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L_1 sub-shell fluorescence yield for lanthanide elements with $58 \leq Z \leq 71$

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Abstract

The lanthanides comprise the largest naturally occurring group in the periodic table, the “rare earth elements” which group the fourteen elements from 58Ce to 71Lu, which are also electropositive and reactive metals, except for yttrium. The researchers used these elements and calculated the yield of fluorescence (ω_{L1}) by theoretical, experimental and analytical methods due to the large number of their applications in various fields of physical chemistry and medical research. In the present work, all the experimental L_1 sub-shell fluorescence yields taken from distinctive sources are studied. A detailed analysis of these data, and a table with weighted average values (ω_{L1W}) of these parameters are presented. New recommended values (ω_{WR}) are obtained dividing the experimental ratios (ω_{exp}) by the weighted ratios (ω_W) and removing out-of-range values (less than 0.8 or greater than 1.2). At that point, new values of average fluorescence yields were deduced using an interpolation that involves the well-known analytical function $[\omega_{Li-}\ /(1-\omega_{Li-WR})]^{1/4}$as function of the atomic number Z, and then semi-empirical data were deduced by fitting the ratio $R = \frac{\bar{\omega}_{Li\text{-}exp}}{\bar{\omega}_{Li\text{-}W}}$, for the three shells. A comparison was made with other theoretical, experimental, and empirical values reported in the literature. An evident correlation was observed between our result and other works.

Keywords: X-rays, atomic fundamental parameters fluorescence yields, recommended weighted average values, semi-empirical calculation.

I. Introduction

X-ray fluorescence parameters ‘’fluorescence yields, production cross-sections, and intensity ratios ...’’ has a great important for increasing need for analysis of new materials. These parameters are required in many applications apart from the atomic physics studies including the surface chemical analysis, dosimetric computations for health physics, cancer therapy and industrial irradiation processing. In the past, several attempts were made to calculate the L_i (i=1,2,3) sub-shell fluorescence yields using a theatrical model, or by fitting the experimental data (empirical and semi-empirical formulae) for a wide range of elements. In this paper, it was focused on the L_1 sub-shell fluorescence yields and the deduction and improvement of their semi-empirical values for $58 \leq Z \leq 71$.

II. Computational method

The reported experimental values of the compiled L_i sub-shell fluorescence yields were extracted from the referenced articles (432 values for L_1 sub-shell in the atomic range $80 \leq Z \leq 96$) were taken in a three to fourth-digit format with their associated errors. While reviewing this data, we noticed that some values are far from each other, so we used the weighted average values given by the following formula [1]:

$$\Omega_W = \left(\sum_{i=1}^{N}(\Delta(\omega_{exp})_i)^{-2}\right)^{-1} \sum_{ji=1}^{N}\left(\omega_{exp} / (\Delta(\omega_{exp})_i)^2\right) \qquad (1)$$

Where $(\omega_{exp})_i$ represents the i^{th} experimental value, $\Delta(\omega_{exp})_i$ is the uncertainty of the i^{th} experimental value, and N indicates the number of experimental data points.

In order to obtain reliable semi-empirical values, we have calculated the ratio of the experimental fluorescence yields with respect to the weighted average value: R= $(\omega)_{exp} / (\omega)_{W}$ then we have plotted the ratio R against the atomic number Z, as shown in Figs. 1. After we examined the weighted average values, we found that most of the experimental data point's ω are centered around the weighted average value of all elements. However, some values are much dispersed compared to the weighted values, in particular for the heavy elements due to the large number of experimental data points in this region, and therefore the large number of references used to collect data, experimental methods and conditions. To obtain a reliable weighted average value and a good semi-empirical result, with sufficient data points, we included only the experimental data points for which the ratio S varies within the range of [0.8 - 1.2].

About 41 values outside the interval [0.8 - 1.2] have been removed. Therefore, using once again formula (1) new recommended weighted average values $\omega_{L\text{-}WR}$ have been obtained. These recommended weighted average values $\omega_{L\text{-}WR}$ were used to calculate the empirical L-shell fluorescence yields. The approximation $(\omega_{L\text{-}WR} / 1\text{-} \omega_{L\text{-}WR})^{1/4}$ is presented as function of Z and plotted in Figure 2. Consequently, we used the following function for these interpolations:

$$(\omega_{Li\text{-}WR} / 1\text{-} \omega_{L\text{-}WR})^{1/4}=f(Z)=\sum_{n=0}^{3} a_n Z^n \quad (2)$$

with:

$$a_0=4{,}65542\pm 24{,}82493, \quad a_1= -0{,}21449\pm 1{,}15888$$

$$a_2=0{,}00358\pm 0{,}01799, \quad a_3= -1{,}93045.10^{-5}\pm 9{,}29352.10^{-5}$$

For the determination of empirical *L* shell fluorescence yields, formula (2) can be rewritten as follows:

$$\omega_{Li\ emp} =(f(z) /1+ f(z))^4 \quad (3)$$

It must be emphasized that the fitting of formula (2) and the associated coefficients are only valid in the region of atomic number $80 \leq Z \leq 96$, and the extension out of this region might take an unpredictable course.

Finally for the determination of the average semi-empirical fluorescence yields, it is calculated using the two expressions (2) and (3) as:

$$\omega_{Li\ S\text{-}emp} = f(z)\ .\ \omega_{Li\ emp} \quad (4)$$

III. RESULTAT AND DISSCUSION

The present calculation of semi-empirical average L sub-shell fluorescence yields according to equation (4) for all elements in the region $58 \leq Z \leq 71$ is listed in Table 1. The theoretical values of Krause at al [2], the fitted results of Puri et a. [3], Campbell. [4], Sahnoun et al [5] and the experimental measurements of Bonzi and Badiger, [6] Bansal et al., [7] Kacal et al., [8] are also added in the same table. Because there are no experimental reported data for the element $_{61}$Pm the value of element is not in this table. The empirical average L_i sub-shell fluorescence yields obtained are compared with the results of Krause at al [2], the fitted results Puri et al. [3], Campbell. [4], Sahnoun et al [5] Bonzi and Badiger, [6] Bansal et al., [7] and Kacal et al., [8] as a function of the atomic number Z and are show in figure 3.

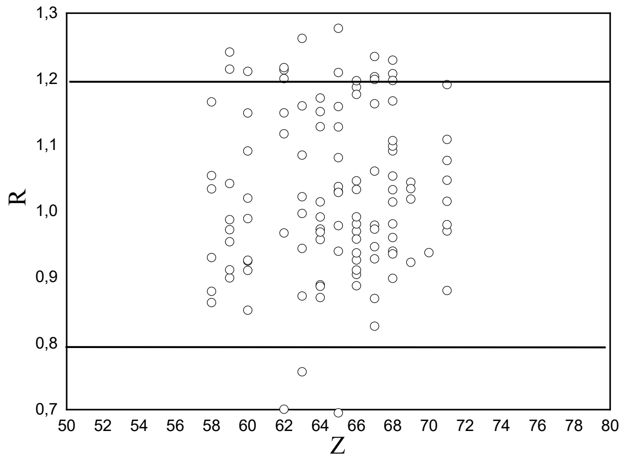

Fig. 1. The distribution of R= $(\omega)_{exp} / (\omega)_{W}$ for each reference from which the databases are extracted according to the atomic number Z.

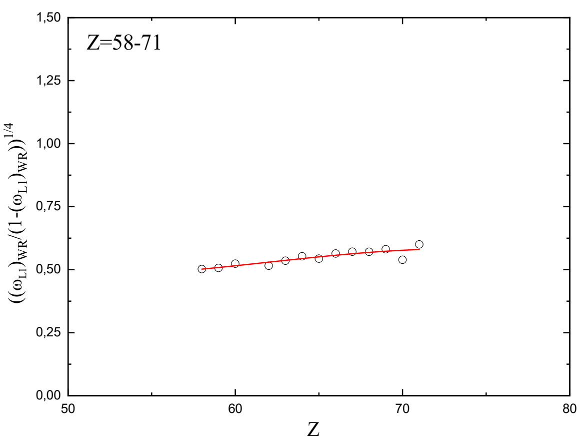

Fig. 2. Distribution of $(\omega_{L\text{-}WR} / 1\text{-} \omega_{L\text{-}WR})^{1/4}$ as a function of atomic number Z.

TABLE I. SEMI-EMPIRICAL (THIS WORK), THEORETICAL, fiTTED AND EXPERIMENTAL (OTHER WORKS) AVERAGE L SUB-SHELL fluORESCENCE YIELDS FOR ALL ELEMENTS IN THE REGION $58 \leq Z \leq 71$.

Z-element	**This work**	**Theo.**	**Fitt**			**Exp**
	Semi-Emp	**[2]**	**[3]**	**[4]**	[5]	
Z = 58, Ce	0,0619	0,058	0,061	--	0,062	--
Z = 59, Pr	0,06772	0,061	0,065	--	0,0663	0,065**[6]**
Z = 60, Nd	0,07383	0,064	0,067	--	0,0706	--
Z = 61, Pm	0,08023	0,066	0,071	--	0,075	--
Z = 62, Sm	0,08688	0,071	0,075	0,075	0,0793	--
Z = 63, Eu	0,09376	0,015	0,078	0,08	0,0836	0,079**[7]**
Z = 64, Gd	0,10085	0,079	0,083	0,09	0,0879	0,085**[7]**
Z = 65, Tb	0,1081	0,083	0,087	0,1	0,0921	--
Z = 66, Dy	0,11549	0,089	0,091	0,1	0,0963	0,096**[7]**
Z = 67, Ho	0,12298	0,094	0,095	0,11	0,1004	0,0107[**7**]
Z = 68, Er	0,13052	0,1	0,105	0,12	0,1043	0,093**[8]**
Z = 69,Tm	0,13807	0,106	0,109	0,13	0,1081	--
Z = 70, Yb	0,14558	0,111	0,114	0,13	0,1118	--
Z = 71, Lu	0,15301	0,12	0,12	0,14	0,1153	0,0115**[8]**

In figure 1, agreement between our empirical L1 sub-shell fluorescence yields results and the theoretical, fitted and experimental values is good, especially in the range 58□Z□62. In addition, our data differ in percentage with the theoretical values of Krause (1979) [2], the argument varies from 6.30% to 13.31% for the first three elements, and deviation varies from 17.73% to 23.75% for Z high. Where the relative difference (RD) between the obtained empirical values and other calculations were obtained using the expression $RD(\%) = \left| (\omega - \omega_{emp}) / \omega_{emp} \right| \times 100$.In what concerns the comparison with previous fitted results, our semi-empirical average L sub-shell fluorescence yields also agree with the values of Campbell.(2003) [4] within 5.8–14.67%, the agreement between other semi-empirical calculation and the fitted and experimental values are not satisfying. The observed deviation varies from16.80% to 21.69% for Puri et al.(1994) [3] except for the five elements (the argument varies from 1.45% to 13.67%), 14.80% to 24.64% for Sahnoune et al.(2016) [5] except for the seven elements (the argument varies from 0.16% to 12.84%).

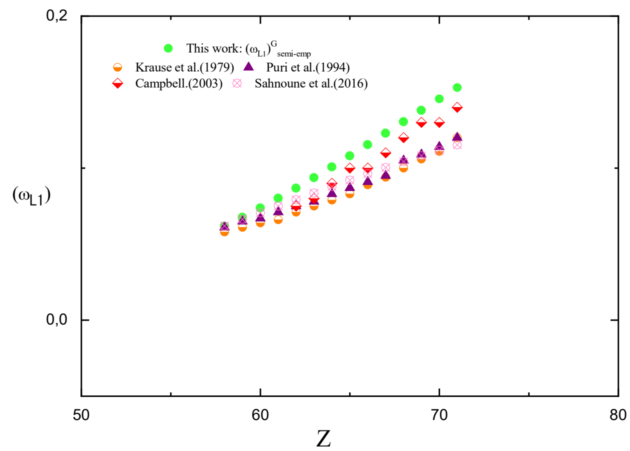

Fig. 3. The investigated semi-empirical L sub-shell fluorescence yields compared to their corresponding calculations Krause [2], Puri et a. [3], Campbell. [4], Sahnoune et al [5], Bonzi and Badiger, [6], Bansal et al., [7] and Kacal et al., [8] as a function of the atomic number Z.

IV. Conclusion

The average L sub-shell fluorescence yield measurements reported in the literature covering the period from 1934 to 2020 have been reviewed and presented in a table form (about 382 measurements). Using simple methods, a new set of L sub-shell fluorescence yields has been determined for elements in the atomic region $58 \le Z \le 71$, The deduced semi-empirical fluorescence yields are in a relatively good agreement with those of other groups for the whole range of atomic number. In addition to available experimental and theoretical average fluorescence yields, current values can be added to databases and made available to workers in the field of atomic inner layer ionization processes.

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