Calculation of K-Shell Fluorescence Yields for Low-Z Elements

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Abstract. The analytical methods based on X-ray fluorescence are advantageous for practical applications in a variety of fields including atomic physics, X-ray fluorescence surface chemical analysis and medical research and so the accurate fluorescence yields (ω_K) are required for these applications. In this contribution we report a new parameters for calculation of K-shell fluorescence yields (ω_K) of elements in the range of 11≤Z≤30. The experimental data are interpolated by using the famous analytical function $\left(\omega_K/(1-\omega_K)\right)^{1/q}$ (were q=3, 3.5 and 4) vs Z to deduce the empirical K-shell fluorescence yields. A comparison is made between the results of the procedures followed here and those theoretical and other semi-empirical fluorescence yield values. Reasonable agreement was typically obtained between our result and other works.

Keywords : Inner-shell ionization process, K-shell fluorescence yields
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INTRODUCTION

The theoretical, experimental and analytical methods for calculation of x-ray production cross sections, the fluorescence yields,… for different elements is very important because of the large number of application in various areas of physics chemistry and medical research. Several attempts were made, in a tabular form [1-4], for measuring and calculating the K-shell fluorescence yields for a wide range of elements. A large deviations were generally observed between the theoretical and the experimental values. These situations motivated the authors to perform fittings with

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analytical functions based on the available experimental data to derive the empirical K-shell fluorescence yields. In this paper the empirical K-shell fluorescence yields of elements in the range 11≤Z≤30 were deduced from the fittings of all the experimental values. Finally, the obtained results were presented in a tabular form and compared with theoretical and other semi-empirical fluorescence yield values.

ANALYTICAL FORMULAS

The database used in the present work rely on our two compilations [5-6]. In addition to these compilations, we extracted other data from a paper published in 2013 [7]. So, the used experimental data is during the period from 1958 till 2013. The first relation to approximation the K shell fluorescence yields as a function of Z, is given by Wentzel [8]; ($(\omega_K = 10^{-6} Z^4 / (1 + 10^{-6} Z^4))$). Similar relation have been used by Haas [9], Arends [10], Gray [11], Kup Aylikci et al. [12] and Kahoul et al. [5] . In this work to deduced the empirical K-shell fluorescence yield we used the weighted means values of ω_K for different measurement for each element, using the formula $\omega_{K\text{-}W} = \left(\sum_{i=1}^{N} (\Delta\omega_i)^{-2} \right)^{-1} \sum_{i=1}^{N} \left[\omega_i / (\Delta\omega_i)^2 \right]$, with, ω_i is the K-shell fluorescence yield, $\Delta\omega_i$ represent the uncertainty of the experimental values and N is the number of experimental data. We calculated empirical K-subshell fluorescence yields by the direct interpolating of the weighted average experimental data for elements from ^{11}Na to ^{30}Zn. Then we calculated the quantity $\left(\frac{\omega_{K\text{-}W\text{-}\exp}}{1-\omega_{K\text{-}W\text{-}\exp}} \right)^{1/3}$, $\left(\frac{\omega_{K\text{-}W\text{-}\exp}}{1-\omega_{K\text{-}W\text{-}\exp}} \right)^{1/3.5}$ and $\left(\frac{\omega_{K\text{-}W\text{-}\exp}}{1-\omega_{K\text{-}W\text{-}\exp}} \right)^{1/4}$ and plotted them vs the atomic number Z separately (see Figure 1); where, $\omega_{K\text{-}W\text{-}\exp}$ is the weighted K-shell fluorescence yield data.

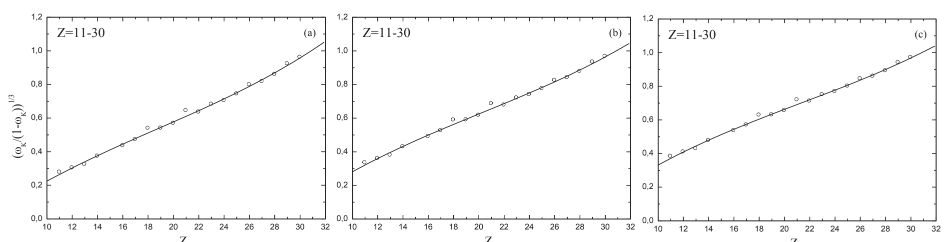

FIGURE 1. Distribution of the experimental Weighted-mean values of the K-shell fluorescence yields $(\omega_K/(1-\omega_K))^{1/q}$, $q = 3, 3.5, 4$ as a function of atomic number. The curve is the fitting according to formula (1)

The analytical function used for the interpolation is the following third degree polynomial:

$$\left(\frac{\omega_K}{1-\omega_K} \right)^{1/q} = \sum_{n=0}^{3} a_n Z^n \quad , q\text{=3, 3.5 and 4} \tag{1}$$

The fitting result is shown in the Figure 1 with a full line.

For the determination of empirical weighted K-shell fluorescence yields we used the formulae:

$$\omega_K = \left(\frac{(f_W(Z))^3}{1+(f_W(Z))^3} \right), \; q=3 \quad (2)$$

$$\omega_K = \left(\frac{(g_W(Z))^{3.5}}{1+(g_W(Z))^{3.5}} \right), \; q=3.5 \quad (3)$$

$$\omega_K = \left(\frac{(h_W(Z))^4}{1+(h_W(Z))^4} \right), \; q=4 \quad (4)$$

with :

$$f_W(Z) = -0.27273 + 0.0726Z - 0.00207Z^2 + 3.40171\times10^{-5}Z^3 \quad (5)$$

$$g_W(Z) = -0.31998 + 0.07125Z - 0.00205Z^2 + 3.63521\times10^{-5}Z^3 \quad (6)$$

$$h_W(Z) = -0.22107 + 0.07271Z - 0.00207Z^2 + 3.23717\times10^{-5}Z^3 \quad (7)$$

RESULTS AND DISCUSSION

We present in Table 1, our empirical K-shell fluorescence yields calculation using the formulae (2), (3) and (4) (for q=3, 3.5 and 4 respectively) for elements in the range 11≤Z≤30. The theoretical values of Kostroun et al. [13], Walters and Bhalla [14] and semiempirical of Bambynek et al. [2], Krause [4] and Hubbell et al. [3] were also introduced. Figure 2 shows the evolution of our K-shell fluorescence yields calculations using the formulae (2), (3) and (4) together with corresponding theoretical calculations of Kostroun et al. [13], Walters and Bhalla [14] and with the semi-empirical values reported by Bambynek et al. [2], Krause [4] and Hubbell et al. [3].

TABLE 1. Present empirical K-shell fluorescence yields compared to Theoretical and Semiempirical values of other authors (a): Kostroun et al. [13], (b): Walters and Bhalla [14], (c): Bambynek et al. [2], (d): Krause [4], (e): Hubbell et al.[5]

Z	This work			Other works				
	Empirical			theoretical		semiempirical fits		
	q=3	q=3.5	q=4	(a)	(b)	(c)	(d)	(e)
11	0.0181	0.0183	0.0187	0.024	0.0224	-	0.023	0.0213
12	0.0270	0.0270	0.0273	0.027	0.0301	-	0.030	0.0291
13	0.0377	0.0376	0.0379	0.033	0.0398	0.036	0.039	0.0387
14	0.0503	0.0500	0,0504	0.044	0.0514	0.047	0.050	0.0504
15	0.0646	0.0643	0,0648	0.057	0.0653	0.060	0.063	0.0642
16	0.0805	0.0803	0,0811	0.073	0.0818	0.076	0.078	0.0804
17	0.0981	0.0980	0.0990	0.091	0.1004	0.094	0.097	0.0989
18	0.1173	0.1173	0.1187	0.111	0.1215	0.115	0.118	0.1199
19	0.1380	0.1382	0.1400	0.132	0.1448	0.138	0.140	0.1432
20	0.1603	0.1606	0.1628	0.155	0.1708	0.163	0.163	0.1687
21	0.1842	0.1845	0.1872	0.183	0.1991	0.190	0.188	0.1962
22	0.2095	0.2100	0.2131	0.212	0.2273	0.219	0.214	0.2256
23	0.2365	0.2369	0.2405	0.243	0.2608	0.249	0.243	0.2564
24	0.2650	0.2654	0.2693	0.276	0.2939	0.281	0.275	0.2885
25	0.2951	0.2954	0.2996	0.310	0.3276	0.314	0.308	0.3213
26	0.3266	0.3268	0.3314	0.344	0.3624	0.347	0.340	0.3546
27	0.3595	0.3596	0.3645	0.379	0.3977	0.381	0.373	0.3880
28	0.3936	0.3937	0.3989	0.414	0.4329	0.414	0.406	0.4212
29	0.4288	0.4289	0.4344	0.448	0.4678	0.446	0.440	0.4538
30	0.4648	0.4650	0.4709	0.482	0.5014	0.479	0.474	0.4857

Despite the quite different procedures have been followed to calculate the K-shell fluorescence yields, the obtained results are generally agree with the theoretical and semi-empirical values for all range of elements $12 \leq Z \leq 30$. The argument for the formula (2) (q=3) is within the range 0% to 12.4% for Kostroun et al. [13], 2.18% to 11.5% for Walters and Bhalla [14], 0% to 7.12% for Bambynek et al. [2], 1.12% to 11% for Krause and 0.12% to 8.87% for Hubbell et al. [3]. The argument for the formula (3) (q=3.5) is within the range 0% to 12.23% for Kostroun et al. [13], 1.55% to 11.48% for Walters and Bhalla [14], 1.44% to 6.68% for Bambynek et al. [2], 0% to 11% for Krause and 0.80% to 8.76% for Hubbell et al. [3]. Finally The argument for the formula (3) (q=4) is within the range 0.51% to 12.92% for Kostroun et al. [13], 0.77% to 10.25% for Walters and Bhalla [14], 1.22% to 7.41% for Bambynek et al. [2], 0% to 2.77% for Krause and 0% to 7.24% for Hubbell et al. [3]. Whereas some differences have been observed with the values of ^{11}Na where we observe a deviation of 32.6% for Kostroun et al. [13], 23.75% for Walters and Bhalla [14], 27.07% for Krause and 17.68% for Hubbell et al. [3] for the empirical values used the formula (2) (q=3). For the formula (3) (q=3.5) the deviation are 31.14% for Kostroun et al. [13], 22.4% for Walters and Bhalla [14], 25.7% for Krause and 16.39% for Hubbell et al. [3]. For q=4 we observed the values of 28.34% for Kostroun et al. [13], 19.78% for Walters and Bhalla [14], 22.99% for Krause and 13.9% for Hubbell et al. [3]. It is thought that this disagreement for this element (Z=11) is due to that the values of K-shell fluorescence yield is small. The measurements of ω_K introduce a supplementary uncertainty on the fluorescence yield than the other elements. Finally, by comparing the deviation between our calculation (formulae (2), (3) and (4)) and the theoretical and semi-empirical ones, we can see that the data of formula (4) (q=4) are more closer than the data deduced for the two other formulae. The formula (4) give a better representation of the experimental data than the other ones (formulae (2) and (3)).

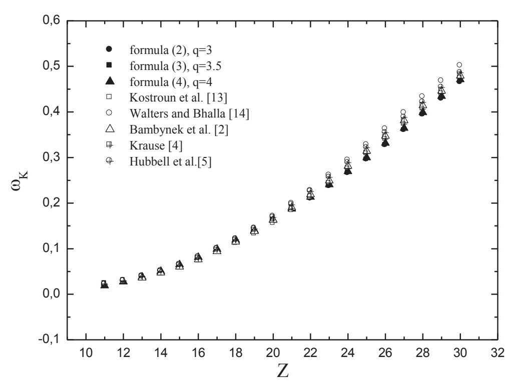

FIGURE 1. The evolution of our K-shell fluorescence yields calculassions using the formulae (2), (3) and (4) together with Theoretical values of Kostroun et al. [13], Walters and Bhalla [14] and with the semi-empirical values reported by Bambynek et al. [2], Krause [4] and Hubbell et al. [3].

CONCLUSION

A new set of K-shell fluorescence yields were determined using simple methods for elements in the atomic region $11 \leq Z \leq 30$. The deduced empirical fluorescence yields according to the different procedures were generally much closer to each other for the whole range of atomic number. The present values were proposed to workers in the field of atomic inner-shell ionization processes.

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