$$

where the first term accounts for the Coulomb interaction, the second term (the Breit term) accounts for magnetic interaction and retardation, and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. In non-relativist methods, operator G only includes the Coulomb interaction term. Hartree-Slater and Hartree-Fock (or Hartree-Slater-Fock) methods were frequently used to achieve the solution of the potential, the energy, and the wave functions of multi-electronic systems using the variational principal to the expected value of the Hamiltonian. Nowadays, these methods have widely been replaced by their relativist versions, the Dirac-Hartree-Slater (often named Dirac-Slater) method, and the Dirac-Hartree-Fock (often named Dirac-Fock)

TABLE 1 Definitions and symbols (from Equations (1) to (8)) of atomic quantities of present work and different references

Present work	"Transition Probability" A	"Total radiative transition probability" $A^{(\mathrm{TR})}$	"Total radiative width" $\Gamma^{(\mathrm{R})}$	"Total radiationless transition probability" $A^{(\mathrm{TA})}$
Kostroun et al.[23]	"transition probability", "transition rate" w	-	"radiative width" Γ_{R}	-
Scofield[16,18,19]	"transition rate", "decay rate", "emission rate" Γ	"total radiative decay rate"	-	-
Chen *et al.*[24,25]	"transition rate" T	-	"radiative width" "radiative width"	-
EADL[12]	"transition rate"	-	Γ_{r}	-
Xraylib[26]	"emission rate"	-	-	-
Pia *et al.*[13–15]	"emission rate"	-	-	-
Bambinek *et al.*[21]	"transition probability", "transition probability per unit time", "rate of emission", "decay probability" w	"total radiative transition probability", "total radiative decay rate", "radiative decay probability"	"radiative width" Γ_{A}	"Auger decay probability" + "Coster-Kronig decay probability"
Salem *et al.*[20]	"transition rate"	-	-	-
Hubbell *et al.*[27]	"transition rate"	-	-	-

TABLE 2 Continuation of Table I

Present work	**"Total radiationless width"** $\Gamma^{(A)}$	**"Total transition probability"** $A^{(T)}$	**"Total state width"** $\Gamma^{(T)}$
	"total radiationless width",		"total level width"
Kostroun *et al.*[23]	"total Auger width", "Auger width" Γ_A	"total transition probability"	Γ
Scofield[16,18,19]	-	"total decay rate"	-
Chen *et al.*[24,25]	"Auger width" Γ_A	-	"total atomic width" Γ
EADL library[12]	"nonradiative width" Γ_{nr}	-	"total width" Γ_t
Xraylib[26]	-	-	"atomic level width"
Pia *et al.*[13–15]	-	-	-
Bambinek *et al.*[21]	"radiatiationless width", "total Auger width total Coster-Kronig width" $\Gamma_A + \Gamma_{CK^*}$	"decay probability of a state"	"total width", "atomic state energy width" Γ

TABLE 3 Continuation of Table II

Present work	**"fluorescence yield"** ω	**"partial fluorescence yield (normalized without accounting radiationless transitions)"** $\omega^{(NA)}$	**partial fluorescence yield** ω
Kostroun *et al.*[23]	"fluorescence yield" ω	-	-
Scofield[16,18,19]	fluorescence yield" ω	-	-
Chen*et al.*[24,25]	"fluorescence yield" ω	-	-
EADL[12]	"fluorescence yield" ω	-	transition probability
Xraylib[26]	"fluorescence yield" ω	"radiative transition probability"	-
Pia *et al.*[13–15]	-	"radiative transition probability"	-
Bambinek *et al.*[21]	"fluorescence yield" ω	-	-
Hubbell *et al.*[27]	"fluorescence yield" ω	-	-
NIST database[28]	"fluorescence yield"	"relative intensity"	-
Kahoul *et al.*[29]	"fluorescence yield" ω	"transition probability"	-
Daoudi *et al.*[30]	"fluorescence yield" ω	-	-

method. In the Hartree-Slater, and Dirac-Hartree-Slater methods, it is considered that each electron is affected by an average field created by all other electrons, while in Hartree-Fock and Dirac-Hartree-Fock methods the average field is represented by the direct and exchange operators, J_D and K_{ex}, such that the average potential is given as:

$$V_{HF}(r) = V_D(r) + V_{ex}(r), \tag{12}$$

where V_D is the direct potential, due to the electron repulsion, and V_{ex} is the exchange potential, which accounts for the exchange of two electrons, due to the anti-symmetrization of the electron wave-functions. With this inclusion, Hartree-Fock accounts for more of the electron-electron interaction than the Hartree-Slater methods, and have generally been shown to be more accurate. Even so, the Hartree-Fock (and Dirac-Hartree-Fock) approaches do not fully describe the Coulomb repulsion between electrons. To obtain high precision results the electronic correlation needs to fully be taken into account, by using methods such as the Multiconfiguration Dirac-Fock, in which the electronic correlation is included by writing the wave function of the atomic system ψ as a linear combination of configuration wave functions φ, which are wave functions for different possible configuration states: $\psi(1, 2, \ldots, N) = \sum_i a_i \varphi_i$, where a_i are mixing

coefficients. This method follow a similar procedure as the Hartree-Fock method. The multiconfiguration Dirac-Fock method is described in detail in other works.[31–34]

3 | OVERVIEW OF THE VALUES FROM DIFFERENT WORKS

We present references containing K-shell fluorescence yields, transition probabilities, partial fluorescence yields, or other atomic parameters, from which K-shell fluorescence yield values ω_K and partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$ and, $\omega_{K\text{-}M_3}$ can be obtained, whether they are libraries, articles, product of theoretical calculations, experimental measurements or the result of combined theoretical and experimental values. Although a huge number of theoretical calculations and experimental results can be found in literature, we selected and described the ones from which comprehensive values can be obtained for large range of transitions and large range of atomic number, which are the ones relevant to the comparisons made in the present work.

The nomenclature of the atomic parameters in the references presented in this section may differ from the nomenclature in the present work. Throughout this section we refer to each quantity using the designations of the present work. The designations used in the original references are presented in Tables 1, 2 and 3.

3.1 | Combination of Kostroun *et al.* Hartree-Slater radiationless transition probability calculations and Scofield's Dirac-Slater radiative transition probability calculations

In 1971, Kostroun *et al.*[23] calculated nonrelativistic K-shell radiationless transition probabilities for selected elements using the Hartree-Slater method (using the non-relativist versions of Equations (9), (10) and (11). In order to derive theoretical total K-shell fluorescence yields, Kostroun *et al.*[23] combined their results with Scofield's earlier Dirac-Slater radiative transition probabilities,[16] which were calculated without considering the finite extent of the nuclear charge distribution. In Kostroun *et al.* work, calculations where only performed for selected elements, the values for the remaining elements where obtained through fits.

In the present work, we present the K-shell fluorescence yield values ω_K extracted directly from Kostroun *et al.* work. These values are compared with values from other works in Section 4, and presented in Table A1 (Section VII). Throughout this work we refer to these values as "Kostroun".

3.2 | Scofield's radiative transition probability calculations based on the Dirac-Slater method

In 1969, using relativistic Hartree-Slater theory, or Dirac-Slater theory (as presented in Section 2.A), Scofield calculated K- and L-shell radiative transition probabilities[16] for selected transitions, and selected elements in the range $13 < Z < 92$. In these calculations, the electrons were treated relativistically and the effect of retardation was included (the second term of operator G from Equation (9)). The electrons were considered as moving independently with their mutual interactions accounted for by a central potential (thus not including the exchange potential from Equation (11)). All multipoles of the radiation field and all transitions from occupied states of the atom were included. Scofield presents the radiative transition probabilities calculated using this model for K- and L-shell transitions.[16] As mentioned in Section 3.A, the calculations in this work did not considered the finite extent of the nuclear charge distribution.

In 1974, Scofield presented K- and L-shell radiative transition probabilities calculated using an improved model, by including nuclear charge distribution of finite extent.[17] In this later work, it is presented values for elements with atomic number ranging $5 \leq Z \leq 104$ and for all possible radiative transitions.

3.3 | Scofield's radiative transition probability calculations based on the Dirac-Fock method

Using relativistic Hartree-Fock theory, or Dirac-Fock theory (as presented in Section 2.A), Scofield calculated K- and L-shell radiative transition probabilities. In Scofield's work, the exchange potential V_{ex} was included (as in Equation (12)). In his work, the values for K-shell are presented for selected transitions, and for selected elements with atomic number ranging $10 \leq Z \leq 98$.[18] The values for L-shell radiative transition probabilities are presented for selected elements with atomic number ranging $18 \leq Z \leq 94$.[19] In other works,[35] it is presented L-shell radiative transition probabilities for more selected elements, which were obtained by interpolation of the probabilities calculated by Scofield.

3.4 | Chen *et al.* radiationless transition probability calculations based on the Dirac-Fock method

Chen *et al.* theoretical approach consists on calculating the radiationless transition probabilities from relativistic perturbation theory, for frozen orbitals, in the Dirac-Hartree-Fock (or Dirac-Fock) approach (thus

including the exchange potential in Equation (12)). Using this approach, Chen *et al.* present calculated radiationless transition probabilities for K- and L-shell, for selected elements with atomic number in the range $18 \leq Z \leq 96$.[24] In a later work, Chen *et al* present radiationless K-shell atomic level widths[25] and present radiationless L-shell atomic level widths.[36,37] for selected elements.

3.5 | EADL

The EADL library[12] contains partial fluorescence yield and radiationless transition yield values, which the Geant4 includes in its library. The radiative transition partial transition yield values are based on Scofield's theoretical approaches[16,17] (which were presented in Section 3.A and Section 3.B) and the radiationless transition yield values are based on Chen's theoretical approaches[24,25,36–38] (which were presented in Section 3.D) complemented by Hubbel's corrections[12] to avoid the over-prediction of the strength of Coster-Kronig transitions resulting from Dirac-Hartree-Slater calculations. The 2014 version of EADL can be found online[39] Recent changes have been performed to EADL library, regarding the binding energy values.

In the present work, we present K-shell partial fluorescence yield values $\omega_{\text{K-L}_2}$, $\omega_{\text{K-L}_3}$, $\omega_{\text{K-M}_2}$, $\omega_{\text{K-M}_3}$, extracted directly from the EADL library.[12] We also present K-shell fluorescence yield values ω_{K} obtained by summing over all radiative transition fluorescence yields, as in Equation (5). These values are compared with values from other works in Section 4, and presented in Section VII (in Tables A1 to A5). Throughout this work we refer to these values as "EADL".

3.6 | Salem *et al.* experimental K- and L-shell X-ray transition ratios

Salem *et al.* compiled selected experimental data for K- and L-shell transition rates, and through least-squares fitting, generated most probable values of K- and L-shell X-ray radiative transition rate ratios.[20] From these ratios, partial fluorescence yield values (normalized without accounting radiationless transitions) $\omega_{ij}^{(\text{NA})}$ can be obtained, as was performed in Pia *et al.* works,[13–15] and in NIST's Fundamental Parameters Database.[28]

3.7 | Bambynek *et al* 1972 semi-empirical fittings to experimental data

In 1972, Bambynek *et al.*[22] fitted a collection of selected K-shell fluorescence yield experimental values, using a semi-empirical fitting formula. The formula and the fitting parameters are presented in Hubbell *et al.* comparisons of several compilations.[27]

We present Bambynek *et al.*[22] K-shell fluorescence yield values ω_{K}, which where extracted directly from Hubbell *et al.* work.[27] These values are compared with values from other works in Section 4, and presented in Section VII (Table A6).

Throughout the work, we refer to the values obtained in this subsection as "Bambynek1972".

3.8 | Krause's 1979 compilation

Krause generated a consistent set of values of K- and L-shell radiative and radiationless yields using the information available up to 1979 on several atomic parameters (fluorescence yields, auger yields, transitions probabilities, level withs, etc).[40] In Krause's work, all pertinent data available in literature, including experimental, theoretical and semi-empirical values, was compiled and evaluated in order to generate K- and L-shell radiative and radiationless yields.

We present the K-shell fluorescence yield ω_{K} values from Krause's compilation.[40] The values are extracted directly from Hubbell *et al.* comparisons of several compilations.[27] These values are compared with values from other works in Section 4, and presented in Section VII (Table A6).

Throughout the work, we refer to the values obtained in this subsection as "Krause1979".

3.9 | Bambynek *et al* 1984 semi-empirical fittings of experimental data

In 1984, Bambynek *et al.* presented a new evaluation[41] of K-shell fluorescence yield values by introducing about 100 new measurements to the Bambynek *et al.* 1972 work.[22] As such, new fitting parameters where obtained, and new fitted values. Hubbell *et al.* comparisons of several compilations[27] present Bambynek's new fitting parameters, new fitted values, and comparisons against Bambynek 1972[22] fitted values.

We present Bambynek *et al.* K-shell fluorescence yield values ω_{K}, which where extracted directly from Hubbell *et al.* comparisons of several compilations.[27] These values are compared with values from other works in Section 4, and presented in Section VII (Table A6).

Throughout the work, we refer to the values obtained in this subsection as "Bambynek1984".

3.10 | Hubbell *et al.* 1994 semi-empirical fittings of experimental data

In 1994, Hubbel *et al.* compiled the measured K-shell, L-shell, and higher atomic shell X-ray fluorescence yield data generated between the period 1978 - 1993.[27] From the compiled data K-, L- and M-shell fluorescence yields were produced by fitting the selected data (the selection

criteria and fitting procedure is explained in their work). They compared their fitted values with earlier fitted values and theoretical values. Hubbel *et al.* fits for K-shell fluorescence yields ω_K are presented in NIST Fundamental Parameters Database[28] even though an erratum[42] informs about extensive anomalies to their fitted values, and as such they advise that the values obtained from Bambynek's 1984 work[41] should be used instead, regarding K-shell fluorescence yield values.

3.11 | NIST Fundamental Parameters Database

Elam accomplished the compilation of a comprehensive database of atomic fundamental parameters relevant to X-ray spectroscopy,[28] which is available in the NIST's web-page. The radiative K-shell fluorescence yield ω_K, tabulated in the database were calculated from the fits to several experimental values by Hubbel *et al.*,[27] discussed in the previous subsection. The radiative L-shell fluorescence yield tabulated in the database are from Krause's revision to experimental and theoretical values[40] with modifications proposed by Jitschin.[43]

The database also presents partial fluorescence yield values (normalized without accounting radiationless transitions) $\omega^{(NA)}$ for K- and L-shell transitions that were calculated using the emission rate ratios presented by Salem *et al* work[20]; the fit process to the data is explained with detail in Elam *et al.*'s work.[28]

We present K-shell fluorescence yields values ω_K, extracted directly from the NIST Fundamental Parameters Database.[28] These values are compared with values from other works in Section 4, and presented in Section VII (Table A6). Throughout the work, the values obtained in this subsection are referred to as "NIST".

3.12 | Combination of Chen *et al.* Dirac Fock transition probabilities and Scofield's Dirac-Slater transition probabilities

In the present work, we calculated K-shell fluorescence yield values ω_K and K-shell partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$ and, $\omega_{K\text{-}M_3}$, using the same references as EADL, i.e. we use Scofield's more recent Dirac-Hartree-Slater calculations of radiative transitions probabilities[17] (which were presented in Section 3.B) and Chen's Dirac-Hartree-Fock calculations of radiationless transition probabilities (which were presented in Section 3.D).

Two different works from Chen *et al.*[24,25] (presented in Section 3.D) can be used to obtain the K-shell total radiationless transition probability $A_K^{(TA)}$. Chen *et al.* later work presents the K-shell total radiationless width $\Gamma_K^{(TA)}$, from which the K-shell total radiationless transition probability $A_K^{(TA)}$ can be derived. The total radiationless transition probability $A_K^{(TA)}$ calculated in Chen *et al* earlier work[24] differs from the calculated value in a later work.[25] Nevertheless, the K-shell fluorescence yield values calculated using the different references have deviations of less than 0.1%, and as such, both references are equivalent. We opted of using Chen *et al.* later work.[25]

Since Chen *et al.* present values for selected elements we derived the values for other elements through fits to the available data.

Thus, we calculate the K-shell fluorescence yields ω_K and radiative transition partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$ and, $\omega_{K\text{-}M_3}$ using Equation (3) and Equation (4), respectively, where the radiative transition probabilities $A_{Kj}^{(R)}$, and the total radiative transition probability $A_K^{(TR)}$ is obtained from Scofield's later Dirac-Slater work,[17] and where the total radiationless transition probability $A_K^{(TA)}$ is obtained from Chen *et al.* later Dirac-Fock work.[25] This combination with Scofield's transition probabilities to derive K-shell fluorescence yield values ω_K had already been performed in Chen *et al.* later work.[25] Unlike EADL, we don't include Hubbel's corrections[44] in any calculations since the procedure of how the EADL library applies these corrections is unclear.

The values obtained in this subsection are compared with values from other works in Section 4, and presented in Section VII (Tables A1 to A5).

Throughout the work, we refer to the values obtained in this subsection as "DF,DS", since they are a combination of Dirac-Fock and Dirac-Slater calculations.

3.13 | Combination of Chen *et al.* Dirac Fock transition probabilities and Scofield's Dirac-Fock transition probabilities

We calculate K-shell fluorescence yield values ω_K and K-shell partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$ and, $\omega_{K\text{-}M_3}$ from the combination of Scofield's radiative transitions Dirac-Hartree-Fock calculations[18] (presented in Section 3.C) and Chen *et al.* later radiationless transitions Dirac-Hartree-Fock calculations[25] (presented in Section 3.D). This combination of values is similar to the combination presented in Section 3.L, however, in this case, Scofield's Dirac-Fock values are used instead of Scofield's Dirac-Slater values, as suggested in Pia *et al.* works.

In Scofield's Dirac-Fock work,[18] it is presented radiative transition probabilities $A^{(R)}$ for a limited number of transitions, and limited number of elements, as well as total radiative transition probability $A^{(TR)}$. From this information, the partial fluorescence yields (normalized without accounting radiationless transitions) $\omega^{(NA)}$ can be obtained using Equation (6). As far as we know, the

xraylib database[26] uses this method, with the exception that the values had to be normalized to satisfy Equation (7). This method is limited to those transitions which are presented in Scofield's work. Pia *et al.* performed a different approach to obtain $\omega^{(NA)}$ values from Scofield's Dirac-Fock work.[18] Since Scofield's work also present radiative transition probability ratios, Pia *et al.* wrote equations to extract the $\omega^{(NA)}$ values from these ratios. Since no transition probability ratio relative to K-$L_{4,5}$ transitions is presented in Scofield's Dirac Fock work, Pia *et al.* made an approximation, by assuming that the K-$M_{4,5}$/K-M_2 Dirac-Fock ratio should be equal to the experimental K-$M_{4,5}$/K-M_2 ratio of Salem *et al.* work.[20] This approximation was justified by the fact that Scofield's Dirac-Slater K-$M_{4,5}$/K-M_2 probability ratio was in good agreement with the experimental ratio, and as such, the Dirac-Fock ratio, although not presented, should also be in good agreement. In the present work, we follow the method employed by Pia *et al.*, but with a different approximation. We found that Scofield's Dirac-Slater K-$M_{4,5}$/K-M_3 ratio was in better agreement with the experimental values, and thus assumed the Dirac-Fock K-$M_{4,5}$/K-M_3 ratio to be equal to the Dirac-Slater K-$M_{4,5}$/K-M_3 ratio. With this method, $\omega^{(NA)}$ values can be obtained for all possible radiative transitions. The method performed in the present work, and the method performed in the xraylib result in different $\omega^{(NA)}_{K\text{-}L_2}$, $\omega^{(NA)}_{K\text{-}L_3}$, $\omega^{(NA)}_{K\text{-}M_2}$, $\omega^{(NA)}_{K\text{-}M_3}$ values. In fact, regarding the $\omega^{(NA)}_{K\text{-}L_2}$, $\omega^{(NA)}_{K\text{-}L_3}$, $\omega^{(NA)}_{K\text{-}M_2}$, $\omega^{(NA)}_{K\text{-}M_3}$ values, the method in the present work (and the method performed in Pia *et al.* works[13–15]) produces values that are overall in slightly closer agreement with the experimental values from Salem *et al.* work[20] than the values obtained from the xraylib method.

We calculated the K-shell fluorescence yield ω_K using Equation (3), where the total radiationless transition probability $A^{(TA)}_K$ is from Chen *et al.* Dirac-Fock work[25] (presented in Section 3.D), and the total radiative transition probability $A^{(TR)}_K$ is from Scofield's Dirac-Fock work[18] (presented in Section 3.C).

The partial fluorescence yields $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$ are calculated from $\omega^{(NA)}_{K\text{-}L_2}$, $\omega^{(NA)}_{K\text{-}L_3}$, $\omega^{(NA)}_{K\text{-}M_2}$, $\omega^{(NA)}_{K\text{-}M_3}$, using Equation (8).

These values obtained on this subsection are compared with values from other works in Section 4, and presented in Section VII (in Tables A1 to A5). Throughout this work, we refer to these values as "DF", as they are a result of Dirac-Fock calculations.

3.14 | Multiconfiguration Dirac-Fock values

We present K-shell fluorescence yield values ω_K calculated using the Multiconfiguration Dirac-Fock method, for selected elements. The values were calculated by different authors.[45–49]

These values are compared with values from other works in Section 4, and presented in Section VII (Table A1). Throughout the present work we refer to these values as "MCDF".

3.15 | Kahoul *et al.* 2012 empirical fittings

In 2012, Kahoul *et al.*[29] compiled experimental data of the K-shell fluorescence yields from the period 1960-2011. From this data, they deduced empirical K-shell fluorescence yield values ω_K from polynomial fittings of the weighted-mean and unweighted-mean values of all the compiled data. The data was separated in three atomic number ranges, $11 \leq Z \leq 20$, $21 \leq Z \leq 50$ and $51 \leq Z \leq 99$, and a polynomial fitting was performed independently for each range.

In the present work, Kahoul *et al.* empirical K-shell fluorescence yield values ω_K, obtained from the Weighted-mean fitting, are presented. The values are extracted directly from Kahoul *et al.* work, and are compared with values from other works in Section 4, and presented in Section VII (Table A6). These values are referred to as "Kahoul2012", throughout the present work.

3.16 | Daoudi *et al.* 2015 empirical fittings

In 2015, Daoudi *et al.*[30] compiled experimental data of the K-shell fluorescence yield values up to the date, relying on existing compilations, and adding new data published in the period 2012-2015. This compilation included 737 experimental values, with atomic number range $3 \leq Z \leq 99$. The data was separated in three atomic number ranges, $11 \leq Z \leq 20$, $21 \leq Z \leq 50$ and $51 \leq Z \leq 99$, and an empiric polynomial fitting was performed independently for each range.

We present the K-shell fluorescence yield values ω_K obtained from Daoudi *et al.*[30] empirical fittings. The values are extracted directly from Daoudi *et al.* work,[30] and are compared with values from other works in Section 4, and presented in Section VII (Table A6). Throughout this work we refer to these values as "Daoudi2015".

3.17 | Combination of semi-empirical or empirical K-shell fluorescence yield values with Salem *et al.* values

From the references regarding semi-empirical or empirical fittings presented so far ("Bambynek1972[22]", "Krause1979[40]", "Bambynek1984[41]", "NIST[28]", "Kahoul2012[29]" and "Daoudi2015[30]"), semi-empirical and empirical values regarding K-shell fluorescence yield ω_K were obtained. In the present work, we calculate partial fluorescence yields $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$ for

each of these references using using Equation (8), where the partial fluorescence yield values (normalized without accounting radiationless transitions) $\omega^{(NA)}$ are those obtained from Salem *et al.* work,[20] which are tabulated in NIST Fundamental Parameters Database. As an example, to derive the K-L_2 partial fluorescence yield $\omega_{K\text{-}L_2}$ from Daoudi *et al.*'s K-shell fluorescence yield ω_K, we write:

$$\omega^{\text{Daoudi,Salem}}_{K\text{-}L_2}(Z) = \omega^{\text{Daoudi}}_{K}(Z) \times \omega^{(NA)\text{Salem}}_{K\text{-}L_2}(Z).$$

We use Salem *et al.* values because they are still up to date considered the most complete references of K- and L-shell experimental transition probability ratios, and their relevance is reinforced by the fact that they are used in the NIST Fundamental Parameters Database, and the fact they are used in Pia *et al.*'s comparisons.

Using this formalism, we present partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$, for each of the semi-empirical and empirical values.

These values are compared with values from other works in Section 4, and presented in Section VII (Tables A7 to A10). Throughout the present work we refer to these values as "Bambynek1972,Salem", "Krause1979,Salem", "Bambynek1984,Salem", "NIST,Salem", "Kahoul2012,Salem" and "Daoudi2015,Salem".

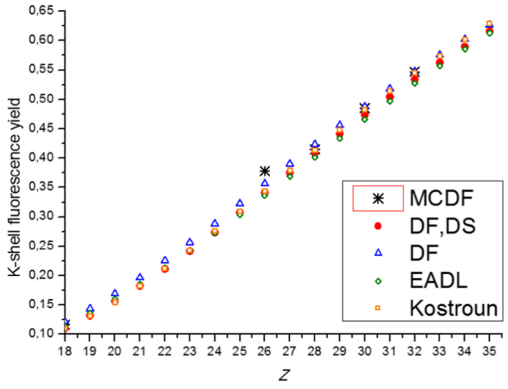
4 | COMPARISON OF VALUES FROM THE DIFFERENT WORKS

We present a comparison of the K-shell fluorescence yield values ω_K, and the K-shell partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$, that were obtained from the different references as explained in Section 3.

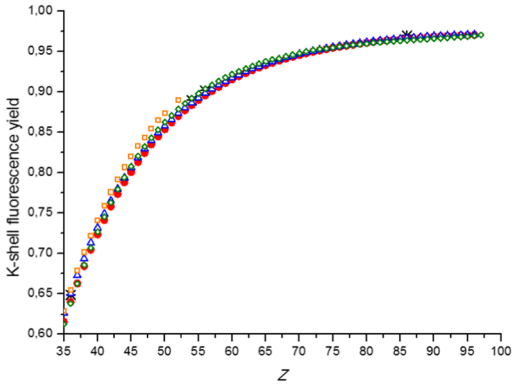
Regarding the K-shell fluorescence yield ω_K, five different theoretical values are presented: "Kostroun",[23] "EADL[12]", "DF,DS[17,25]", "DF[18,25]" and "MCDF[45–48]". Values from four semi-empirical fittings are presented regarding K-shell fluorescence yield ω_K: "Bambynek1972",[22] "Krause1979",[40] "Bambynek1984",[41] and "NIST".[28] The values from two empirical fittings are presented: "Kahoul2012"[29] and "Daoudi2015".[30]

In what concerns the theoretical partial fluorescence yield values $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$, we present the theoretical values "EADL[12]", "DF,DS[17,25]" and "DF[18,25]", we do not present values from Kostroun work[23] since they are calculated non-relativistically. As to semi-empirical and empirical values, as explained in Section 3.Q we present the semi-empirical values: "Bambynek1972,Salem",[20,22] "Krause1979,Salem",[20,40] "Bambynek1984,Salem"[20,41] and "NIST,Salem",[20,28] and the empirical values: "Kahoul2012,Salem"[20,29] and "Daoudi2015,Salem".[20,30]

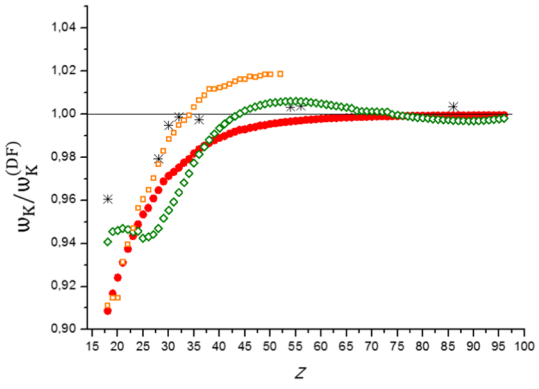
We also present the relative difference between values from different references. For an element with atomic



(a) Theoretical K-shell fluorescence yield values ($18 \leq Z \leq 35$)

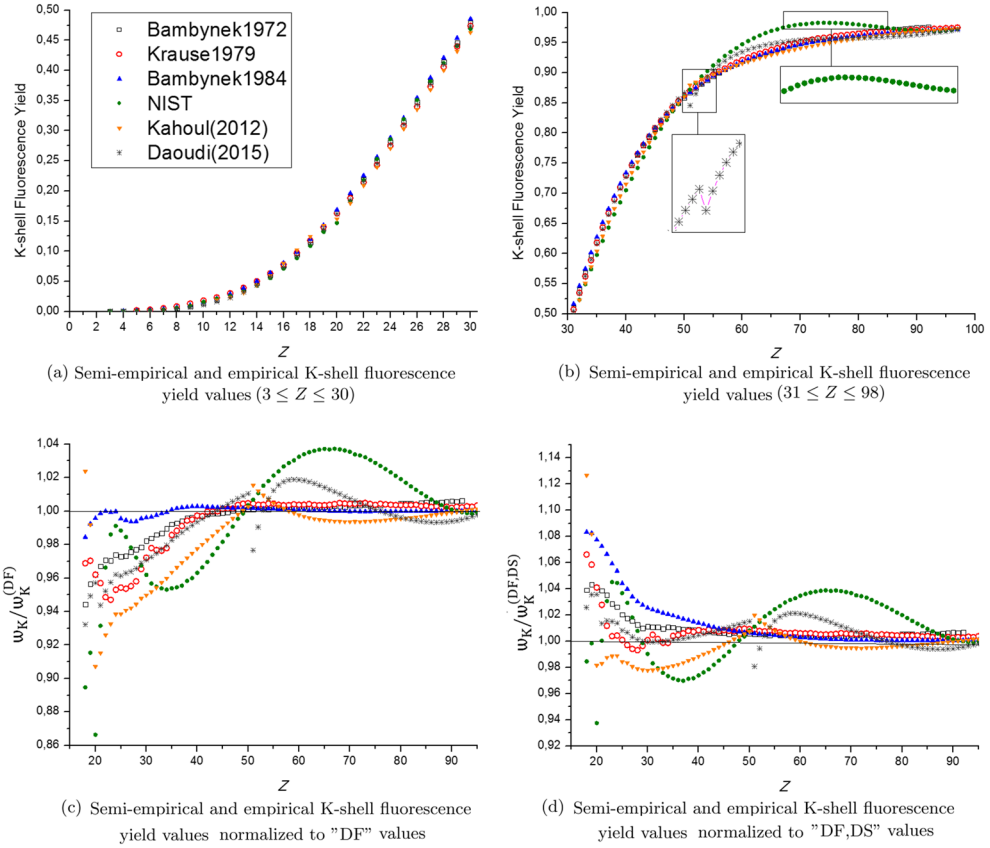


(b) Theoretical K-shell fluorescence yield values ($35 \leq Z \leq 96$)



(c) Theoretical K-shell fluorescence yield values normalized to "DF" values

FIGURE 1 Kostroun: values obtained from the combination of Kostroun *et al.* calculations[23] and Scofield's radiative Dirac-Slater calculations.[16] "DF,DS": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Slater calculations.[17] "DF": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Fock calculations.[18] "EADL": values obtained from the Evaluated Atomic Data Library.[12]



(a) Semi-empirical and empirical K-shell fluorescence yield values ($3 \leq Z \leq 30$)

(b) Semi-empirical and empirical K-shell fluorescence yield values ($31 \leq Z \leq 98$)

(c) Semi-empirical and empirical K-shell fluorescence yield values normalized to "DF" values

(d) Semi-empirical and empirical K-shell fluorescence yield values normalized to "DF,DS" values

FIGURE 2 "Bambynek1972": Values from Bambynek *et al.* earlier semi-empirical fit.[22] "Krause1979": values from Krause's semi-empirical fit.[40] "Bambynek1984": values from Bambynek *et al.* later semi-empirical fit.[41] "NIST": semi-empirical fit values presented in NIST's Fundamental Parameters Database.[28] "Kahoul": values from Kahoul *et al.* empirical fit.[29] "Daoudi": values from Daoudi *et al.* empirical fit.[30]

number Z, and a radiative transition ij, the relative difference of the partial fluorescence yield from reference 1 and reference 2 is given as:

$$\Delta\omega_{ij}^{\text{ref1,ref2}}(Z) = \frac{\left(\omega_{ij}^{\text{ref1}}(Z) - \omega_{ij}^{\text{ref2}}(Z)\right) \times 100\%}{\frac{\omega_{ij}^{\text{ref1}}(Z)+\omega_{ij}^{\text{ref2}}(Z)}{2}}. \quad (13)$$

And the average relative difference is given by averaging the absolute value of the relative difference for all elements available in both references:

$$\Delta\omega_{ij}^{\text{ref1,ref2}} = \frac{\sum_Z \left|\Delta\omega_{ij}^{\text{ref1,ref2}}(Z)\right|}{N}, \quad (14)$$

where N is the number of elements.

4.1 | K-shell Fluorescence Yield Comparison

4.1.1 | Theoretical K-shell fluorescence yield values

The K-shell fluorescence yield theoretical values are presented in Figure 1a,b (the values are divided in two atomic ranges to better visualization), and in Section VII (Table A1). The same theoretical K-shell fluorescence yield values are normalized to their corresponding "DF" values and presented in Figure 1c.

From the comparisons in Figure 1a,b it is highlighted that the K-shell fluorescence yield values increase monotonically with increasing atomic number for all theoretical references. While "Kostroun" values are in relatively good agreement with "DF,DS" values for low atomic numbers, their disagreement increases as atomic number increases. The "EADL" values are in good agreement with "DF,DS" values, which is to be expected since they are calculated using the transition probabilities from the same references (with the excetion that the EADL library introduces a correction that we did not introduce in "DF,DS" calculations). "DF,DS" and "DF" values are obtained using the same reference for radiationless transition probabilities, but using different references from Scofield regarding the radiative transitions probabilities. Scofield's radiative transition probabilities calculated using the Dirac-Fock method are overall higher than those calculated using the

TABLE 4 K-shell fluorescence yield average relative difference

$\Delta\omega_K(\%)$	DS,DF	DF
Bambynek 1972	0.93245	0.85845
Krause 1979	0.74575	1.1053
Bambynek1984	1.30666	0.15352
NIST	2.10472	2.7279
Kahoul 2012	1.02286	1.80249
Daoudi 2015	0.88204	1.47661

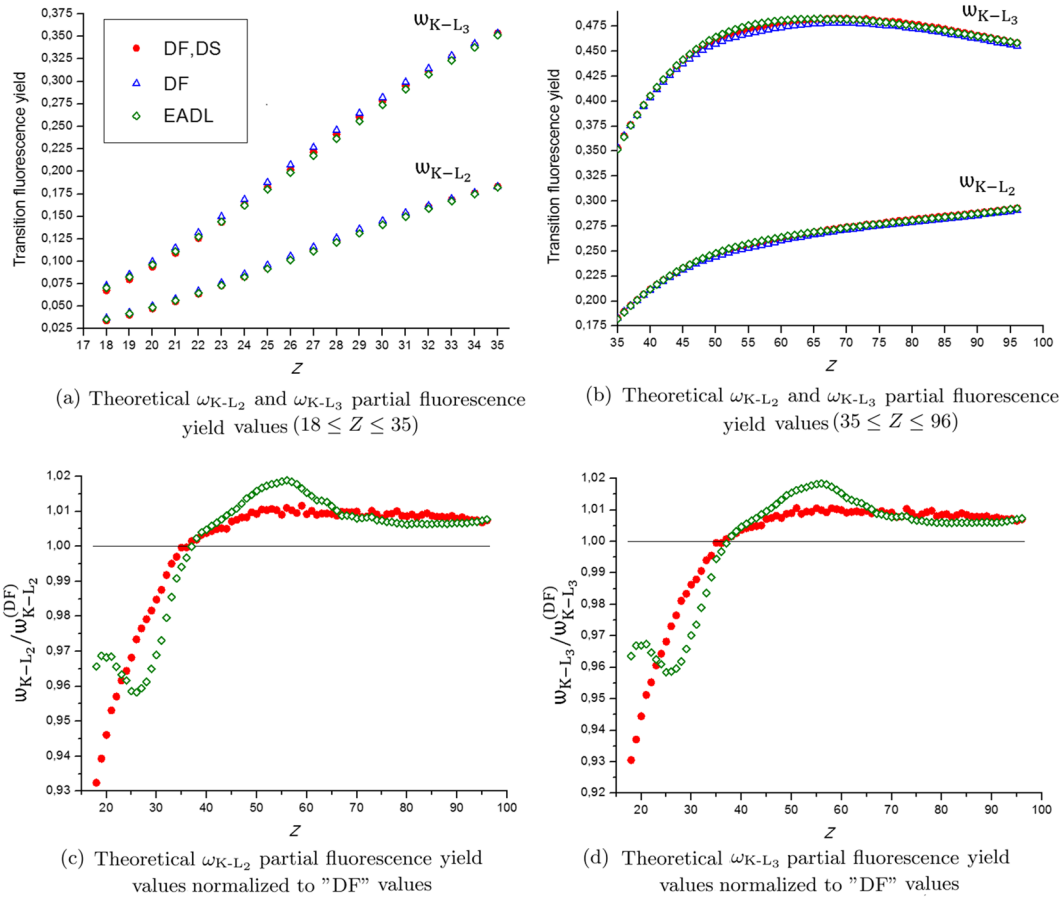
Dirac-Slater method. As such, "DF" K-shell fluorescence yield values are overall higher than "DF,DS" values, as shown in Figure 1c. For low atomic numbers, "DF,DS" and "DF" values differ by almost 10% difference, but as the atomic number increases they become more and more in agreement. In fact, for $42 < Z < 74$ they differ less than 1%, and from $75 < Z < 96$ they differ less than 0.1%

The "MCDF" values are in better agreement with "DF" values among other theoretical values.

4.1.2 | Semi-empirical and empirical K-shell fluorescence yield values

The semi-empirical and emperical K-shell fluorescence yield values are compared in Figure 2a,b (the values are divided in two atomic ranges to better visualization). The same values are presented in Table A6 (in Section VII). Table A6 also presents, for each atomic number, the minimum and the maximum value from the compared references, and the relative difference from those values, with the intent of presenting the highest deviations of the available semi-empirical and empirical references. In Figure 2c,d, the semi-empirical and empirical values are normalized to the corresponding theoretical "DF" values, and "DF,DS" values, respectively.

Unlike the theoretical values presented in Figure 1, some of the semi-empirical and empirical values presented in Figure 2a,b exhibit non-monotonically behaviour with increasing atomic number. Such is highlighted in Figure 2b zooms, where it is visible that in the range $70 < Z < 85$ NIST's values decrease as atomic number increases, and that "Daoudi" values decrease for $Z = 50$. The decrease in "Daoudi" values can be explained by the fact that they divided the experimental results in three ranges of atomic number and performed different fittings for each range. From Figure 2b (and Table A6) it is visible that in the range $60 < Z < 80$ "NIST" values are in clear disagreement with all other semi-empirical and empirical values. The different semi-empirical and empirical K-shell fluorescence yield values present worse agreement between each other for low atomic numbers. In the range $3 < Z < 18$, differences higher than 10% can be found between some of the references. As the atomic number



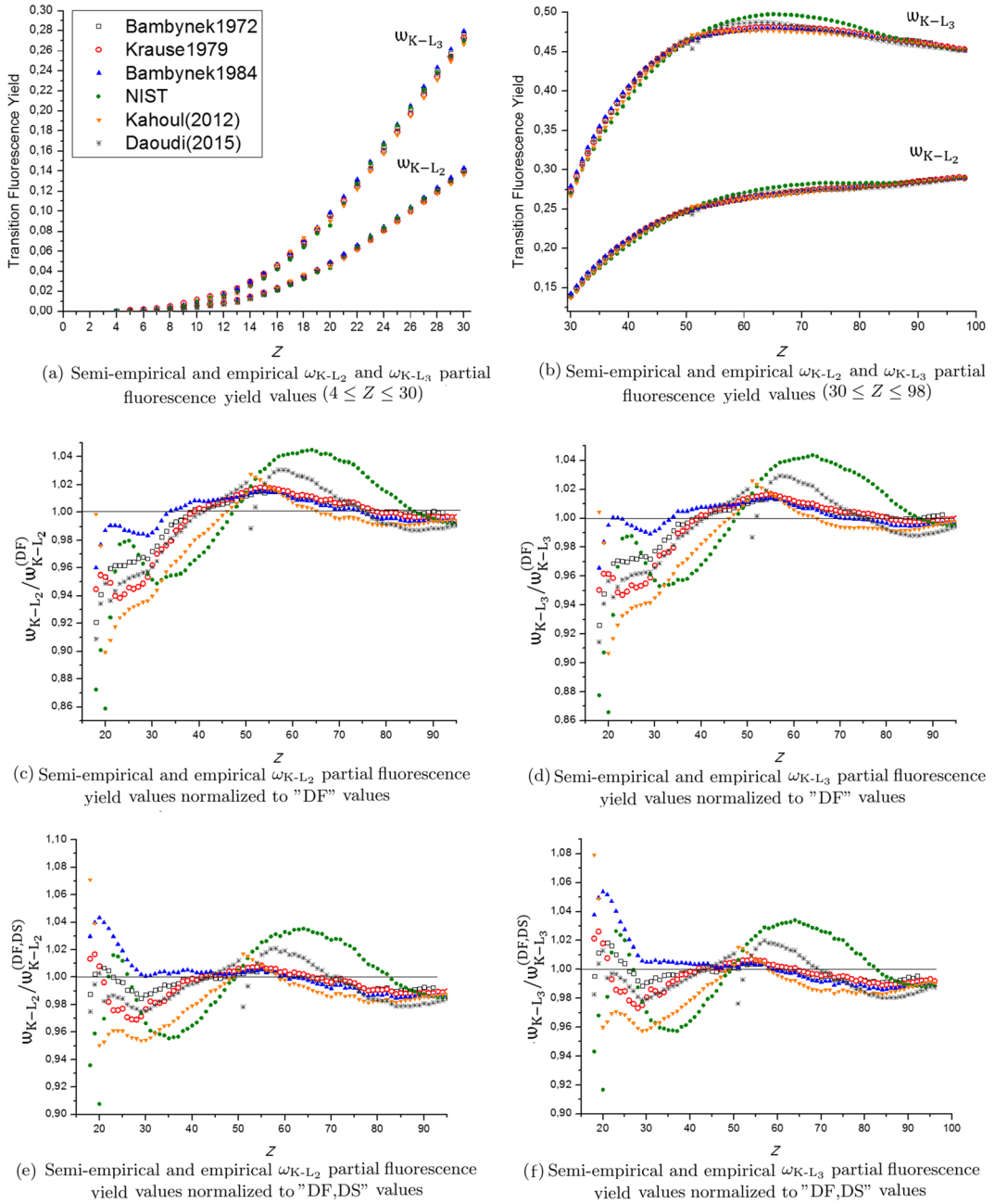
(a) Theoretical $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ partial fluorescence yield values ($18 \leq Z \leq 35$)

(b) Theoretical $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ partial fluorescence yield values ($35 \leq Z \leq 96$)

(c) Theoretical $\omega_{K\text{-}L_2}$ partial fluorescence yield values normalized to "DF" values

(d) Theoretical $\omega_{K\text{-}L_3}$ partial fluorescence yield values normalized to "DF" values

FIGURE 3 "DF,DS": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Slater calculations.[17] "DF": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Fock calculations.[18] "EADL": values obtained from the Evaluated Atomic Data Library.[12]



(a) Semi-empirical and empirical $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ partial fluorescence yield values ($4 \leq Z \leq 30$)

(b) Semi-empirical and empirical $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ partial fluorescence yield values ($30 \leq Z \leq 98$)

(c) Semi-empirical and empirical $\omega_{K\text{-}L_2}$ partial fluorescence yield values normalized to "DF" values

(d) Semi-empirical and empirical $\omega_{K\text{-}L_3}$ partial fluorescence yield values normalized to "DF" values

(e) Semi-empirical and empirical $\omega_{K\text{-}L_2}$ partial fluorescence yield values normalized to "DF,DS" values

(f) Semi-empirical and empirical $\omega_{K\text{-}L_3}$ partial fluorescence yield values normalized to "DF,DS" values

FIGURE 4 "Bambynek1972": Values from Bambynek *et al.* earlier semi-empirical fit.[22] "Krause1979": values from Krause's semi-empirical fit.[40] "Bambynek1984": values from Bambynek *et al.* later semi-empirical fit [41]. "NIST": semi-empirical fit values presented in NIST's Fundamental Parameters Database.[28] "Kahoul": values from Kahoul *et al.* empirical fit.[29] "Daoudi": values from Daoudi *et al.* empirical fit.[30]

increases, better agreement is generally found between the different references. Such is to be expected, since experimental measurement of K-shell fluorescence yields for low atomic numbers generally result in higher uncertainties due to the higher predominance of radiationless transition in these elements. In the range $19 < Z < 50$ the difference between the different values is comprised between 10% to 1%, and in the range $51 < Z < 99$ the agreement is comprised between 1% to 0.4%.

The comparison in Figure 2c highlights that "Bambynek1984" values are in excellent agreement with "DF" values, their relative difference is always lower than 0.2%. "Bambynek1972" and "Krause1979" values are also in good agreement with the "DF" values, especially in the $Z > 40$ range, where they converge to the "DF" values as the atomic number increases. The more recent empirical and semi-empirical values, "NIST", "Kahoul2012", and "Daoudi2015", present worse agreement with "DF" values

than "Bambynek1972", "Krause1979", "Bambynek1984" values. In the range $0 < Z < 40$ the semi-empirical and empirical values are generally lower than "DF" values. The "NIST" values present the worst agreement with the "DF" values.

From Figure 2d one can see that "Bambynek1972", "Krause1979" and "Bambynek1984" values are in good agreement with "DF,DS" values, and their agreement increases with increasing atomic number. "Kahoul2012" and "Daoudi2015" values are also in good agreement but their values do not converge to those of "DF,DS" values as the atomic number increases. As for the "NIST" values, they present as the ones with worse agreement with "DF,DS" values.

It is worthwhile mentioning that from the comparisons presented in this subsection, the K-shell fluorescence yield values from "DF,DS", "DF", "EADL", "Bambynek1972", "Krause1979" and "Bambynek1984", converge as atomic number increases, presenting very good agreement in the range $Z > 40$, while the most recent values "NIST", Kahoul" and "Daoudi2015" do not exhibit this behaviour.

In Table 4 the average relative difference between each semi-empirical and empirical values and the "DF,DS" and "DF" values is presented. From this Table it is shown that the "Bambynek 1972" and "Bambynek 1984" values are in closer agreement with the "DF" values, while all the other references are in better agreement with the "DF,DS" values. Although, with the exception of "NIST" values, all values are in good agreement with the "DF" and "DF,DS" values, presenting average relative difference lower than 2%. The "Bambynek 1984" values are in excellent agreement with "DF" values, presenting less than 0.2% difference.

4.2 | K-L_2 and K-L_3 partial fluorescence yield comparison

4.2.1 | Theoretical K-L_2 and K-L_3 partial fluorescence yield values

The theoretical partial fluorescence yields $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ of "DF,DS", "DF", and "EADL" values are compared in Figure 3a,b (values are divided in two ranges of atomic number to better visualization), and presented in Tables A2 and A3 (in Section VII). In Figure 3c,d, the "DF,DS" and "EADL" partial fluorescence yields $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ are normalized to the "DF" values.

From Figure 3a,b (and Tables A2 and A3) it is highlighted that "DF,DS" partial fluorescence yields $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ are lower than "DF" values in the range $18 < Z < 36$, and higher than "DF" values in the range $36 < Z \leq 97$. For low atomic numbers the difference between "DF,DS" and "DF" references is significantly high for both $\omega_{K\text{-}L_2}$, and $\omega_{K\text{-}L_3}$, the difference is close to 7% for Z=18. For high atomic numbers better agreement is shown, in the range $Z > 60$ the difference is always lower than 1%.

4.2.2 | Semi-empirical and empirical K-L_2 and K-L_3 partial fluorescence yield values

In Figure 4a,b, the semi-empirical and empirical $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ partial fluorescence yield values are compared (the values are divided in two ranges of atomic number to better visualization), which are obtained from the combination of semi-empirical or empirical K-shell fluorescence yield values with Salem *et al.* transition probability values (as explained in Section 3.Q). The same values are presented in Tables A7 and A8 (Section VII). In Figure 4c,d, $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ values of semi-empirical and empirical references are normalized to the respective "DF" values, and, in Figure 4e,f, are normalized to the respective "DF,DS" values.

The values presented in Figure 4a,b (also presented in Tables A7 and A8) exhibit significantly high relative differences from each other, especially at low atomic numbers. In the range $3 \leq Z < 20$ differences of 10% to 100% are found between some of the references. As the atomic number increases better agreement is observed. In the range $20 < Z < 80$, the values have relative differences within 10%, and in the range $80 < Z < 96$ lower than 2%.

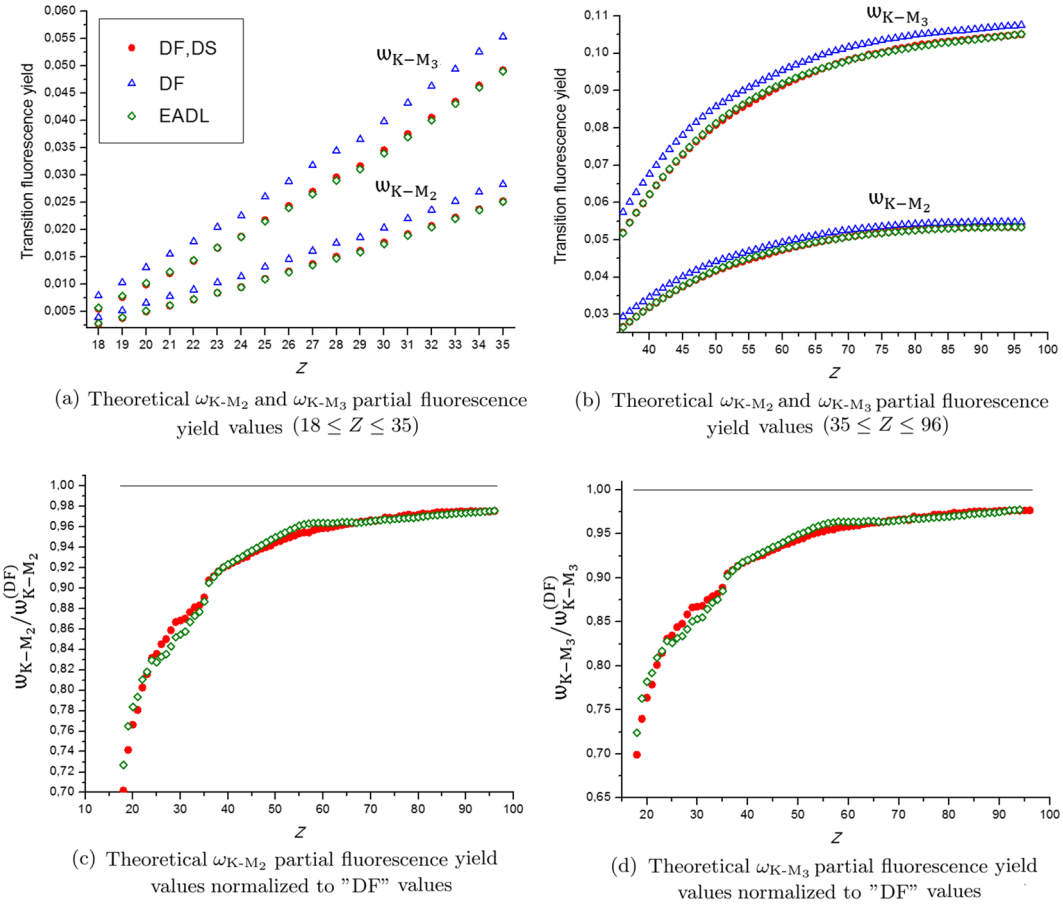
The comparisons in Figure 4c,d, 4.e and 4.f, show that at low atomic numbers, better agreement is seen in the comparison with "DF,DS" values, with the exception of the "Bambynek1984, Salem" values, which are in better agreement with "DF" values. For higher atomic numbers the semi-empirical and empirical values are generally in better agreement with "DF" values.

TABLE 5 $\omega_{K\text{-}L_2}$ fluorescence yield average relative difference

$\Delta\omega_{K\text{-}L_2}$(%)	DS,DF	DF
Bambynek 1972	1.10103	1.3122
Krause 1979	1.39625	1.57368
Bambynek1984	1.43885	0.89263
NIST	2.86495	3.11976
Kahoul 2012	2.53726	2.12996
Daoudi 2015	1.87931	2.08348

TABLE 6 $\omega_{K\text{-}L_3}$ fluorescence yield average relative difference

$\Delta\omega_{K\text{-}L_3}$(%)	DS,DF	DF
Bambynek 1972	0.5014	1.10359
Krause 1979	0.81386	1.38566
Bambynek1984	1.06974	0.62827
NIST	2.18804	2.90847
Kahoul 2012	1.87117	1.98114
Daoudi 2015	1.16017	1.84538



(a) Theoretical $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ partial fluorescence yield values $(18 \leq Z \leq 35)$

(b) Theoretical $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ partial fluorescence yield values $(35 \leq Z \leq 96)$

(c) Theoretical $\omega_{K\text{-}M_2}$ partial fluorescence yield values normalized to "DF" values

(d) Theoretical $\omega_{K\text{-}M_3}$ partial fluorescence yield values normalized to "DF" values

FIGURE 5 "DF,DS": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Slater calculations.[17] "DF": values obtained from the combination of Chen *et al.* radiationless Diroc-Fock calculations[25] and Scofield's radiative Dirac-Fock calculations.[18] "EADL": values obtained from the Evaluated Atomic Data Library.[12]

Table 5 presents the average relative difference between each semi-empirical or empirical $\omega_{K\text{-}L_2}$ values and the "DF,DS" and "DF" values. In Table 6 the same is presented, but regarding $\omega_{K\text{-}L_3}$ values. From these Tables, we infer that all semi-empirical and empirical values are in closer agreement with "DF,DS" values than the "DF" values, with the exception of "Bambynek1984, Salem" (for both $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$), and "Kahoul 2012" (for $\omega_{K\text{-}L_2}$). It is worthwhile noting that the average deviation between the semi-empirical and empirical values in relation to "DF,DS" or "DF" values is for all cases lower than 3%, and in many cases lower than 1%.

4.3 | K-M_2 and K-M_3 fluorescence yield comparison

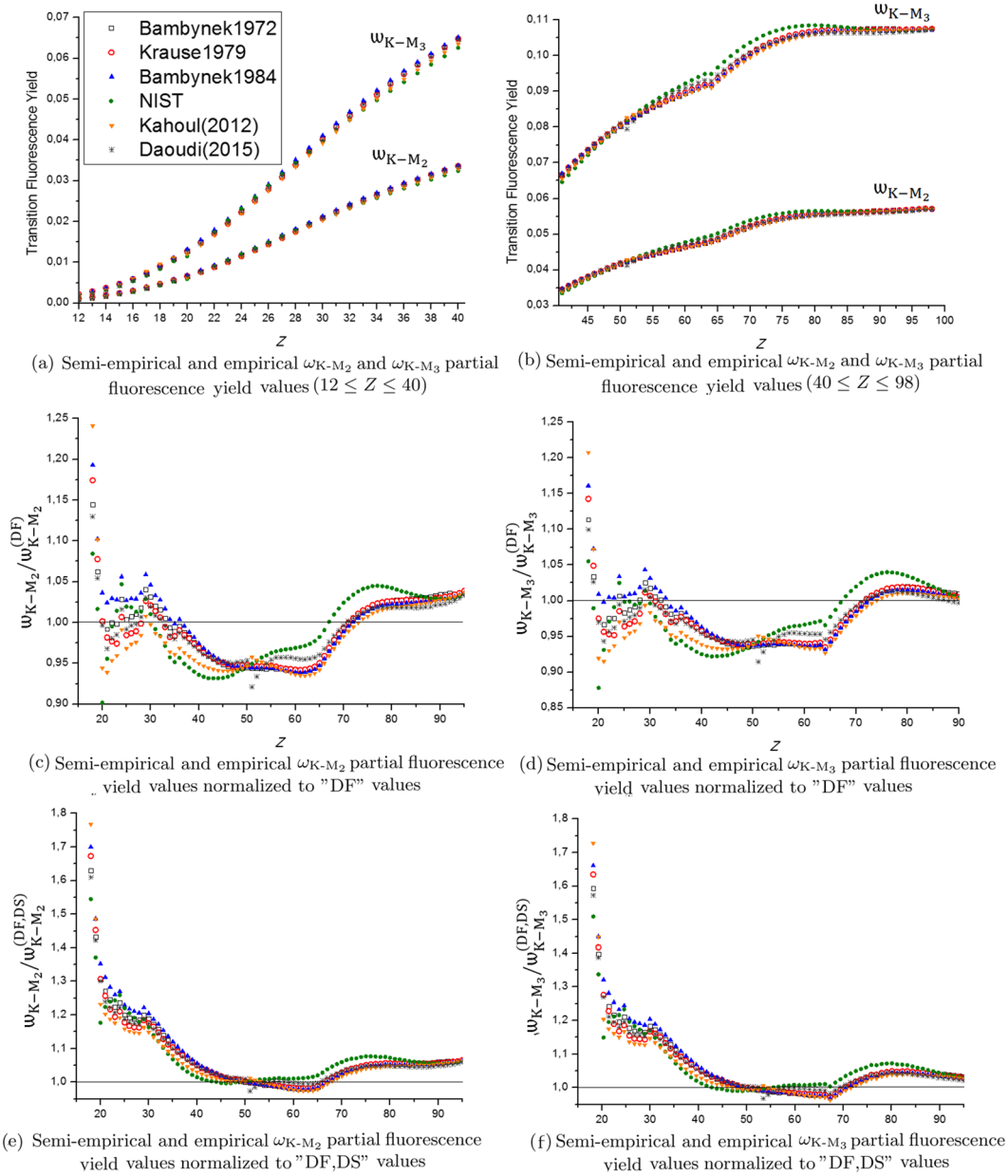
4.3.1 | Theoretical K-M_2 and K-M_3 partial fluorescence yield values

A comparison of the theoretical partial fluorescence yield values $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ is presented in Figure 5a,b (values are divided in two ranges of atomic number to better visualization). The same values are presented in Tables A4 and A5 (in Section VII). In Figure 5c,d, these values are normalized to the respective "DF" values.

Figure 5 indicates that the partial fluorescence yields $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ from "DF" values are higher than the respective "DF,DS" values for all atomic numbers. These values are in higher disagreement at low atomic numbers, where at $Z = 18$ the relative difference is around 35%. At higher atomic numbers the agreement improves, and at $Z = 95$ the difference is lower than 3%.

4.3.2 | Semi-empirical and empirical K-M_2 and K-M_3 partial fluorescence yield values

In Figure 6a,b, the semi-empirical and empirical partial fluorescence yields $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ are compared (the values are divided in two ranges of atomic number to better visualization). The same values are presented in Tables A9 and A10. These values are obtained from the combination of semi-empirical or empirical K-shell fluorescence yield values with Salem *et al.* transition probability values (as presented in Section 3.Q). From these figures and tables, it is clear that the semi-empirical and empirical partial



(a) Semi-empirical and empirical $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ partial fluorescence yield values ($12 \leq Z \leq 40$)

(b) Semi-empirical and empirical $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ partial fluorescence yield values ($40 \leq Z \leq 98$)

(c) Semi-empirical and empirical $\omega_{K\text{-}M_2}$ partial fluorescence yield values normalized to "DF" values

(d) Semi-empirical and empirical $\omega_{K\text{-}M_3}$ partial fluorescence yield values normalized to "DF" values

(e) Semi-empirical and empirical $\omega_{K\text{-}M_2}$ partial fluorescence yield values normalized to "DF,DS" values

(f) Semi-empirical and empirical $\omega_{K\text{-}M_3}$ partial fluorescence yield values normalized to "DF,DS" values

FIGURE 6 "Bambynek1972": Values from Bambynek *et al.* earlier semi-empirical fit.[22] "Krause1979": values from Krause's semi-empirical fit.[40] "Bambynek1984": values from Bambynek *et al.* later semi-empirical fit.[41] "NIST": semi-empirical fit values presented in NIST's Fundamental Parameters Database.[28] "Kahoul": values from Kahoul *et al.* empirical fit.[29] "Daoudi": values from Daoudi *et al.* empirical fit.[30]

fluorescence yields exhibit significantly high differences between each other, especially at low atomic numbers. In the range $3 \leq Z < 20$ some references present 10% to 100% difference to other references. As the atomic number increases better agreement is observed between all references. In the range $20 < Z < 80$, the values are comprised within 10% difference from each other, and in the range $80 < Z < 96$, differences are lower than 2%.

The $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ semi-empirical and empirical values are normalized with the respective "DF" theoretical values in Figure 6c,d, and with the respective theoretical "DF,DS" values in Figure 6e,f. These comparisons highlight that the empirical and semi-empirical values are higher than "DF,DS" values for almost all atomic numbers. Better agreement is found when comparing with the "DF" values.

Table 7 presents the average relative difference between each semi-empirical or empirical $\omega_{K\text{-}M_2}$ values and the "DF,DS" and "DF" values. In Table 8 the same is presented, but regarding $\omega_{K\text{-}M_3}$ values. From these Tables, we infer that all semi-empirical and empirical values are in closer agreement with "DF" values.

TABLE 7 $\omega_{K\text{-}M_2}$ fluorescence yield average relative difference

$\Delta\omega_{K\text{-}M_2}(\%)$	DS,DF	DF
Bambynek 1972	7.51496	3.38598
Krause 1979	7.1521	3.41098
Bambynek1984	7.87296	3.66588
NIST	6.99792	3.79644
Kahoul 2012	6.35466	3.9817
Daoudi 2015	6.82589	2.92917

TABLE 8 $\omega_{K\text{-}M_3}$ fluorescence yield average relative difference

$\Delta\omega_{K\text{-}M_3}(\%)$	DS,DF	DF
Bambynek 1972	6.66471	3.36447
Krause 1979	6.13335	3.35167
Bambynek1984	6.88758	3.11984
NIST	5.92833	3.61726
Kahoul 2012	5.37293	4.10008
Daoudi 2015	5.77349	2.9606

5 | CONCLUSIONS

The comparisons between all theoretical, empirical, and semi-empirical K-shell fluorescence yield values, ω_K, from the different references exhibit that NIST's Fundamental Parameters Database values disagree with the other references, especially in the atomic number range $60 \leq Z \leq 80$. As such, we suggest a change to values obtained from other references.

The ω_K, $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$, $\omega_{K\text{-}M_3}$ partial fluorescence yields values from EADL and from Dirac-Fock/Dirac-Slater calculations ("DF,DS") exhibit some disagreement even though they were obtained from the same references. Pia et al.[13–15] had already pointed out this disagreement in their comparisons of partial fluorescence yields (normalized without accounting for radiationless transitions). Part of this disagreement can be due to the fact EADL includes a correction to the radiationless transition probabilities that we do not included in the present work.

Pia *et al.* work[13–15] highlighted that partial fluorescence yields (normalized without accounting for radiationless transitions) $\omega_{ij}^{(NA)}$ obtained from Scofield's Hartree-Fock work[18] are in better agreement with the experimental values of Salem *et al.*,[20] and as such, EADL should adopt Scofield's Hartree-Fock values. In the present work, the comparison consisted in partial fluorescence yields ω_{ij} that where normalized accounting for radiationless transitions, as are presented in EADL. The comparisons from the present work highlight that regarding ω_K, $\omega_{K\text{-}L_2}$ and $\omega_{K\text{-}L_3}$ values, when comparing the values obtained from using Scofield's Dirac-Slater calculations "DF,DS", and the values obtained using Scofield's Dirac-Fock calculations "DF", the "DF,DS" values are actually in better agreement with most of the semi-empirical and empirical values. The exception to the previous statement is the case of Bambynek *et al.* 1984 semi-empirical values, which are in excellent agreement with "DF" values. As for the $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ partial fluorescence yields, the "DF" values are in better agreement with all semi-empirical and empirical values. The comparisons in the present work do not support that the change in the EADL library, regarding what Scofield's values are adopted, will make EADL's partial fluorescence yield values in better agreement with the semi-empirical and empirical values available in literature. As such, we suggest that such a change in EADL should be backed up with further studies.

The present work introduced a method to obtain partial fluorescence yields $\omega_{K\text{-}L_2}$, $\omega_{K\text{-}L_3}$, $\omega_{K\text{-}M_2}$ and $\omega_{K\text{-}M_3}$ from the combination of semi-empirical or empirical fitting functions with Salem *et al.*[20] ratios (as described in Section 3.Q). This method can be a viable alternative of obtaining comprehensive values for data libraries, covering a large range of atomic number and a large range of transitions, as an alternative to relying in the existing theoretical data. However, some of the existing empirical and semi-empirical values present significant deviations between each other, especially at low atomic numbers, where differences around 100 % can be found between some of the references. In the range $Z > 20$ the deviations between the different references are comprised within 10% to a few percent.

From the comparisons of the present work, we concluded that the "DF" values are in excellent agreement with Bambynek *et al.* 1984 semi-empirical values. In fact, no pair of references presented better agreement.

The method used in this work to obtain partial fluorescence yield values (normalized without accounting for radiationless transitions), which is based on Pia *et al.* method,[13–15] allows to obtain values for all radiative transitions. The method used in the xraylib library is limited to those transitions that the transition probability values[26] are presented in Scofield's work.[18] Furthermore, the $\omega_{K\text{-}L_2}^{(NA)}$, $\omega_{K\text{-}L_3}^{(NA)}$, $\omega_{K\text{-}M_2}^{(NA)}$ and $\omega_{K\text{-}M_3}^{(NA)}$ values obtained using this method are slightly in better agreement with the experimental values of Salem *et al.*[20] Thus, we suggest that the xraylib library[26] could consider using the method described in the present work, or the method used in Pia *et al.* work.[13–15]

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APPENDIX A: FLUORESCENCE YIELD AND PARTIAL FLUORESCENCE YIELD

TABLE A1 Theoretical K-shell fluorescence yield values

Z	Kostroun	DF,DF	DF	EADL	MCDF
10	2.04E-02				1.59E-02[45]
12	2.72E-02				
14	4.41E-02				
16	7.27E-02				
18	1.11E-01	1.11E-01	1.22E-01		1.17E-01[45]
20	1.55E-01	1.57E-01	1.69E-01		
22	2.12E-01	2.12E-01	2.26E-01	2.14E-01	
24	2.76E-01	2.74E-01	2.89E-01		
26	3.44E-01	3.41E-01	3.57E-01	3.36E-01	3.78E-01[46]
28	4.14E-01	4.09E-01	4.24E-01	4.01E-01	4.15E-01[49]
30	4.82E-01	4.74E-01	4.88E-01	4.66E-01	4.85E-01[46]
32	5.45E-01	5.34E-01	5.48E-01		5.47E-01[47]
34	6.02E-01	5.90E-01	6.02E-01		
36	6.55E-01	6.40E-01	6.51E-01		6.49E-01[45]
38	7.02E-01	6.85E-01	6.94E-01		
40	7.41E-01	7.24E-01	7.32E-01	7.27E-01	
42	7.76E-01	7.58E-01	7.65E-01	7.63E-01	
44	8.07E-01	7.88E-01	7.94E-01		
46	8.33E-01	8.14E-01	8.19E-01		
48	8.55E-01	8.35E-01	8.40E-01		
50	8.74E-01	8.54E-01	8.58E-01	8.63E-01	
52	8.90E-01	8.70E-01	8.74E-01		
54		8.84E-01	8.87E-01		8.90E-01[45]
56		8.96E-01	8.99E-01		9.02E-01[48]
58		9.06E-01	9.09E-01		
60		9.16E-01	9.18E-01	9.22E-01	
62		9.23E-01	9.25E-01		
64		9.30E-01	9.32E-01		
66		9.36E-01	9.37E-01		
68		9.41E-01	9.43E-01		
70		9.46E-01	9.47E-01	9.48E-01	
72		9.50E-01	9.51E-01		
74		9.53E-01	9.54E-01		
76		9.56E-01	9.57E-01		
78		9.59E-01	9.59E-01		
80		9.61E-01	9.62E-01	9.60E-01	
82		9.63E-01	9.64E-01	9.61E-01	
84		9.65E-01	9.65E-01		
86		9.66E-01	9.67E-01		9.70E-01[45]
88		9.67E-01	9.68E-01		
90		9.69E-01	9.69E-01		
92		9.69E-01	9.70E-01		
94		9.70E-01	9.71E-01		
96		9.71E-01	9.71E-01		

TABLE A2 Theoretical K-L_2 fluorescence yield values

Z	DF,DS	DF	EADL
18	3.44E-02	3.69E-02	
20	4.76E-02	5.03E-02	
22	6.40E-02	6.69E-02	6.46E-02
24	8.28E-02	8.59E-02	
26	1.03E-01	1.06E-01	1.01E-01
28	1.23E-01	1.26E-01	1.21E-01
30	1.43E-01	1.45E-01	1.41E-01
32	1.61E-01	1.62E-01	
34	1.76E-01	1.76E-01	
36	1.89E-01	1.89E-01	
38	2.01E-01	2.01E-01	
40	2.12E-01	2.11E-01	2.12E-01
42	2.21E-01	2.20E-01	2.21E-01
44	2.29E-01	2.28E-01	
46	2.36E-01	2.34E-01	
48	2.42E-01	2.40E-01	
50	2.47E-01	2.44E-01	2.48E-01
52	2.51E-01	2.48E-01	
54	2.54E-01	2.51E-01	
56	2.57E-01	2.54E-01	
58	2.60E-01	2.57E-01	
60	2.63E-01	2.60E-01	2.64E-01
62	2.65E-01	2.63E-01	
64	2.67E-01	2.65E-01	
66	2.70E-01	2.67E-01	
68	2.72E-01	2.69E-01	
70	2.74E-01	2.71E-01	2.73E-01
72	2.75E-01	2.73E-01	
74	2.77E-01	2.74E-01	
76	2.79E-01	2.76E-01	
78	2.80E-01	2.78E-01	
80	2.81E-01	2.79E-01	2.81E-01
82	2.83E-01	2.80E-01	2.82E-01
84	2.84E-01	2.82E-01	
86	2.85E-01	2.83E-01	
88	2.87E-01	2.84E-01	
90	2.88E-01	2.86E-01	
92	2.90E-01	2.87E-01	
94	2.91E-01	2.89E-01	
96	2.93E-01	2.91E-01	

TABLE A3 Theoretical K-L_3 fluorescence yield values

Z	DF,DS	DF	EADL
18	6.79E-02	7.30E-02	
20	9.39E-02	9.94E-02	
22	1.26E-01	1.32E-01	1.27E-01
24	1.63E-01	1.69E-01	
26	2.02E-01	2.07E-01	1.99E-01
28	2.41E-01	2.46E-01	2.36E-01
30	2.78E-01	2.82E-01	2.74E-01
32	3.11E-01	3.14E-01	
34	3.40E-01	3.42E-01	
36	3.65E-01	3.65E-01	
38	3.86E-01	3.86E-01	
40	4.05E-01	4.04E-01	4.05E-01
42	4.21E-01	4.19E-01	4.22E-01
44	4.34E-01	4.32E-01	
46	4.46E-01	4.42E-01	
48	4.54E-01	4.51E-01	
50	4.61E-01	4.57E-01	4.64E-01
52	4.66E-01	4.62E-01	
54	4.70E-01	4.66E-01	
56	4.73E-01	4.69E-01	
58	4.76E-01	4.71E-01	
60	4.78E-01	4.74E-01	4.81E-01
62	4.80E-01	4.76E-01	
64	4.81E-01	4.76E-01	
66	4.82E-01	4.78E-01	
68	4.83E-01	4.78E-01	
70	4.83E-01	4.78E-01	4.82E-01
72	4.81E-01	4.78E-01	
74	4.81E-01	4.77E-01	
76	4.80E-01	4.76E-01	
78	4.79E-01	4.74E-01	
80	4.77E-01	4.73E-01	4.76E-01
82	4.75E-01	4.71E-01	4.74E-01
84	4.73E-01	4.69E-01	
86	4.71E-01	4.67E-01	
88	4.68E-01	4.65E-01	
90	4.66E-01	4.62E-01	
92	4.63E-01	4.60E-01	
94	4.61E-01	4.58E-01	
96	4.58E-01	4.55E-01	

TABLE A4 Theoretical K-M_2 fluorescence yield values

Z	DF,DS	DF	EADL
18	2.81E-03	4.01E-03	
20	5.06E-03	6.61E-03	
22	7.26E-03	9.04E-03	7.33E-03
24	9.52E-03	1.14E-02	
26	1.24E-02	1.47E-02	1.22E-02
28	1.51E-02	1.76E-02	1.48E-02
30	1.77E-02	2.03E-02	1.74E-02
32	2.07E-02	2.36E-02	
34	2.38E-02	2.69E-02	
36	2.66E-02	2.94E-02	
38	2.94E-02	3.21E-02	
40	3.19E-02	3.46E-02	3.20E-02
42	3.43E-02	3.70E-02	3.44E-02
44	3.64E-02	3.91E-02	
46	3.84E-02	4.10E-02	
48	4.01E-02	4.27E-02	
50	4.17E-02	4.41E-02	4.19E-02
52	4.30E-02	4.53E-02	
54	4.42E-02	4.64E-02	
56	4.52E-02	4.74E-02	
58	4.63E-02	4.84E-02	
60	4.73E-02	4.93E-02	4.75E-02
62	4.81E-02	5.01E-02	
64	4.89E-02	5.08E-02	
66	4.96E-02	5.15E-02	
68	5.03E-02	5.21E-02	
70	5.08E-02	5.26E-02	5.08E-02
72	5.13E-02	5.30E-02	
74	5.17E-02	5.34E-02	
76	5.21E-02	5.37E-02	
78	5.25E-02	5.40E-02	
80	5.27E-02	5.42E-02	5.26E-02
82	5.29E-02	5.44E-02	5.28E-02
84	5.31E-02	5.45E-02	
86	5.32E-02	5.46E-02	
88	5.33E-02	5.47E-02	
90	5.34E-02	5.48E-02	
92	5.34E-02	5.48E-02	
94	5.34E-02	5.48E-02	
96	5.34E-02	5.48E-02	

TABLE A5 Theoretical K-M_3 fluorescence yield values

Z	DF,DS	DF	EADL
18	5.56E-03	7.95E-03	
20	1.00E-02	1.31E-02	
22	1.43E-02	1.79E-02	1.45E-02
24	1.88E-02	2.26E-02	
26	2.44E-02	2.89E-02	2.40E-02
28	2.96E-02	3.45E-02	2.90E-02
30	3.46E-02	3.98E-02	3.40E-02
32	4.05E-02	4.63E-02	
34	4.64E-02	5.26E-02	
36	5.20E-02	5.74E-02	
38	5.73E-02	6.27E-02	
40	6.22E-02	6.76E-02	6.23E-02
42	6.67E-02	7.22E-02	6.69E-02
44	7.09E-02	7.63E-02	
46	7.46E-02	7.99E-02	
48	7.79E-02	8.30E-02	
50	8.08E-02	8.57E-02	8.13E-02
52	8.34E-02	8.80E-02	
54	8.56E-02	9.00E-02	
56	8.77E-02	9.18E-02	
58	8.96E-02	9.36E-02	
60	9.14E-02	9.54E-02	9.19E-02
62	9.31E-02	9.70E-02	
64	9.45E-02	9.82E-02	
66	9.59E-02	9.96E-02	
68	9.72E-02	1.01E-01	
70	9.82E-02	1.02E-01	9.81E-02
72	9.90E-02	1.02E-01	
74	9.99E-02	1.03E-01	
76	1.01E-01	1.04E-01	
78	1.01E-01	1.04E-01	
80	1.02E-01	1.05E-01	1.02E-01
82	1.03E-01	1.05E-01	1.02E-01
84	1.03E-01	1.06E-01	
86	1.03E-01	1.06E-01	
88	1.04E-01	1.06E-01	
90	1.04E-01	1.07E-01	
92	1.04E-01	1.07E-01	
94	1.05E-01	1.07E-01	
96	1.05E-01	1.08E-01	

TABLE A6 Semi-empirical and empirical K-shell fluorescence yield values

Z	Bambynek 1972	Krause 1979	Bambynek 1984	NIST	Kahoul 2012	Daoudi 2015	Min	Max	$\Delta\omega_K$
4	4.51E-04		6.93E-04	3.30E-05		3.60E-04	3.30E-05	6.93E-04	1.82E+02
6	1.98E-03	2.80E-03	2.58E-03	1.40E-03		1.45E-03	1.40E-03	2.80E-03	6.67E+01
8	5.79E-03	8.30E-03	6.91E-03	5.80E-03		4.40E-03	4.40E-03	8.30E-03	6.14E+01
10	1.34E-02	1.80E-02	1.52E-02	1.60E-02		1.09E-02	1.09E-02	2.04E-02	6.09E+01
12	2.65E-02	3.00E-02	2.91E-02	2.60E-02	2.33E-02	2.31E-02	2.31E-02	3.01E-02	2.63E+01
14	4.69E-02	5.00E-02	5.04E-02	4.30E-02	4.32E-02	4.34E-02	4.30E-02	5.14E-02	1.78E+01
16	7.60E-02	7.80E-02	8.04E-02	7.10E-02	7.97E-02	7.34E-02	7.10E-02	8.18E-02	1.41E+01
18	1.15E-01	1.18E-01	1.20E-01	1.09E-01	1.25E-01	1.14E-01	1.09E-01	1.25E-01	1.35E+01
20	1.63E-01	1.63E-01	1.69E-01	1.47E-01	1.54E-01	1.62E-01	1.47E-01	1.71E-01	1.51E+01
22	2.19E-01	2.14E-01	2.26E-01	2.18E-01	2.09E-01	2.15E-01	2.09E-01	2.27E-01	8.44E+00
24	2.81E-01	2.75E-01	2.89E-01	2.86E-01	2.71E-01	2.78E-01	2.71E-01	2.94E-01	8.18E+00
26	3.47E-01	3.40E-01	3.55E-01	3.51E-01	3.35E-01	3.43E-01	3.35E-01	3.62E-01	7.74E+00
28	4.14E-01	4.06E-01	4.21E-01	4.12E-01	4.00E-01	4.09E-01	4.00E-01	4.33E-01	7.85E+00
30	4.79E-01	4.74E-01	4.86E-01	4.69E-01	4.63E-01	4.73E-01	4.63E-01	5.01E-01	7.94E+00
32	5.40E-01	5.35E-01	5.46E-01	5.23E-01	5.23E-01	5.34E-01	5.23E-01	5.65E-01	7.78E+00
34	5.96E-01	5.89E-01	6.02E-01	5.74E-01	5.78E-01	5.90E-01	5.74E-01	6.23E-01	8.19E+00
36	6.46E-01	6.43E-01	6.52E-01	6.21E-01	6.29E-01	6.41E-01	6.21E-01	6.75E-01	8.39E+00
38	6.91E-01	6.90E-01	6.96E-01	6.65E-01	6.75E-01	6.87E-01	6.65E-01	7.21E-01	8.09E+00
40	7.30E-01	7.30E-01	7.34E-01	7.05E-01	7.16E-01	7.27E-01	7.05E-01	7.61E-01	7.65E+00
42	7.64E-01	7.65E-01	7.67E-01	7.42E-01	7.52E-01	7.63E-01	7.42E-01	7.95E-01	6.91E+00
44	7.93E-01	7.94E-01	7.96E-01	7.76E-01	7.84E-01	7.95E-01	7.76E-01	8.24E-01	5.89E+00
46	8.18E-01	8.20E-01	8.20E-01	8.07E-01	8.13E-01	8.22E-01	8.07E-01	8.49E-01	5.08E+00
48	8.40E-01	8.43E-01	8.42E-01	8.36E-01	8.38E-01	8.46E-01	8.35E-01	8.71E-01	4.14E+00
50	8.59E-01	8.62E-01	8.60E-01	8.61E-01	8.60E-01	8.67E-01	8.54E-01	8.89E-01	3.99E+00
52	8.75E-01	8.77E-01	8.75E-01	8.83E-01	8.84E-01	8.65E-01	8.65E-01	9.05E-01	4.44E+00
54	8.88E-01	8.91E-01	8.88E-01	9.03E-01	8.93E-01	8.94E-01	8.84E-01	9.03E-01	2.12E+00
56	9.00E-01	9.02E-01	9.00E-01	9.20E-01	9.01E-01	9.13E-01	8.96E-01	9.20E-01	2.65E+00
58	9.11E-01	9.12E-01	9.10E-01	9.35E-01	9.09E-01	9.26E-01	9.06E-01	9.35E-01	3.09E+00
60	9.20E-01	9.21E-01	9.18E-01	9.47E-01	9.15E-01	9.35E-01	9.15E-01	9.47E-01	3.43E+00
62	9.27E-01	9.29E-01	9.26E-01	9.58E-01	9.22E-01	9.41E-01	9.22E-01	9.58E-01	3.85E+00
64	9.34E-01	9.35E-01	9.32E-01	9.66E-01	9.27E-01	9.46E-01	9.27E-01	9.66E-01	4.12E+00
66	9.40E-01	9.41E-01	9.38E-01	9.72E-01	9.32E-01	9.50E-01	9.32E-01	9.72E-01	4.19E+00
68	9.45E-01	9.47E-01	9.43E-01	9.77E-01	9.37E-01	9.52E-01	9.37E-01	9.77E-01	4.24E+00
70	9.50E-01	9.51E-01	9.47E-01	9.80E-01	9.41E-01	9.54E-01	9.41E-01	9.80E-01	4.12E+00
72	9.54E-01	9.55E-01	9.51E-01	9.82E-01	9.45E-01	9.55E-01	9.45E-01	9.82E-01	3.90E+00
74	9.57E-01	9.58E-01	9.54E-01	9.83E-01	9.48E-01	9.56E-01	9.48E-01	9.83E-01	3.59E+00
76	9.60E-01	9.61E-01	9.57E-01	9.83E-01	9.52E-01	9.57E-01	9.52E-01	9.83E-01	3.23E+00
78	9.63E-01	9.63E-01	9.59E-01	9.82E-01	9.55E-01	9.57E-01	9.55E-01	9.82E-01	2.80E+00
80	9.66E-01	9.65E-01	9.62E-01	9.80E-01	9.57E-01	9.58E-01	9.57E-01	9.80E-01	2.35E+00
82	9.68E-01	9.67E-01	9.63E-01	9.78E-01	9.60E-01	9.58E-01	9.58E-01	9.78E-01	1.99E+00
84	9.70E-01	9.68E-01	9.65E-01	9.76E-01	9.62E-01	9.59E-01	9.59E-01	9.76E-01	1.68E+00
86	9.72E-01	9.69E-01	9.67E-01	9.73E-01	9.64E-01	9.60E-01	9.60E-01	9.73E-01	1.36E+00
88	9.73E-01	9.70E-01	9.68E-01	9.71E-01	9.66E-01	9.61E-01	9.61E-01	9.73E-01	1.20E+00
90	9.75E-01	9.71E-01	9.69E-01	9.70E-01	9.68E-01	9.63E-01	9.63E-01	9.75E-01	1.24E+00
92	9.76E-01	9.72E-01	9.70E-01	9.69E-01	9.70E-01	9.65E-01	9.65E-01	9.76E-01	1.14E+00
94		9.73E-01	9.71E-01	9.69E-01	9.71E-01	9.67E-01	9.67E-01	9.73E-01	5.93E-01
96		9.74E-01	9.72E-01	9.71E-01	9.73E-01	9.70E-01	9.70E-01	9.74E-01	4.27E-01
98		9.75E-01	9.72E-01	9.74E-01	9.74E-01	9.73E-01	9.72E-01	9.75E-01	2.88E-01

TABLE A7 Semi-empirical and empirical K-L_2 fluorescence yield values

Z	Bambynek 1972, ,Salem	Krause 1979 ,Salem	Bambynek 1984 ,Salem	NIST ,Salem	Kahoul 2012 ,Salem	Daoudi 2015 ,Salem	Min	Max	$\Delta\omega_{K\text{-}L_2}$
4	1.51E-04	0.00E+00	2.32E-04	1.10E-05		1.20E-04	1.10E-05	2.32E-04	1.82E+02
6	6.62E-04	9.36E-04	8.61E-04	4.68E-04		4.85E-04	4.68E-04	9.36E-04	6.67E+01
8	1.93E-03	2.77E-03	2.31E-03	1.94E-03		1.47E-03	1.47E-03	2.77E-03	6.14E+01
10	4.48E-03	6.02E-03	5.08E-03	5.35E-03		3.64E-03	3.64E-03	6.02E-03	4.93E+01
12	7.88E-03	8.92E-03	8.65E-03	7.73E-03	6.93E-03	6.87E-03	6.87E-03	8.92E-03	2.60E+01
14	1.39E-02	1.48E-02	1.49E-02	1.28E-02	1.28E-02	1.29E-02	1.28E-02	1.49E-02	1.58E+01
16	2.25E-02	2.31E-02	2.38E-02	2.10E-02	2.36E-02	2.17E-02	2.10E-02	2.38E-02	1.24E+01
18	3.39E-02	3.48E-02	3.54E-02	3.22E-02	3.68E-02	3.35E-02	3.22E-02	3.69E-02	1.36E+01
20	4.80E-02	4.80E-02	4.97E-02	4.32E-02	4.52E-02	4.77E-02	4.32E-02	5.03E-02	1.52E+01
22	6.43E-02	6.29E-02	6.63E-02	6.41E-02	6.14E-02	6.31E-02	6.14E-02	6.69E-02	8.60E+00
24	8.26E-02	8.08E-02	8.48E-02	8.41E-02	7.96E-02	8.16E-02	7.96E-02	8.59E-02	7.59E+00
26	1.02E-01	1.00E-01	1.04E-01	1.03E-01	9.86E-02	1.01E-01	9.86E-02	1.06E-01	7.01E+00
28	1.22E-01	1.20E-01	1.24E-01	1.21E-01	1.18E-01	1.20E-01	1.18E-01	1.26E-01	6.67E+00
30	1.41E-01	1.40E-01	1.43E-01	1.38E-01	1.36E-01	1.39E-01	1.36E-01	1.45E-01	6.21E+00
32	1.59E-01	1.58E-01	1.61E-01	1.54E-01	1.54E-01	1.57E-01	1.54E-01	1.62E-01	5.02E+00
34	1.75E-01	1.73E-01	1.77E-01	1.68E-01	1.70E-01	1.73E-01	1.68E-01	1.77E-01	4.75E+00
36	1.88E-01	1.88E-01	1.90E-01	1.81E-01	1.83E-01	1.87E-01	1.81E-01	1.90E-01	4.82E+00
38	2.01E-01	2.01E-01	2.02E-01	1.93E-01	1.96E-01	2.00E-01	1.93E-01	2.02E-01	4.50E+00
40	2.11E-01	2.11E-01	2.13E-01	2.04E-01	2.07E-01	2.11E-01	2.04E-01	2.13E-01	4.03E+00
42	2.21E-01	2.21E-01	2.22E-01	2.14E-01	2.17E-01	2.20E-01	2.14E-01	2.22E-01	3.34E+00
44	2.29E-01	2.29E-01	2.30E-01	2.24E-01	2.26E-01	2.29E-01	2.24E-01	2.30E-01	2.46E+00
46	2.36E-01	2.36E-01	2.37E-01	2.33E-01	2.34E-01	2.37E-01	2.33E-01	2.37E-01	1.85E+00
48	2.42E-01	2.43E-01	2.42E-01	2.41E-01	2.41E-01	2.44E-01	2.40E-01	2.44E-01	1.62E+00
50	2.47E-01	2.48E-01	2.47E-01	2.48E-01	2.48E-01	2.50E-01	2.44E-01	2.50E-01	2.12E+00
52	2.52E-01	2.52E-01	2.52E-01	2.54E-01	2.55E-01	2.49E-01	2.48E-01	2.55E-01	2.54E+00
54	2.55E-01	2.56E-01	2.55E-01	2.59E-01	2.57E-01	2.57E-01	2.51E-01	2.59E-01	3.11E+00
56	2.58E-01	2.59E-01	2.58E-01	2.64E-01	2.59E-01	2.62E-01	2.54E-01	2.64E-01	3.69E+00
58	2.61E-01	2.61E-01	2.61E-01	2.68E-01	2.60E-01	2.65E-01	2.57E-01	2.68E-01	4.03E+00
60	2.63E-01	2.64E-01	2.63E-01	2.71E-01	2.62E-01	2.68E-01	2.60E-01	2.71E-01	4.16E+00
62	2.66E-01	2.66E-01	2.65E-01	2.74E-01	2.64E-01	2.70E-01	2.63E-01	2.74E-01	4.29E+00
64	2.68E-01	2.68E-01	2.67E-01	2.77E-01	2.66E-01	2.71E-01	2.65E-01	2.77E-01	4.41E+00
66	2.69E-01	2.70E-01	2.69E-01	2.78E-01	2.67E-01	2.72E-01	2.67E-01	2.78E-01	4.19E+00
68	2.71E-01	2.72E-01	2.71E-01	2.81E-01	2.69E-01	2.73E-01	2.69E-01	2.81E-01	4.24E+00
70	2.73E-01	2.73E-01	2.72E-01	2.81E-01	2.70E-01	2.74E-01	2.70E-01	2.81E-01	4.12E+00
72	2.75E-01	2.75E-01	2.74E-01	2.83E-01	2.72E-01	2.75E-01	2.72E-01	2.83E-01	3.90E+00
74	2.76E-01	2.76E-01	2.75E-01	2.83E-01	2.73E-01	2.76E-01	2.73E-01	2.83E-01	3.59E+00
76	2.77E-01	2.77E-01	2.76E-01	2.83E-01	2.74E-01	2.76E-01	2.74E-01	2.83E-01	3.23E+00
78	2.78E-01	2.78E-01	2.77E-01	2.83E-01	2.75E-01	2.76E-01	2.75E-01	2.83E-01	2.80E+00
80	2.79E-01	2.79E-01	2.78E-01	2.83E-01	2.77E-01	2.77E-01	2.77E-01	2.83E-01	2.35E+00
82	2.80E-01	2.80E-01	2.79E-01	2.83E-01	2.78E-01	2.78E-01	2.78E-01	2.83E-01	1.99E+00
84	2.81E-01	2.81E-01	2.80E-01	2.83E-01	2.79E-01	2.78E-01	2.78E-01	2.84E-01	2.14E+00
86	2.83E-01	2.82E-01	2.81E-01	2.83E-01	2.81E-01	2.79E-01	2.79E-01	2.85E-01	2.12E+00
88	2.84E-01	2.83E-01	2.83E-01	2.84E-01	2.82E-01	2.81E-01	2.81E-01	2.87E-01	2.08E+00
90	2.86E-01	2.85E-01	2.84E-01	2.84E-01	2.84E-01	2.82E-01	2.82E-01	2.88E-01	1.95E+00
92	2.87E-01	2.86E-01	2.86E-01	2.85E-01	2.86E-01	2.84E-01	2.84E-01	2.90E-01	1.88E+00
94		2.88E-01	2.87E-01	2.87E-01	2.87E-01	2.86E-01	2.86E-01	2.91E-01	1.70E+00
96		2.89E-01	2.89E-01	2.88E-01	2.89E-01	2.88E-01	2.88E-01	2.93E-01	1.62E+00
98		2.90E-01	2.89E-01	2.89E-01	2.89E-01	2.89E-01	2.89E-01	2.90E-01	2.88E-01

TABLE A8 Semi-empirical and empirical K-L_3 fluorescence yield values

Z	Bambynek 1972 , Salem	Krause 1979 ,Salem	Bambynek 1984 ,Salem	NIST ,Salem	Kahoul 2012 ,Salem	Daoudi 2015 ,Salem	Min	Max	$\Delta\omega_{K\text{-}L_3}$
4	3.00E-04	0.00E+00	4.61E-04	2.20E-05	0.00E+00	2.40E-04	2.20E-05	4.61E-04	1.82E+02
6	1.32E-03	1.86E-03	1.71E-03	9.32E-04		9.65E-04	9.32E-04	1.86E-03	6.67E+01
8	3.85E-03	5.53E-03	4.60E-03	3.86E-03		2.93E-03	2.93E-03	5.53E-03	6.14E+01
10	8.92E-03	1.20E-02	1.01E-02	1.07E-02		7.24E-03	7.24E-03	1.20E-02	4.93E+01
12	1.57E-02	1.78E-02	1.72E-02	1.54E-02	1.38E-02	1.37E-02	1.37E-02	1.78E-02	2.60E+01
14	2.77E-02	2.95E-02	2.98E-02	2.54E-02	2.55E-02	2.56E-02	2.54E-02	2.98E-02	1.58E+01
16	4.48E-02	4.60E-02	4.74E-02	4.18E-02	4.70E-02	4.33E-02	4.18E-02	4.74E-02	1.24E+01
18	6.76E-02	6.94E-02	7.05E-02	6.41E-02	7.33E-02	6.67E-02	6.41E-02	7.33E-02	1.35E+01
20	9.56E-02	9.56E-02	9.89E-02	8.61E-02	9.01E-02	9.51E-02	8.61E-02	9.94E-02	1.44E+01
22	1.28E-01	1.25E-01	1.32E-01	1.27E-01	1.22E-01	1.26E-01	1.22E-01	1.32E-01	7.69E+00
24	1.64E-01	1.60E-01	1.68E-01	1.67E-01	1.58E-01	1.62E-01	1.58E-01	1.69E-01	6.73E+00
26	2.01E-01	1.97E-01	2.06E-01	2.04E-01	1.95E-01	1.99E-01	1.95E-01	2.07E-01	6.26E+00
28	2.39E-01	2.35E-01	2.43E-01	2.38E-01	2.31E-01	2.37E-01	2.31E-01	2.46E-01	6.06E+00
30	2.76E-01	2.73E-01	2.80E-01	2.70E-01	2.67E-01	2.73E-01	2.67E-01	2.82E-01	5.65E+00
32	3.10E-01	3.07E-01	3.13E-01	3.00E-01	3.00E-01	3.06E-01	3.00E-01	3.14E-01	4.77E+00
34	3.39E-01	3.35E-01	3.42E-01	3.26E-01	3.29E-01	3.35E-01	3.26E-01	3.42E-01	4.75E+00
36	3.64E-01	3.62E-01	3.67E-01	3.50E-01	3.54E-01	3.61E-01	3.50E-01	3.67E-01	4.82E+00
38	3.86E-01	3.85E-01	3.88E-01	3.71E-01	3.76E-01	3.83E-01	3.71E-01	3.88E-01	4.50E+00
40	4.04E-01	4.04E-01	4.07E-01	3.91E-01	3.96E-01	4.03E-01	3.91E-01	4.07E-01	4.03E+00
42	4.21E-01	4.21E-01	4.22E-01	4.09E-01	4.14E-01	4.20E-01	4.09E-01	4.22E-01	3.34E+00
44	4.34E-01	4.35E-01	4.36E-01	4.25E-01	4.30E-01	4.35E-01	4.25E-01	4.36E-01	2.46E+00
46	4.45E-01	4.46E-01	4.46E-01	4.39E-01	4.42E-01	4.47E-01	4.39E-01	4.47E-01	1.85E+00
48	4.54E-01	4.56E-01	4.55E-01	4.52E-01	4.53E-01	4.58E-01	4.51E-01	4.58E-01	1.51E+00
50	4.62E-01	4.64E-01	4.62E-01	4.63E-01	4.63E-01	4.66E-01	4.57E-01	4.66E-01	1.96E+00
52	4.68E-01	4.69E-01	4.68E-01	4.72E-01	4.73E-01	4.63E-01	4.62E-01	4.73E-01	2.32E+00
54	4.72E-01	4.73E-01	4.72E-01	4.80E-01	4.75E-01	4.75E-01	4.66E-01	4.80E-01	2.97E+00
56	4.75E-01	4.76E-01	4.75E-01	4.85E-01	4.76E-01	4.82E-01	4.69E-01	4.85E-01	3.55E+00
58	4.77E-01	4.78E-01	4.76E-01	4.90E-01	4.76E-01	4.85E-01	4.71E-01	4.90E-01	3.85E+00
60	4.79E-01	4.79E-01	4.78E-01	4.93E-01	4.77E-01	4.87E-01	4.74E-01	4.93E-01	4.02E+00
62	4.80E-01	4.81E-01	4.79E-01	4.96E-01	4.77E-01	4.87E-01	4.76E-01	4.96E-01	4.11E+00
64	4.81E-01	4.81E-01	4.80E-01	4.97E-01	4.77E-01	4.87E-01	4.76E-01	4.97E-01	4.28E+00
66	4.81E-01	4.81E-01	4.79E-01	4.97E-01	4.77E-01	4.86E-01	4.77E-01	4.97E-01	4.19E+00
68	4.80E-01	4.81E-01	4.79E-01	4.97E-01	4.76E-01	4.84E-01	4.76E-01	4.97E-01	4.24E+00
70	4.80E-01	4.80E-01	4.78E-01	4.95E-01	4.75E-01	4.82E-01	4.75E-01	4.95E-01	4.12E+00
72	4.79E-01	4.80E-01	4.78E-01	4.93E-01	4.75E-01	4.80E-01	4.75E-01	4.93E-01	3.90E+00
74	4.78E-01	4.79E-01	4.77E-01	4.91E-01	4.74E-01	4.78E-01	4.74E-01	4.91E-01	3.59E+00
76	4.77E-01	4.77E-01	4.75E-01	4.88E-01	4.73E-01	4.75E-01	4.73E-01	4.88E-01	3.23E+00
78	4.75E-01	4.75E-01	4.73E-01	4.84E-01	4.71E-01	4.72E-01	4.71E-01	4.84E-01	2.80E+00
80	4.74E-01	4.73E-01	4.71E-01	4.80E-01	4.69E-01	4.70E-01	4.69E-01	4.80E-01	2.35E+00
82	4.71E-01	4.70E-01	4.69E-01	4.76E-01	4.67E-01	4.66E-01	4.66E-01	4.76E-01	1.99E+00
84	4.69E-01	4.68E-01	4.67E-01	4.72E-01	4.65E-01	4.64E-01	4.64E-01	4.73E-01	2.03E+00
86	4.67E-01	4.66E-01	4.64E-01	4.68E-01	4.63E-01	4.61E-01	4.61E-01	4.71E-01	1.98E+00
88	4.65E-01	4.63E-01	4.62E-01	4.64E-01	4.62E-01	4.59E-01	4.59E-01	4.68E-01	1.92E+00
90	4.63E-01	4.61E-01	4.60E-01	4.61E-01	4.60E-01	4.57E-01	4.57E-01	4.66E-01	1.77E+00
92	4.61E-01	4.59E-01	4.58E-01	4.58E-01	4.58E-01	4.56E-01	4.56E-01	4.63E-01	1.59E+00
94		4.57E-01	4.56E-01	4.55E-01	4.56E-01	4.55E-01	4.55E-01	4.61E-01	1.37E+00
96		4.55E-01	4.53E-01	4.53E-01	4.54E-01	4.53E-01	4.53E-01	4.58E-01	1.25E+00
98		4.53E-01	4.52E-01	4.52E-01	4.53E-01	4.52E-01	4.52E-01	4.53E-01	2.88E-01

TABLE A9 Semi-empirical and empirical K-M_2 fluorescence yield values

Z	Bambynek 1972 , Salem	Krause 1979 ,Salem	Bambynek 1984 ,Salem	NIST ,Salem	Kahoul 2012 ,Salem	Daoudi 2015 ,Salem	Min	Max	$\Delta\omega_{K\text{-}M_2}$
12	9.99E-04	1.13E-03	1.10E-03	9.81E-04	8.79E-04	8.71E-04	8.71E-04	1.13E-03	2.60E+01
14	1.80E-03	1.92E-03	1.94E-03	1.65E-03	1.66E-03	1.67E-03	1.65E-03	1.94E-03	1.58E+01
16	2.98E-03	3.05E-03	3.15E-03	2.78E-03	3.12E-03	2.87E-03	2.78E-03	3.15E-03	1.24E+01
18	4.59E-03	4.70E-03	4.78E-03	4.35E-03	4.97E-03	4.53E-03	2.81E-03	4.97E-03	5.55E+01
20	6.62E-03	6.62E-03	6.85E-03	5.96E-03	6.24E-03	6.58E-03	5.06E-03	6.85E-03	3.00E+01
22	9.04E-03	8.83E-03	9.31E-03	8.99E-03	8.62E-03	8.86E-03	7.26E-03	9.31E-03	2.48E+01
24	1.18E-02	1.15E-02	1.21E-02	1.20E-02	1.13E-02	1.16E-02	9.52E-03	1.21E-02	2.38E+01
26	1.48E-02	1.45E-02	1.51E-02	1.49E-02	1.43E-02	1.46E-02	1.22E-02	1.51E-02	2.11E+01
28	1.79E-02	1.75E-02	1.82E-02	1.78E-02	1.73E-02	1.77E-02	1.48E-02	1.82E-02	2.05E+01
30	2.10E-02	2.08E-02	2.13E-02	2.06E-02	2.03E-02	2.07E-02	1.74E-02	2.13E-02	2.02E+01
32	2.40E-02	2.38E-02	2.43E-02	2.33E-02	2.32E-02	2.37E-02	2.07E-02	2.43E-02	1.59E+01
34	2.68E-02	2.64E-02	2.70E-02	2.58E-02	2.59E-02	2.65E-02	2.38E-02	2.70E-02	1.28E+01
36	2.92E-02	2.91E-02	2.95E-02	2.81E-02	2.84E-02	2.90E-02	2.66E-02	2.95E-02	1.01E+01
38	3.15E-02	3.14E-02	3.17E-02	3.03E-02	3.07E-02	3.13E-02	2.94E-02	3.21E-02	8.73E+00
40	3.36E-02	3.36E-02	3.37E-02	3.24E-02	3.29E-02	3.34E-02	3.19E-02	3.46E-02	8.09E+00
42	3.55E-02	3.55E-02	3.57E-02	3.45E-02	3.49E-02	3.55E-02	3.43E-02	3.70E-02	7.59E+00
44	3.72E-02	3.73E-02	3.74E-02	3.65E-02	3.68E-02	3.73E-02	3.64E-02	3.91E-02	7.17E+00
46	3.88E-02	3.89E-02	3.89E-02	3.83E-02	3.86E-02	3.90E-02	3.83E-02	4.10E-02	6.86E+00
48	4.03E-02	4.05E-02	4.04E-02	4.01E-02	4.02E-02	4.06E-02	4.01E-02	4.27E-02	6.19E+00
50	4.17E-02	4.18E-02	4.17E-02	4.18E-02	4.17E-02	4.21E-02	4.17E-02	4.41E-02	5.67E+00
52	4.28E-02	4.29E-02	4.28E-02	4.32E-02	4.33E-02	4.23E-02	4.23E-02	4.53E-02	6.85E+00
54	4.38E-02	4.39E-02	4.38E-02	4.45E-02	4.41E-02	4.41E-02	4.38E-02	4.64E-02	5.79E+00
56	4.47E-02	4.48E-02	4.47E-02	4.57E-02	4.48E-02	4.53E-02	4.47E-02	4.74E-02	5.83E+00
58	4.56E-02	4.56E-02	4.55E-02	4.68E-02	4.55E-02	4.63E-02	4.55E-02	4.84E-02	6.19E+00
60	4.64E-02	4.64E-02	4.63E-02	4.78E-02	4.62E-02	4.71E-02	4.62E-02	4.93E-02	6.58E+00
62	4.71E-02	4.72E-02	4.71E-02	4.87E-02	4.69E-02	4.79E-02	4.69E-02	5.01E-02	6.75E+00
64	4.80E-02	4.80E-02	4.79E-02	4.96E-02	4.76E-02	4.86E-02	4.76E-02	5.08E-02	6.43E+00
66	4.93E-02	4.94E-02	4.92E-02	5.10E-02	4.89E-02	4.98E-02	4.89E-02	5.15E-02	5.13E+00
68	5.09E-02	5.10E-02	5.07E-02	5.26E-02	5.04E-02	5.12E-02	5.03E-02	5.26E-02	4.54E+00
70	5.22E-02	5.23E-02	5.20E-02	5.39E-02	5.17E-02	5.24E-02	5.08E-02	5.39E-02	5.92E+00
72	5.33E-02	5.33E-02	5.31E-02	5.48E-02	5.27E-02	5.33E-02	5.13E-02	5.48E-02	6.74E+00
74	5.41E-02	5.42E-02	5.39E-02	5.56E-02	5.36E-02	5.41E-02	5.17E-02	5.56E-02	7.21E+00
76	5.48E-02	5.49E-02	5.46E-02	5.61E-02	5.43E-02	5.46E-02	5.21E-02	5.61E-02	7.40E+00
78	5.53E-02	5.53E-02	5.51E-02	5.64E-02	5.48E-02	5.50E-02	5.25E-02	5.64E-02	7.20E+00
80	5.57E-02	5.57E-02	5.54E-02	5.65E-02	5.52E-02	5.52E-02	5.26E-02	5.65E-02	7.26E+00
82	5.59E-02	5.59E-02	5.56E-02	5.65E-02	5.54E-02	5.54E-02	5.28E-02	5.65E-02	6.75E+00
84	5.61E-02	5.60E-02	5.58E-02	5.64E-02	5.57E-02	5.55E-02	5.31E-02	5.64E-02	6.06E+00
86	5.63E-02	5.61E-02	5.60E-02	5.64E-02	5.59E-02	5.56E-02	5.32E-02	5.64E-02	5.78E+00
88	5.64E-02	5.62E-02	5.61E-02	5.63E-02	5.60E-02	5.57E-02	5.33E-02	5.64E-02	5.64E+00
90	5.67E-02	5.64E-02	5.63E-02	5.64E-02	5.63E-02	5.60E-02	5.34E-02	5.67E-02	5.99E+00
92	5.68E-02	5.66E-02	5.65E-02	5.64E-02	5.64E-02	5.62E-02	5.34E-02	5.68E-02	6.12E+00
94		5.68E-02	5.66E-02	5.65E-02	5.67E-02	5.64E-02	5.34E-02	5.68E-02	6.04E+00
96		5.70E-02	5.69E-02	5.68E-02	5.69E-02	5.67E-02	5.34E-02	5.70E-02	6.46E+00
98		5.71E-02	5.69E-02	5.70E-02	5.70E-02	5.69E-02	5.69E-02	5.71E-02	2.88E-01

TABLE A10 Semi-empirical and empirical K-M_3 fluorescence yield values

Z	Bambynek 1972 , Salem	Krause 1979 ,Salem	Bambynek 1984 ,Salem	NIST ,Salem	Kahoul 2012 ,Salem	Daoudi 2015 ,Salem	Min	Max	$\Delta\omega_{K\text{-}M_3}$
12	1.93E-03	2.18E-03	2.12E-03	1.89E-03	1.70E-03	1.68E-03	1.68E-03	2.18E-03	2.60E+01
14	3.48E-03	3.71E-03	3.74E-03	3.19E-03	3.21E-03	3.22E-03	3.19E-03	3.74E-03	1.58E+01
16	5.74E-03	5.90E-03	6.08E-03	5.37E-03	6.02E-03	5.55E-03	5.37E-03	6.08E-03	1.24E+01
18	8.85E-03	9.08E-03	9.23E-03	8.39E-03	9.60E-03	8.74E-03	5.56E-03	9.60E-03	5.33E+01
20	1.28E-02	1.28E-02	1.32E-02	1.15E-02	1.20E-02	1.27E-02	1.00E-02	1.32E-02	2.77E+01
22	1.74E-02	1.70E-02	1.80E-02	1.74E-02	1.66E-02	1.71E-02	1.43E-02	1.80E-02	2.25E+01
24	2.27E-02	2.22E-02	2.33E-02	2.31E-02	2.19E-02	2.25E-02	1.88E-02	2.33E-02	2.17E+01
26	2.85E-02	2.79E-02	2.91E-02	2.88E-02	2.76E-02	2.82E-02	2.40E-02	2.91E-02	1.93E+01
28	3.45E-02	3.39E-02	3.51E-02	3.44E-02	3.34E-02	3.41E-02	2.90E-02	3.51E-02	1.90E+01
30	4.05E-02	4.01E-02	4.11E-02	3.97E-02	3.92E-02	4.01E-02	3.40E-02	4.11E-02	1.89E+01
32	4.64E-02	4.59E-02	4.69E-02	4.49E-02	4.49E-02	4.58E-02	4.05E-02	4.69E-02	1.46E+01
34	5.16E-02	5.10E-02	5.22E-02	4.97E-02	5.01E-02	5.11E-02	4.64E-02	5.26E-02	1.25E+01
36	5.64E-02	5.61E-02	5.69E-02	5.42E-02	5.49E-02	5.60E-02	5.20E-02	5.74E-02	9.99E+00
38	6.08E-02	6.07E-02	6.12E-02	5.85E-02	5.93E-02	6.04E-02	5.73E-02	6.27E-02	9.05E+00
40	6.48E-02	6.48E-02	6.51E-02	6.26E-02	6.35E-02	6.45E-02	6.22E-02	6.76E-02	8.37E+00
42	6.85E-02	6.86E-02	6.88E-02	6.66E-02	6.75E-02	6.85E-02	6.66E-02	7.22E-02	8.12E+00
44	7.19E-02	7.20E-02	7.21E-02	7.04E-02	7.11E-02	7.20E-02	7.04E-02	7.63E-02	8.02E+00
46	7.49E-02	7.51E-02	7.51E-02	7.39E-02	7.45E-02	7.53E-02	7.39E-02	7.99E-02	7.74E+00
48	7.76E-02	7.79E-02	7.78E-02	7.73E-02	7.75E-02	7.82E-02	7.73E-02	8.30E-02	7.14E+00
50	8.03E-02	8.05E-02	8.03E-02	8.04E-02	8.04E-02	8.10E-02	8.03E-02	8.57E-02	6.54E+00
52	8.26E-02	8.28E-02	8.26E-02	8.33E-02	8.34E-02	8.17E-02	8.17E-02	8.80E-02	7.47E+00
54	8.45E-02	8.48E-02	8.45E-02	8.59E-02	8.50E-02	8.50E-02	8.45E-02	9.00E-02	6.32E+00
56	8.63E-02	8.65E-02	8.63E-02	8.82E-02	8.64E-02	8.75E-02	8.63E-02	9.18E-02	6.24E+00
58	8.80E-02	8.81E-02	8.79E-02	9.03E-02	8.78E-02	8.94E-02	8.78E-02	9.36E-02	6.45E+00
60	8.95E-02	8.96E-02	8.94E-02	9.22E-02	8.91E-02	9.10E-02	8.91E-02	9.54E-02	6.84E+00
62	9.10E-02	9.12E-02	9.09E-02	9.40E-02	9.05E-02	9.24E-02	9.05E-02	9.70E-02	6.94E+00
64	9.17E-02	9.18E-02	9.15E-02	9.49E-02	9.10E-02	9.29E-02	9.10E-02	9.82E-02	7.61E+00
66	9.51E-02	9.52E-02	9.48E-02	9.83E-02	9.43E-02	9.60E-02	9.43E-02	9.96E-02	5.48E+00
68	9.80E-02	9.82E-02	9.77E-02	1.01E-01	9.71E-02	9.87E-02	9.71E-02	1.01E-01	4.24E+00
70	1.00E-01	1.01E-01	1.00E-01	1.04E-01	9.95E-02	1.01E-01	9.81E-02	1.04E-01	5.49E+00
72	1.03E-01	1.03E-01	1.02E-01	1.06E-01	1.02E-01	1.03E-01	9.90E-02	1.06E-01	6.54E+00
74	1.04E-01	1.04E-01	1.04E-01	1.07E-01	1.03E-01	1.04E-01	9.99E-02	1.07E-01	6.85E+00
76	1.05E-01	1.06E-01	1.05E-01	1.08E-01	1.05E-01	1.05E-01	1.01E-01	1.08E-01	7.00E+00
78	1.06E-01	1.06E-01	1.06E-01	1.08E-01	1.05E-01	1.06E-01	1.01E-01	1.08E-01	6.63E+00
80	1.07E-01	1.07E-01	1.06E-01	1.09E-01	1.06E-01	1.06E-01	1.02E-01	1.09E-01	6.46E+00
82	1.07E-01	1.07E-01	1.07E-01	1.08E-01	1.06E-01	1.06E-01	1.02E-01	1.08E-01	5.80E+00
84	1.07E-01	1.07E-01	1.07E-01	1.08E-01	1.07E-01	1.06E-01	1.03E-01	1.08E-01	4.77E+00
86	1.08E-01	1.07E-01	1.07E-01	1.08E-01	1.07E-01	1.06E-01	1.03E-01	1.08E-01	4.08E+00
88	1.08E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.06E-01	1.04E-01	1.08E-01	3.66E+00
90	1.08E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.06E-01	1.04E-01	1.08E-01	3.35E+00
92	1.08E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.06E-01	1.04E-01	1.08E-01	3.05E+00
94	0.00E+00	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.05E-01	1.07E-01	2.40E+00
96	0.00E+00	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.05E-01	1.08E-01	2.35E+00
98	0.00E+00	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	1.07E-01	2.88E-01