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M-Shell Fluorescence Yields Curve of heavy elements

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Abstract

Accurate experimental data regarding the X-ray production (XRP) cross sections, ionization cross sections and the fluorescence yields are very important because of the large number of their applications in various areas of physical chemistry and medical research.
The average M-shell fluorescence yields, $\overline{\omega}_M$, have been evaluated for element $_{79}$Au using our database of measured experimental values. We have calculated the average M-shell fluorescence yield using the experimental data measured by different groups covering the wide period. We have interpolated these values of the experimental data by using the analytical function $(\overline{\omega_M}/(1-\overline{\omega_M}))^{1/4}$ as function of the atomic number (Z) to deduce the empirical average M-shell fluorescence yield. The results have been compared with other theoretical, experimental and empirical values reported in the literature and a reasonable agreement has beenobtained.

Keywords: Average M-shell fluorescence yield, empirical fluorescence yields.

Introduction

The theoretical, experimental and analytical methods for calculating the x-ray production cross sections, fluorescence yields, vacancy transfer probabilities and intensity ratios of different elements are very important because of the large number of their applications in various areas of physical chemistry and medical research. Therefore, an accurate average M-shell fluorescence yield ($\overline{\omega_M}$)is required for these applications. Several attempts were made in the past to measure and estimate the average M-shell fluorescence yields for a wide range of elements. McGuire [1] calculated the Auger, Coster-Kronig, super Coster-Kronig and radiative transition rates using the non-relativistic Hartree-Fock-Slater (HFS) wave function with Herman-Skillman potential for elements in the range of 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 photon energy of 6 keV for elements with 29≤Z≤100. For the measured values, the authors used different techniques that vary according to the experimental conditions such as the ionization process, the target material and the type of detectors. In 1984 Shatendra et al. [3] measured the average M-shell fluorescence yields in ^{79}Au, ^{82}Pb, ^{90}Th and ^{92}U using the photoionization of the M shell by 5.9 keV X-rays from a ^{55}Fe radioactive source and analyzing the M X-rays by a Si(Li) low-energy photon spectrometer. The average M shell fluorescence yields were computed by Puri et al. [4] using the M X-ray production (XRF) cross section values and the theoretical M shell photoionization cross section for the elements with 71≤Z≤92 at incident photon energy of 5.96 keV. In this paper we have performed the fittings using analytical function based on the available experimental data to derive the empirical average M-shell fluorescence yields for elements with 70≤Z≤92. These values of the experimental data have been interpolated by using the analytical function$(\overline{\omega_M}/(1-\overline{\omega_M}))^{1/4}$as function of Z to deduce the empirical average M-shell fluorescence yield. Finally, the obtained results have been presented in a tabular form and compared with theoretical, fitted and other experimental works.

1. Method and Results

The empirical average M-shell fluorescence yields are calculated using the experimental values published in the period 1955 to 2005 [5]. First, we have presented the quantities $\left((\overline{\omega_M})_{exp}/1-(\overline{\omega_M})_{exp}\right)^{1/4}$ as function of Z, with $(\overline{\omega}_M)_{exp}$ is the experimental average M shell fluorescence yields. The reduced experimental data $\left((\overline{\omega_M})_{exp}/1-(\overline{\omega_M})_{exp}\right)^{1/4}$ are plotted in Figure 1 as a function of the atomic number Z. As seen in the Figure1 there is a linear dependence between $\left((\overline{\omega_M})_{exp}/1-(\overline{\omega_M})_{exp}\right)^{1/4}$ and Z. Consequently we used a simple linear function for these interpolations:

$$\left((\overline{\omega_M})_{exp}/1-(\overline{\omega_M})_{exp}\right)^{1/4} = f(Z) = a_1 = a_2 \times Z \quad (1)$$

With
$a_1 = (-84.407 \pm 13.431) \times 10^{-3}$ *and* $a_2 = (6.235 \pm 0.1654) \times 10^{-3}$.

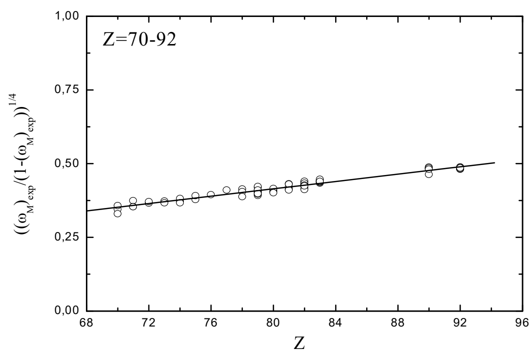

Figure 1. The distribution of the reduced experimental values $\left((\overline{\omega_M})_{exp}/1-(\overline{\omega_M})_{exp}\right)^{1/4}$as a function of atomic number Z. The curve is the fitting according to Eq.1 .

Fig. 1 shows the fitting results according to the equation (1) (full line). To deduce the empirical average M-shell fluorescence yields of elements in the range 70≤Z≤92 we used the formula:

$$(\overline{\omega_M})_{emp} = \left(\frac{f^4(Z)}{1+f^4(Z)}\right) \quad (2)$$

Table 1.a and table 1.b presents our average M-shell fluorescence yields according to equations (2) for the elements in the atomic range 70≤Z≤92. In the same table we have also presented the theoretical calculation of McGuire [1], the fitted values of Öz et al. [2] and Hubbell et al. [6] and the experimental results of Apaydin et al. [7] and Puri et al. [4], and added the fitted values of Kaur and Mittal [8] using the non-relativistic HFS values of McGuire [1] and the relativistic DHS values of Chen et al. [9, 10] respectively. For the fitted average M-shell fluorescence yields of Kaur and Mittal [8] we used the M-subshell fluorescence yields $\omega_{Mi}(i = 1-5)$ and Coster-Kronig yield $f_{Mij}(i = 1-4, j = 2-5)$deduced from the MFCKYLD

code and the M-shell photoionization cross section $\sigma_{Mi}(i = 1 - 5)$ at 8 keV of Scofield [11].

Table 1.a Present empirical average M shell fluorescence yields derived from Eq. (1) compared to theoretical, fitted and experimental values of other authors.

Z	This work	Theoretical		Fitted			
						Kaur and Mittal [8]	
	$(\overline{\omega}_M)_{emp}$	McGuire [1]	Chen et al. [9,10]	Öz et al. [2]	Hubbell et al. [6]	McGuire's values	Chen's values
Z=70,Yb	0.0151	0.0154	-	0.0159	0.0136	0.0156	0.0158
Z=71,Lu	0.0162	0.0169	0.0172	0.0173	0.0146	0.0172	0.0162
Z=72,Hf	0.0173	0.0186	0.0183	0.0186	0.0156	0.0188	0.0175
Z=73,Ta	0.0185	0.0208	0.0193	0.0201	0.0167	0.0204	0.0189
Z=74,W	0.0198	0.0211	-	0.0213	0.0179	0.0218	0.0203
Z=75,Re	0.0211	0.0221	-	0.0226	0.0191	0.0229	0.0217
Z=76,Os	0.0225	0.0234	-	0.0239	0.0203	0.0235	0.0230
Z=77,Ir	0.0239	0.0236	0.0240	0.0251	0.0216	0.0232	0.0242
Z=78,Pt	0.0254	0.0247	0.0254	0.0264	0.0230	0.0249	0.0255
Z=79,Au	0.0270	0.0270	0.0268	0.0276	0.0245	0.0270	0.0268
Z=80,Hg	0.0286	0.0288	-	0.0289	0.0260	0.0290	0.0283
Z=81,Tl	0.0304	0.0305	0.0298	0.0303	0.0275	0.0307	0.0299
Z=82,Pb	0.0321	0.0320	0.0313	0.0317	0.0292	0.0322	0.0315
Z=83,Bi	0.0340	0.0334	0.0329	0.0332	0.0310	0.0333	0.0331
Z=84,Po	0.0359	0.0344	-	0.0348	0.0328	0.0344	0.0347
Z=85,At	0.0379	0.0357	-	0.0366	0.0347	0.0357	0.0364
Z=86,Rn	0.0400	0.0374	-	0.0385	0.0366	0.0372	0.0381
Z=87,Fr	0.0422	0.0404	-	0.0407	0.0387	0.0394	0.0399
Z=88,Ra	0.0444	0.0442	-	0.0431	0.0408	0.0426	0.0416
Z=89,Ac	0.0467	0.0488	-	0.0458	0.0430	0.0470	0.0432
Z=90,Th	0.0491	0.0543	0.0451	0.0486	0.0453	0.0541	0.0447
Z=91,Pa	0.0516	-	-	0.0522	0.0477	-	-
Z=92,U	0.0542	-	0.0491	0.0560	0.0502	-	-

Table 1.b Present empirical average M shell fluorescence yields derived from Eq. (1) compared to experimental values of other authors.

Z	This work $(\overline{\omega}_M)_{emp}$	Experimental Apaydin et al. [7]	Experimental Puri et al. [4]
Z=70,Yb	0.0151	0.0140	-
Z=71,Lu	0.0162	0.0192	0.0154
Z=72,Hf	0.0173	-	0.0176
Z=73,Ta	0.0185	-	0.0190
Z=74,W	0.0198	0.0188	-
Z=75,Re	0.0211	0.0200	-
Z=76,Os	0.0225	-	-
Z=77,Ir	0.0239	-	0.0276
Z=78,Pt	0.0254	-	0.0285
Z=79,Au	0.0270	0.0266	0.0300
Z=80,Hg	0.0286	0.0269	-
Z=81,Tl	0.0304	0.0305	-
Z=82,Pb	0.0321	0.0312	0.0334
Z=83,Bi	0.0340	0.0341	0.0356
Z=84,Po	0.0359	-	-
Z=85,At	0.0379	-	-
Z=86,Rn	0.0400	-	-
Z=87,Fr	0.0422	-	-
Z=88,Ra	0.0444	-	-
Z=89,Ac	0.0467	-	-
Z=90,Th	0.0491	-	0.0512
Z=91,Pa	0.0516	-	-
Z=92,U	0.0542	0.0516	0.0514

In order to present the deviation of the various empirical M-shell fluorescence yields, figure 2 show the theoretical calculation of McGuire [1] and Chen et al.[9,10], the fitted values Öz et al. [2], Hubbell et al. [6] and Kaur and Mittal [8] and the experimental results of Apaydin et al. [7] and Puri et al. [4] and the empirical results deduced from equations (2) as function of Z. It can be seen that the present empirical average M-shell fluorescence yields are in good agreement with the theoretical, fitted and experimental values for all elements in the range of 70≤Z≤92.

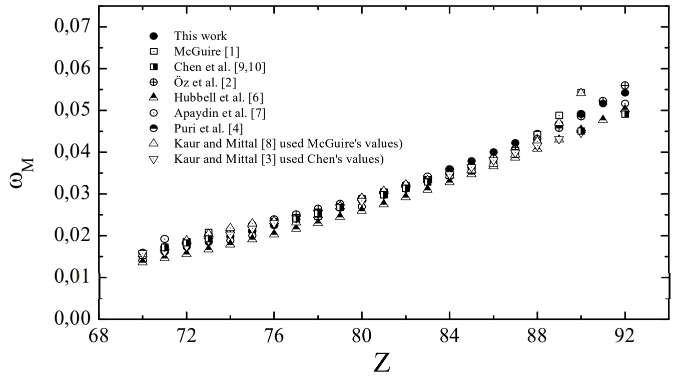

Figure 2. The theoretical calculation of McGuire [1] and Chen et al. [9, 10], the fitted values of Öz et al. [2], Hubbell et al. [6] and Kaur and Mittal [8] (used the non-relativistic Hartree-Fock-Slater (HFS) values of McGuire [1] and the relativistic Dirac-Hartree-Slater (DHS) values of Chen et al. [9,10]) and the experimental results of Apaydin et al. [7] and Puri et al. [4] and the present empirical average M-shell fluorescence yieldsfrom this work as a function of atomic number Z.

2. Conclusion

The average M-shell fluorescence yield measurements reported in the literature were used to deduce the empirical 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≤Z≤90. The deduced empirical fluorescence yields according to the different procedures were generally in a good agreement with other groups. Our results are important for future measurements in the field of atomic inner-shell ionization processes and other application in physical chemistry.

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