Average M Shell Fluorescence Yields for Elements with 70≤Z≤92

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Abstract. The theoretical, experimental and analytical methods for the calculation of average M-shell fluorescence yield ($\overline{\omega}_M$) of different elements are very important because of the large number of their applications in various areas of physical chemistry and medical research. In this paper, the bulk of the average M-shell fluorescence yield measurements reported in the literature, covering the period 1955 to 2005 are interpolated by using an analytical function to deduce the empirical average M-shell fluorescence yield in the atomic range of 70≤Z≤92. The results were compared with the theoretical and fitted values reported by other authors. Reasonable agreement was typically obtained between our result and other works.

Keywords: average M-shell fluorescence yield, weighted- and unweighted-mean values.
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INTRODUCTION

Several attempts were made, for measuring and calculating the average M-shell fluorescence yields for a wide range of elements. McGuire [1] were used the calculated Auger, Coster-Kronig, super Coster-Kronig, and radiative transition rates to compute atomic *M*-shell Auger, Coster-Kronig, and fluorescence yields for elements in the range 20≤Z≤90. Öz et al. [2] calculated the average M shell fluorescence yields and the total M-shell x-ray fluorescence (MXRF) cross section at 6 keV for elements with 29≤Z≤100. In this paper our research group performs fittings with analytical functions based on the available experimental data to derive the empirical average M shell fluorescence yields for elements with 70≤Z≤92. The experimental data were

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taken from different sources published from 1955 to 2005. Finally, the obtained results were presented in a tabular form and were compared with theoretical and fitted works.

CALCULATION OF AVERAGE M SHELL FLUORESCENCE YIELD

Several attempts have been made to fit experimentally the average M-shell fluorescence yields by empirical formulas. In 1955 Burhop [3] interpolated the available experimental data using the formula $\overline{\omega}_M = 1.7\times10^{-9}(Z-13)^4$. Hubbell et al. [4] have proposed the relation $\overline{\omega}_M = 1.29\times10^{-9}(Z-13)^4$ to determine the average M-shell fluorescence yields in the range 19≤Z≤100. Based on these formulae, the bulk of the average M-shell fluorescence yield measurements for elements from ^{70}Yb to ^{92}U reported in the literature [5-19], covering the period 1955 to 2005 are used to calculate the empirical $\overline{\omega}_M$. First, the quantity $\overline{\omega}_{M-\exp}/(Z-13)^4$ and plotted them vs the atomic number Z for all element in the range 70≤Z≤92. The data are presented in Figure 1 (dots) as a function of the atomic number Z. The analytical function used for the interpolation is the following expression:

$$\frac{\overline{\omega}_{M-\exp}}{(Z-13)^4} = A \qquad (1)$$

To determine the constant A we calculate the average of the quantities $\overline{\omega}_{M-\exp}/(Z-13)^4$ for all elements from ^{70}Yb to ^{92}U, finally we deduced the value of A as: $A = 1.41\times10^{-9}$ The average value of A is shown in Figure 1. To deduce empirical $\overline{\omega}_M$ we used the relation:

$$\overline{\omega}_{M-\exp} = 1.41\times10^{-9}(Z-13)^4 \qquad (2)$$

Second, depending on the famous formula $(\omega/1-\omega)^{1/4} = \sum_{n=0}^{3} b_n Z^n$, we derived a second formula to deduce the empirical average M-shell fluorescence yields. We calculated the quantities $\left(\overline{\omega}_{M\text{-}\exp}/(1-\overline{\omega}_{M\text{-}\exp})\right)^{1/4}$ and plotted them vs the atomic number Z. The data $\left(\overline{\omega}_{M\text{-}\exp}/(1-\overline{\omega}_{M\text{-}\exp})\right)^{1/4}$ are presented in Figure 2 (dots) as a function of the atomic number Z. The analytical function used for the fitting is the following polynomial:

$$\left((\overline{\omega}_{M\text{-}\exp})/(1-\overline{\omega}_{M\text{-}\exp})\right)^{1/4} = \sum_{n=0}^{3} a_n Z^n \qquad (3)$$

Figure 2 shows the fitting results according to the equation (3). To deduce the empirical average M-shell fluorescence yields of elements in the range 70≤Z≤92 for the second method we used the expression:

$$(\overline{\omega}_M)_{emp} = \left((f^4(z))/(1+f^4(z))\right) \qquad (4)$$

with : $f(Z) = 4.18763 - 0.15517\,Z + 0.00202\,Z^2 - 8.38359 \times 10^{-6} Z^3$

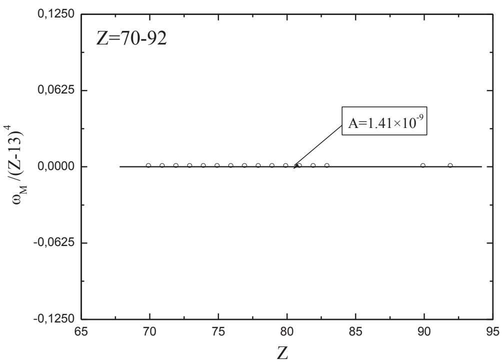

FIGURE 1. Distribution of the experimental average M-shell fluorescence yields $\overline{\omega}_{M-\exp}/(Z-13)^4$ as a function of atomic number Z. The average value of the constant A are also shown.

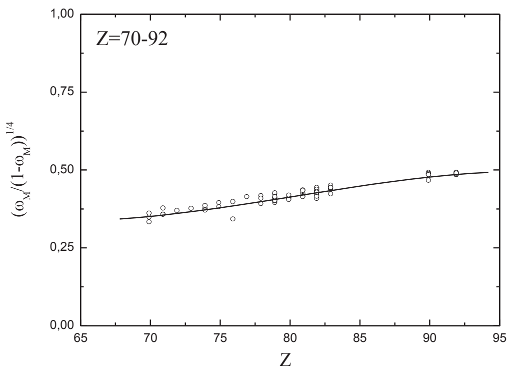

FIGURE 2. Distribution of the experimental values of the M-shell fluorescence yields $\left(\omega_{M\text{-}\exp}/\left(1-\omega_{M\text{-}\exp}\right)\right)^{1/4}$ as a function of atomic number Z. The curve is the fitting according to formula (3)

RESULTS AND DESCUSSION

The calculated empirical average M-shell fluorescence yields according to the different methods mentioned before (formulae (1) and (3)) in the atomic range $70 \leq Z \leq 92$ have been tabulated in Table 1. In the same table we presented the theoretical calculation of McGuire [1] and the fitted values of Öz et al. [2] and Hubbell et al. [20].

TABLE 1. Present empirical average M shell fluorescence yields $\overline{\omega}_M$ compared to the theoretical calculation of McGuire [1] and the fitted values of Öz et al. [2] and Hubbell et al. [20].

	Empirical (this work)		Theoretical	Fitted	
Z	*Formula (1)*	*Formula (3)*	McGuire [1]	Öz et al. [2]	Hubbell et al. [20]
^{70}Yb	0.0149	0.0145	0.0154	0.0159	0.0136
^{71}Lu	0.0160	0.0153	0.0169	0.0173	0.0146
^{72}Hf	0.0171	0.0161	0.0186	0.0186	0.0156
^{73}Ta	0.0183	0.0171	0.0208	0.0201	0.0167
^{74}W	0.0195	0.0183	0.0211	0.0213	0.0179
^{75}Re	0.0208	0.0195	0.0221	0.0226	0.0191
^{76}Os	0.0222	0.0209	0.0234	0.0239	0.0203
^{77}Ir	0.0237	0.0223	0.0236	0.0251	0.0216
^{78}Pt	0.0252	0.0239	0.0247	0.0264	0.0230
^{79}Au	0.0268	0.0256	0.0270	0.0276	0.0245
^{80}Hg	0.0284	0.0274	0.0288	0.0289	0.0260
^{81}Tl	0.0301	0.0293	0.0305	0.0303	0.0275
^{82}Pb	0.0320	0.0312	0.0320	0.0317	0.0292
^{83}Bi	0.0339	0.0333	0.0334	0.0332	0.0310
^{84}Po	0.0358	0.0353	0.0344	0.0348	0.0328
^{85}At	0.0379	0.0374	0.0357	0.0366	0.0347
^{86}Rn	0.0400	0.0396	0.0374	0.0385	0.0366
^{87}Fr	0.0423	0.0417	0.0404	0.0407	0.0387
^{88}Ra	0.0446	0.0437	0.0442	0.0431	0.0408
^{89}Ac	0.0470	0.0457	0.0488	0.0458	0.0430
^{90}Th	0.0496	0.0476	0.0543	0.0486	0.0453
^{91}Pa	0.0522	0.0493	-	0.0522	0.0477
^{92}U	0.0549	0.0508	-	0.0560	0.0502

To display our calculation graphically Figure 3 shows the empirical calculation (using formulae (1) and (3)) normalized to their corresponding theoretical calculations of McGuire [1] and the fitted values of Öz et al. [2] and Hubbell et al [3] have been evaluated as a function of the atomic number Z. Despite the quite different procedures have been followed to calculate the average M-shell fluorescence yields, the obtained results are generally agree with the theoretical and fitted values in all the range of atomic number $70 \leq Z \leq 92$ for the two methods (formulae (1) and (3)). The argument in the formula (1) is within the range 0.12% to 12.14% for McGuire [1], 0.07% to 9.08% for Öz et al. [2] and 9.06% to 9.62% for Hubbell et al. [20]. For the formula (3), the deviation is within the range 0% to 10.49% for McGuire [1], 0.30% to 13.07% for Öz et al. [2] and 0% to 11.04% for Hubbell et al. [20]. It is noted from the above discussion that the present results can be used for analytical applications and more experimental and empirical determinations are needed to give more insights for the full knowledge of the average M-shell fluorescence yields.

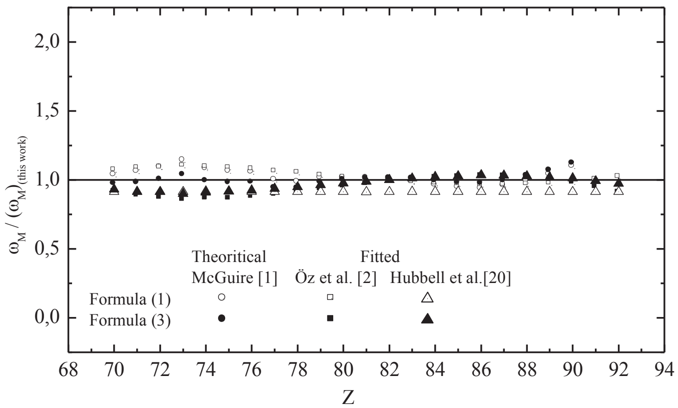

FIGURE 3. The empirical calculation (using formulae (1) and (3)) normalized to their corresponding theoretical calculations of McGuire [1] and the fitted values of Öz et al. [2] and Hubbell et al [3] as function of the atomic number Z.

CONCLUSION

The fluorescence yield measurements reported in the literature covering the period 1955 to 2005 were used to calculate the average M-shell fluorescence yields. A new set of average M-shell fluorescence yields were determined using simple methods for elements in the atomic region $70 \leq Z \leq 92$. The deduced empirical fluorescence yields according to the different procedures were generally much closer to each other for the whole range of atomic number. In addition to the available experimental and theoretical average M-shell fluorescence yields, the present values were proposed to workers in the field of atomic inner-shell ionization processes.

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