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Empirical *L* Shell Fluorescence Yields for Elements with $40 \le Z \le 92$

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Based on the fact that ratio of ionization to X-ray production cross-sections are independent of the excitation energy of projectile for a given target, we have deduced a new values of L shell average fluorescence yield from existing experimental compilation (till 2014) for a wide range of elements ($40 \le Z \le 92$) by proton impact (up to 10.0 MeV) of ionization and X-ray production cross-sections which are found to be universal when plotted as a function of the scaled velocity of projectile. The obtained empirical cross-sections are found reliable and then exploited to derive new values of average fluorescence yield. The obtained values are compared with earlier theoretical and experimental results and an agreement is observed for all elements.

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1. Introduction

Accurate values of average fluorescence yield are important in many uses of inner shell ionization and related phenomena such as particle induced X-ray emission (PIXE) analysis that uses the inner shell fluorescence yields to predict or compare theoretical X-ray cross-sections with those measured experimentally. The collected data base [1] consists of 991 and 5266 experimental points for total ionization and X-ray production cross-sections, respectively. Sometimes a remarkable dispersion is pointed out in experimental values. This situation motivates the need to a consistent and reliable new set of average L shell fluorescence yields.

2. Ionisation and X-ray production cross-sections

Figure 1 displays the available experimental points of L shell total ionization (Fig. 1a) and X-ray production cross-sections of existing compilation (Fig. 1b) [2] and other data extracted from curves [1]. Also, we introduce the dispersion criterion, within [0.5–1.5], of the existing experimental data from their corresponding calculated by ECPSSR model [3] with correct exact integration limits [4]. In such model Smit and Lapicki indicated that it would be wrong to evaluate the exact limits for momentum transfers of integration in calculating form factors

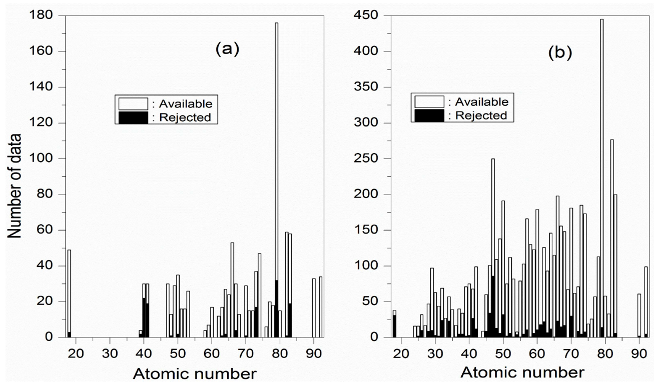

Fig. 1. Ionization (a) and X-ray production (b) experimental points and their corresponding rejected data.

($Q_{\min}$ and $Q_{\max}$) by replacing η_s with η_S^R ($\eta_S^R = m_S^R \eta_S$), where η_S^R is the reduced ion energy and m_S^R is the relativistic correction function [5]. As a solution of this problem, they proposed that the factor m_S^R should multiply electron rest mass m wherever it occurs. This led to the correct integration limits given by Eq. (1) from reference of Smit and Lapicki [4] given as

$$Q_{\substack{\min \\ \max}} = \left(\frac{M}{m_S^R m}\right)^2 \eta_S^R \left(1 \mp \sqrt{1-\frac{m_S^R m W}{\eta_S^R M}}\right)^2, \quad (1)$$

where W is the transferred energy from projectile to the ejected electron and Q is the square of the transferred momentum of the projectile.

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TABLE I

r_0, r_1, r, and $\varepsilon_{\rm rms}$ for both X-ray production and ionization cross-sections for selected elements.

Z	r_0	r_1	r	$\varepsilon_{\rm rms}$	Z	r_0	r_1	r	$\varepsilon_{\rm rms}$
X-ray production									
47	8.87953	–3.68271	1.04256	5.82	79	7.18089	–2.50234	0.8929	3.15
60	8.56443	–3.50094	1.02185	2.25	90	7.20063	–2.70441	0.97536	0.91
Ionization									
47	11.01748	–2.64373	0.78201	1.22	79	8.41193	–2.59343	0.90628	3.91
60	14.1901	–7.12786	1.88901	0.54	90	11.53568	–5.94973	1.63783	0.94

TABLE II

Ratio (R) to the present calculation of other values of $\bar{\omega}_L$ as a function of atomic number (Z).

Z	R [6]	R [8]	R [7] fit	R [7]	R [9]	R [14]	R [13]	R [12]	R [11]	R [10]
40	1.17	1.23	1.16	1.19	1.16				0.97	
46	1.07	1.19	1.16	1.05	1.12			1.14	1.04	
50	1.03	1.17	1.19	1.01	1.11			1.20	1.05	
56	1.00	1.16	1.09	0.99	1.10	1.09	1.11			
62	0.99	1.15	1.06	0.99	1.11	1.10	1.19			
64	0.99	1.14	1.06	1.00	1.11	1.13	1.04			
75	1.02	1.13	1.07	1.03	1.08	1.05				0.86
83	1.06	1.12	1.06	1.05	1.07	1.03				1.02
92	1.07	1.11	1.06	1.07	1.06	1.05				1.03

The present compilations are found to be universal when plotted, in a logarithmic scale, as a function of the scaled velocity $\xi_L = (\xi_{L_1} + \xi_{L_2} + 2\xi_{L_3})/4$. This is shown in Fig. 2a for $_{79}$Au. Universal character of cross-sections allows us to derive an empirical cross-section for each elements by interpolating these cross-sections by a first order exponential decay function as

$$\ln \sigma_{\rm emp} = r_0 + r_1 \exp(-r \ln \xi_M) \qquad (2)$$

The result of interpolation is shown in Fig. 2a with a full line.

The root-mean-square error ($\varepsilon_{\rm rms}$) is considered as a criterion of the quality of the calculated empirical cross-section. This error is expressed as the total deviation of the experimental cross-sections ($\sigma_{\rm exp}$) from their corresponding empirical ($\sigma_{\rm emp}$) values. The interpolation coefficients (r_0, r_1 and r) with the values of $\varepsilon_{\rm rms}$, are listed in Table I for selected elements.

3. Fluorescence yields of the L-shell

The total L-shell ionization cross-section is related to total X-ray production one through $\sigma_L^X = \bar{\omega}_L \sigma_L^I$, where $\bar{\omega}_L$ is the average fluorescence yield of the L-shell. This formula can be exploited to deduce empirical values of the average fluorescence yield for elements with $40 \leq Z \leq 92$ as follows.

First, $\sigma_{\rm emp}^X$ and $\sigma_{\rm emp}^I$ are plotted together as a function of the scaled velocity ξ_L (see Fig. 2a), where $\sigma_{\rm emp}^X$ is the total empirical X-ray production cross-section and $\sigma_{\rm emp}^I$ is the total empirical ionization one, both deduced from the previous section.

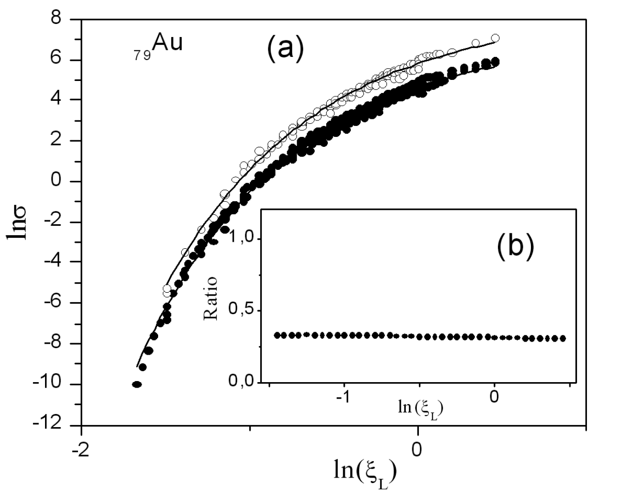

Fig. 2. Ionization (open circles) and X-ray production (dark points) cross-sections as a function of the scaled velocity ξ_L, in a logarithmic scale, for $_{79}$Au (a). The ratio between them are also included (b).

Second, the ratio $\sigma_{\rm emp}^X/\sigma_{\rm emp}^I$ is depicted in the same Fig. 2b, inner figure. It can be seen that this ratio presents, approximately, a constant value for each element over the whole range of the scaled velocity ξ_L. This situation makes the ratio $\sigma_{\rm emp}^X/\sigma_{\rm emp}^I$ to be independent of the scaled velocity ξ_L and allows us to take the mean value of this ratio for each element.

Third, the previous result can be served to calculate the empirical average fluorescence yield. This latter is affected to the corresponding mean value of the ratio for each element.

Then, the values of the empirical average fluorescence yield $\bar{\omega}_L$ deduced from the procedure described in the three previous steps, are interpolated as a function of the atomic number, using the famous formula

$$\sqrt[4]{\frac{\bar{\omega}_L}{1-\bar{\omega}_L}} = a + bZ, \tag{4}$$

where $a = -0.02177$ and $b = 0.01073$ are deduced from the present study.

Finally, ratio (R) to the present calculation of $\bar{\omega}_L$ is presented in Table II of theoretical [2, 3, 5–9] and experimental values [10–14]. Generally, the results obtained from this procedure present a good compromise between theory and experiment.

4. Conclusion

Based on the empirical ionization and X-ray production cross-sections by proton impact, where the ratio ionization to production of the cross-section is found to be independent of the excitation energy for a given element. This procedure allows us to deduce the average fluorescence yield of elements for which we do not dispose of the experimental ionization or X-ray production cross-sections and to cover the whole range of elements from zirconium to uranium.

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