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# Semi-empirical and empirical calculation of Kβ/Kα intensity ratios for lanthanides

**Assala Hamidani[1,2*], Abdelhalim Kahoul[1,2], José P. Marques[3,4], Salim Daoudi[1,2], Jorge M. Sampaio[3,4], Fernando Parente[5], Nuray Kup Aylikci[6], Volkan Aylikci[7], Yazid Kasri[8], Kaouther Meddouh[1,2]**

[1]*Department of Matter Sciences, Faculty of Sciences and Technology, Mohamed El Bachir El Ibrahimi University, Bordj-Bou-Arreridj 34030, Algeria.*
[2]*Laboratory of Materials Physics, Radiation and Nanostructures (LPMRN), Faculty of Sciences and Technology, Mohamed El Bachir El Ibrahimi University, Bordj-Bou-Arreridj 34030, Algeria.*
[3]*LIP – Laboratório de Instrumentação e Física Experimental de Partículas, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal.*
[4]*Faculdade de Ciências da Universidade de Lisboa, Campo Grande, C8, 1749-016 Lisboa, Portugal.*
[5]*Laboratory of Instrumentation, Biomedical Engineering and Radiation Physics (LIBPhys-UNL), Department of Physics, NOVA School of Science andTechnology, NOVA University Lisbon, 2829-516 Caparica, Portugal.*
[6]*Department of Energy Systems Engineering, Faculty of Engineering and Natural Sciences, Iskenderun Technical University, 31200 Iskenderun, Hatay, Turkey.*
[7]*Department of Metallurgical and Materials Engineering, Faculty of Engineering and Natural Sciences, Iskenderun Technical University, 31200 Iskenderun, Hatay, Turkey.*
[8]*Theoretical Physics Laboratory, Physics Department, University of Bejaia, 06000 Bejaia, Algeria.*
**Corresponding author E-mail address: assala.hamidani@univ-bba.dz*
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## Abstract

The aim of this work is to presenta study of the Kβ/Kα X-ray intensity ratios for elements from $_{57}$La to $_{71}$Lu taken exclusively from experimental data. New recommended weighted average values $(K\beta/K\alpha)_{WR}$ are obtained dividing the experimental ratios $(K\beta/K\alpha)_{Exp}$ by the weighted ratios $(K\beta/K\alpha)_{W}$, then eliminating the values not between 0.9 and 1.1.

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Also, empirical average Kβ/KαX rays intensity ratios are established for elements from $_{57}$La to $_{71}$Lu using a method based on the interpolation of a popular analytical functionas a function of the atomic number *Z*. In addition to that, fitting the ratio S = $(K\beta/K\alpha)_{Exp}$ / $(K\beta/K\alpha)_W$ enabled to deduce new semi-empirical average Kβ/KαX rays intensity ratios.Finally, comparing our results with other theoretical, experimental and empirical values reported in the literature shows that there is a good agreement between the different values.

**Keywords:** Semi-empirical calculation, weighted average values, X-rays intensity ratios.

## 1. Introduction

In manyapplications, including physical chemistry and medical research, calculating X-ray production cross sections and intensity ratios is crucial. Additionally, the determination of Kβ/Kα intensity ratios is employed to verify the validity of theoretical theories based on various atomic models. Numerous authors have already studiedKβ/Kα intensity ratio values, whether through experimentation under a varietyof conditions [1–3] or through theoretical investigation, such as Scofield's significant calculation utilizing Hartree–Slater theory [4]. However, it was discovered that both theoretical and experimental values and the experimental data itself differ, especially when it comes to lanthanides. In light of this, our study team chose to calculate semi-empirical Kβ/Kα intensity ratios for lanthanides by fitting the existing experimental data using analytical functions. The Kβ/Kα intensity ratios and weighted average values that were obtained from the database [5] are used to calculate the weighted recommended averages values $(K\beta/K\alpha)_{WR}$. These were fitted with a polynomial fit to generate the empirical average Kβ/Kα X rays intensity ratios for elements from $_{57}$Lu to $_{71}$La, while the experimental data, which were then normalized to the corresponding weighted averages values $(K\beta/K\alpha)_W$were fitted to obtain the semi-empirical intensity ratios. Our findings were then compiled and compared with data from other theories and experiments.

## 2. Method

### *2.1Weighted and weighted recommended average values*

It should be noted that, the weighted average values of the intensity ratios $(K\beta/K\alpha)_W$have already been calculated in [5]. These were initially estimated because there are several published experimental results

$(K\beta/K\alpha)_{Exp}$for a single atomic element. The formula used is the following:

$$\left(\frac{K_\beta}{K_\alpha}\right)_W \pm \varepsilon = \frac{1}{\sum_{i=1}^{N}\frac{1}{\left(\Delta\left(\frac{K_\beta}{K_\alpha}\right)_{Exp-i}\right)^2}} \sum_{i=1}^{N}\frac{\left(\frac{K_\beta}{K_\alpha}\right)_{Exp-i}}{\left(\Delta\left(\frac{K_\beta}{K_\alpha}\right)_{Exp-i}\right)^2} \pm \frac{1}{\left(\sum_{i=1}^{N}\frac{1}{\left(\Delta\left(\frac{K_\beta}{K_\alpha}\right)_{Exp-i}\right)^2}\right)^{\frac{1}{2}}} \quad (1)$$

where $(K\beta/K\alpha)_{Exp-i}$ is the experimental intensity ratio, $\Delta(K\beta/K\alpha)_{Exp-i}$represents the uncertainty of the $i^{th}$ experimental value, and $N$ is the number of experimental data. Figure 1 illustrates the Kβ/Kα experimental values for lanthanides normalized to their corresponding weighted averages values$(K\beta/K\alpha)_W$. We can observe that there is a considerable gap between the weighted average values $(K\beta/K\alpha)_W$ and some experimental data $(K\beta/K\alpha)_{exp}$, especially for the elements $_{62}$Sm, $_{63}$Eu, $_{64}$Gd, $_{65}$Tb, and $_{68}$Er. The abundance of data used in this study is the main cause of this dispersion. All of the experimental values shown in Fig. 1 that were outside of the range [0.9,1.1] have been eliminated in order to remedy this issue. Therefore, new reliable weighted recommended average values $(K\beta/K\alpha)_{WR}$ have been generated using the formula (1) once more. For elements with $Z$ from 57 to 71, these values were used to calculate the empirical and semi-empirical Kβ/Kα intensity ratios.

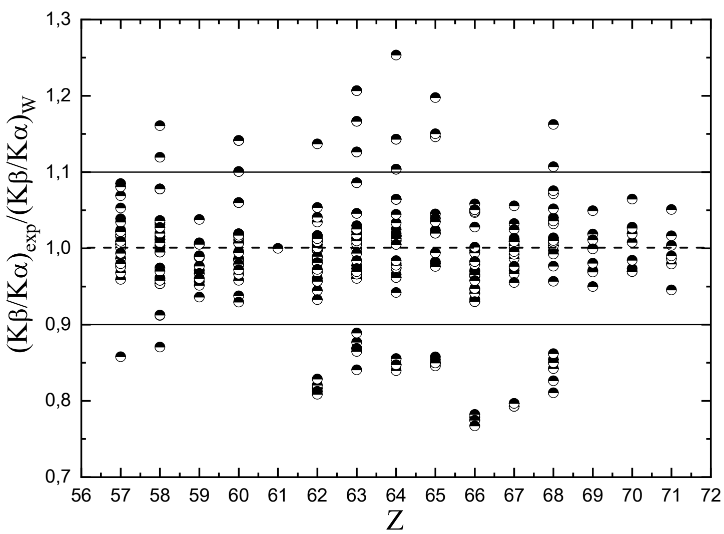


**Figure 1.**The distribution of $(\boldsymbol{K\beta/K\alpha})_{\boldsymbol{exp}}/\ (\boldsymbol{K\beta/K\alpha})_{\boldsymbol{W}}$according to the atomic number $Z$ for lanthanides.

### *2.2 Empirical and Semi-empirical calculations*

The formula below was used to get the empirical and semi-empirical average Kβ/Kα X ray intensity ratios for elements ranging from $_{57}$Lu to $_{71}$La:

$$((K\beta/K\alpha)_{WR}/(1-(K\beta/K\alpha)_{WR}))^{\frac{1}{4}} = \sum_i a_i Z^i \quad (2)$$

Several researchers have already used a method based on this formula, including [6, 7, 5]. In order to use this method, the term$((K\beta/K\alpha)_{WR}/(1-(K\beta/K\alpha)_{WR})^{\frac{1}{4}}$must be fitted after being plotted against the atomic number *Z*, as seen in Fig. 2. A basic third-degree polynomial is employed for fitting:

$$((K\beta/K\alpha)_{WR}/(1-(K\beta/K\alpha)_{WR})^{\frac{1}{4}} = \sum_{n=0}^{3} a_n Z^n = g(z) \quad (3)$$

with: $a_0$=1.95251; $a_1$=-0.06514; $a_2$= 0.00113; and $a_3$=-6.34467 × 10$^{-6}$.
where $(K\beta/K\alpha)_{WR}$ refers to the weighted recommended average values of the intensity ratios.

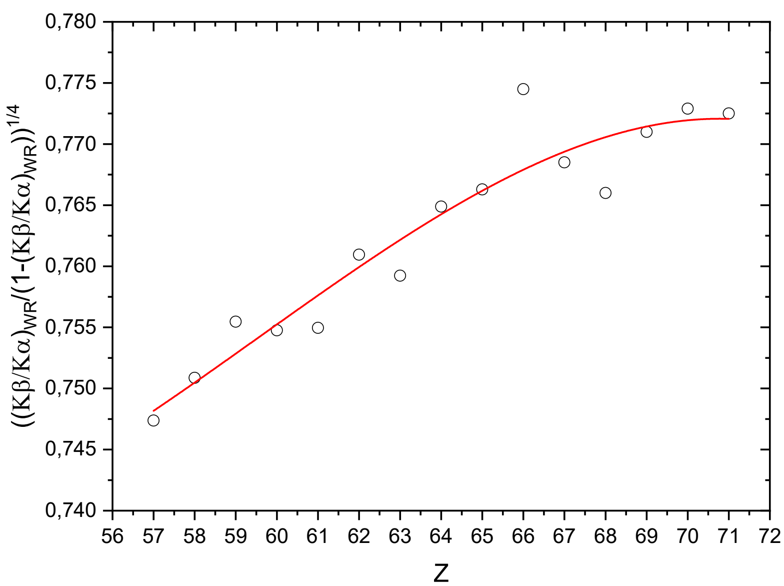


**Figure 2.** Distribution of $((K\beta/K\alpha)_{WR}/(1-(K\beta/K\alpha)_{WR})^{\frac{1}{4}}$ as a function of The atomic number*Z*.

As a result, new empirical average Kβ⁄Kα X-ray intensity ratios $(K\beta/K\alpha)_{emp}$ have been determined using the following equation:

$$\left(\frac{K\beta}{K\alpha}\right)_{emp} = \frac{g(Z)^4}{1+g(Z)^4} \quad (4)$$

After the out-of-range data in Fig.3 were removed, the remaining points were fitted by another third-degree polynomial:

$$S = \frac{(K\beta/K\alpha)_{Exp}}{(K\beta/K\alpha)_W} = \sum_{i=1}^{3} b_i Z^i = f(Z) \quad (5)$$

with: $b_0$=18.22832; $b_1$= -0.81243; $b_2$= 0.01273; and $b_3$=-6.6332× $10^{-5}$.
Semi-empirical average Kβ⁄Kα X ray intensity ratios can be expressed as follows by considering both equations (4) and (5):

$$\left(\frac{K\beta}{K\alpha}\right)_{Semi-emp} = f(Z) \times \frac{g(Z)^4}{1+g(Z)^4} \quad (6)$$

Table 1 summarizes the semi-empirical and empirical calculations of the Kβ/Kα intensity ratios for lanthanides.

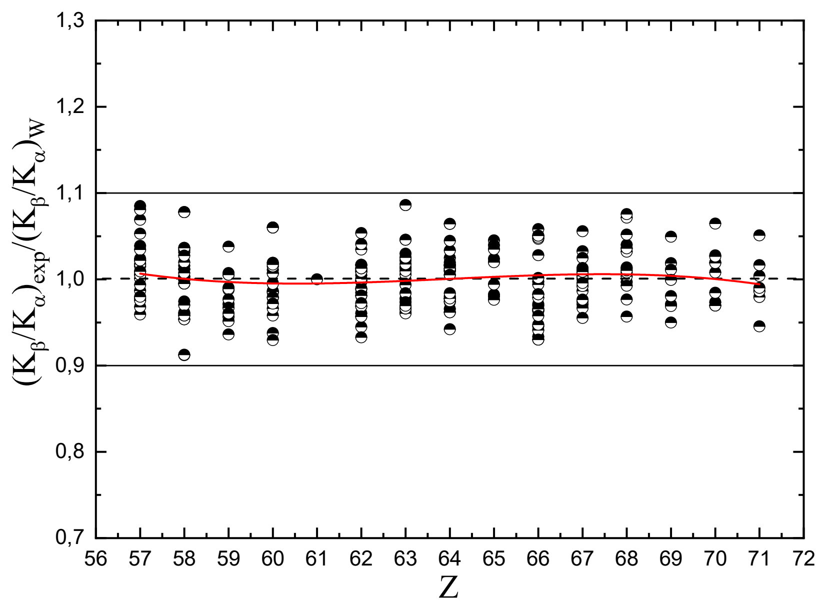


**Figure 3.**The distribution of $(K\beta/K\alpha)_{Exp}/\ (K\beta/K\alpha)_W$ according to the atomic number *Z* for lanthanides, after the out-of-range data was removed.

**Table 1.** The semi-empirical and empirical calculations of Kβ/Kα intensity ratios for lanthanides.

| Z | Empirical | Semi-empirical |
|---|---|---|
| 57 | 0.2268 | 0.2257 |
| 58 | 0.2286 | 0.2260 |
| 59 | 0.2304 | 0.2269 |
| 60 | 0.2323 | 0.2283 |
| 61 | 0.2341 | 0.2300 |
| 62 | 0.2359 | 0.2319 |
| 63 | 0.2376 | 0.2339 |
| 64 | 0.2392 | 0.2359 |
| 65 | 0.2406 | 0.2378 |
| 66 | 0.2418 | 0.2393 |
| 67 | 0.2428 | 0.2404 |
| 68 | 0.2434 | 0.2409 |
| 69 | 0.2438 | 0.2407 |
| 70 | 0.2438 | 0.2397 |
| 71 | 0.2434 | 0.2377 |

## 3. Results anddiscussion

Fig. 4 illustrates the comparison between our semi-empirical calculation, theoretical values from Scofield [4], experimental measurements from Ertugrul [3], and semi-empirical values from Daoudi [8]. It can be seen that the theoretical, experimental, and semi-empirical values agree fairly

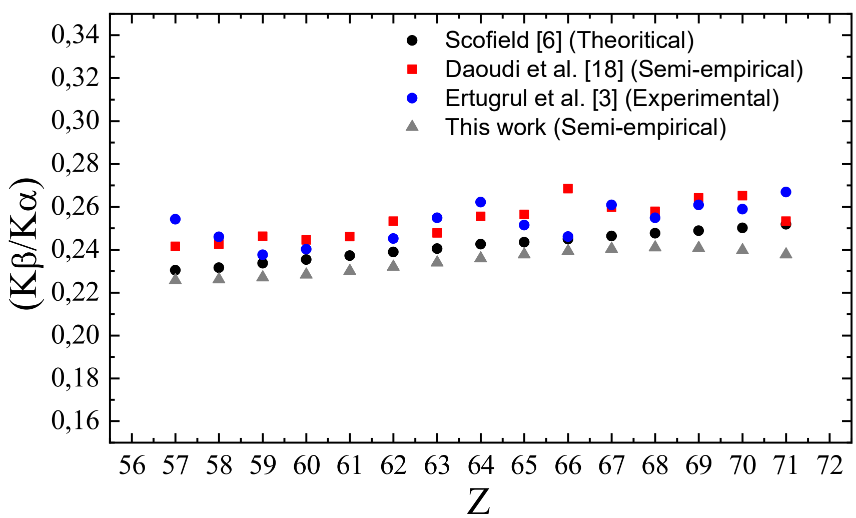


**Figure 4.**Comparison between the theoretical values of Scofield [4], the semi-empirical values of Daoudi et al. [8], the experimental data of Ertuğrul [3] and our results.

well with one another. Despite some elements as: $_{57}$La and $_{66}$Dy showing a deviation of 12.6% and 12.2% with [3] and [8], respectively, the four plots are generally in a very good agreement.

## 5. Conclusion

In this research, newaverage Kβ/KαX-ray intensity ratios for lanthanides, have been determined empirically and semi-empirically, and presented, together with their fitting parameters. Our results were in good agreement with other published values for the chosen atomic number range.

## References


[1] M. I. Marques, M. C. Martins et J. G. Ferreira, "The experimental relative intensity Kβ/Kα in elements with 33⩽ Z⩽ 57," J. Phys. B: Atom. Mol. Phys.**13** (1980) 41–45.

[2] M. E. Şahin, L. Demir et G. Budak, "Measurement of K X-ray fluorescence cross-sections and yields for 5.96 keV photons," Appl. Radiat. Isot.**63**(2005) 141–145.

[3] B. Ertuğral, G. Apaydın, U. Çevik, M. Ertuğrul et A. İ. Kobya, "Kβ/Kα X-ray intensity ratios for elements in the range 16⩽ Z⩽ 92 excited by 5.9, 59.5 and 123.6 keV photons," Radiat. Phys. Chem.**76**(2007) 15–22.

[4] J. H. Scofield, "Relativistic Hartree-Slater values for K and L X-ray emission rates," At. Data Nucl. Data Tables.**14** (1974) 121–137.

[5] A. Hamidani, S. Daoudi, A. Kahoul, J. M. Sampaio, J. P. Marques, F. Parente, S. Croft, A. Favalli, N. Kup Aylikci, V. Aylikci, Y. Kasri, K. Meddouh, "Updated database, semi-empirical and theoretical calculation of Kβ/Kα intensity ratios for elements ranging from 11Na to 96Cm". At. Data Nucl. Data Tables. (2022) 101549.

[6] N. K. Aylikci, V. Aylikci, A. Kahoul, E. N. Tiraşoğlu, I. H. Karahan et E. R. Cengiz, "Effect of p H treatment on K-shell x-ray intensity ratios and K-shell x-ray-production cross sections in ZnCo alloys," Phys. Rev. A. **84** (2011) 042509.

[7] A. Kahoul, N. K. Aylikci, V. Aylikci, B. Deghfel, Y. Kasri et M. Nekkab, "New procedure calculation of photon-induced Kβ/Kα intensity ratios for elements 16S to 92U," J. Radiat. Res. Appl. Sci.**7** (2014) 346–362.

[8] S. Daoudi, A. Kahoul, N. K. Aylikci, J. M. Sampaio, J. P. Marques, V. Aylikci, Y. Sahnoune, Y. Kasri et B. Deghfel, "Review of experimental photon-induced Kβ/Kα intensity ratios," At. Data Nucl. Data Tables. **132** (2020) 101308.