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Calculation of Coster-Kronig Enhancement Factors and L Subshell X-Ray Fluorescence Cross-Sections for ^{55}Cs

R. YILMAZ* and K. ARICI
Department of Physics, Faculty of Sciences and Arts, Yuzuncu Yil University, Van, Turkey
E-mail: ryilmaz@yyu.edu.tr

X-Ray fluorescence cross-sections (σ_{Li}, i = α, β, ℓ, γ) of the ^{55}Cs element were calculated theoretically at excitation energies for each L_i (i = 1, 2 and 3) subshell, respectively. Coster-Kronig transitions (f_{12}, f_{23} and f_{13}) are non-radiative transitions in which an inner shell vacancy is transferred from one subshell of an atom to another. The increase in L X-ray intensity due to the effect the Coster-Kronig transitions on L X-ray fluorescence cross sections were calculated theoretically. These calculated values were compared with other experimental and theoretical values. Calculations showed that the alteration in absolute intensities of L_α and L_ℓ lines arising from Coster-Kronig transitions are greater than that of L_β.

Key Words: X-Ray fluorescence, Non-radiative transitions, Coster-Kronig enhancement factors.

INTRODUCTION

Determination of X-ray fluorescence (XRF) cross-sections are important in many practical applications, such as elemental analysis by X-ray emissions technique, basic studies of nuclear and atomic processes leading to emission of X-rays and Auger electrons and dosimetric computations for medical physics and irradiational processes.

The X-ray fluorescence cross-section is defined as the product of corresponding photoelectric cross-section and fluorescence yield at a given excitation energy. However, in the case of the L-shell, particularly the L_3 subshell X-ray lines, estimation of XRF cross-sections is not so straightforward because of the possibility of the so-called Coster-Kronig transitions. These transitions are non-radiative transitions, in which the two inner shells electrons are situated on two different subshells of the same inner shell (*e.g.*, L_1 and L_3). Such transitions between L_1 and L_3 and between L_2 and L_3 sublevels cause an additional excitation of L_3 subshell state, thereby enhancing the fluorescence cross-sections for L_α and other subshell X-ray lines[1,2].

Recently, many researchers have investigated Coster-Kronig transitions for various elements; Ertugrul[3-5], Oz *et al.*[6,7], Simsek[8], Sogut *et al.*[9] have investigated chemical

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†Department of Physics, Faculty of Sciences and Arts, 7 Aralik University, Kilis, Turkey.

effects on enhancement of Coster-Kronig transition of L_3 X-rays. The effect of fluorescence and Coster-Kronig yields on L X-ray emission cross-section has been studied by Hallak[10]. L X-ray production cross-sections, L subshell fluorescence yields and K-L vacancy transfer probabilities have been measured by Han *et al.*[11]. Puri and Singh[12] determined L_i subshell fluorescence yields (ω_i) and L_1-L_3 Coster-Kronig transition (f_{13}) for elements with $70 \leq Z \leq 92$ using photoionization technique. Kaya *et al.*[13] measured L subshell fluorescence cross-sections and subshell yields in elements $55 \leq Z \leq 81$ by 59.5 keV photons. Besides, the Coster-Kronig enhancement factors have investigated both experimentally and theoretically for some elements, recently. Oz *et al.*[14,15] have investigated theoretical and experimental Coster-Kronig enhancement factors of some elements with $66 \leq Z \leq 72$ and $74 \leq Z \leq 90$. In a previous work[16], we measured Coster-Kronig enhancement factors for Yb, Lu, Os and Pt elements.

In this paper, we studied the physical quantities that are affected by non-radiative transitions for lines. To investigate the role of Coster-Kronig transitions on L XRF cross-sections and the effect on the enhancement of L X-ray intensity, L subshells of for each element, excitation energies were chosen according to binding energies. It means that the cases are $B_{L_3} < E < B_{L_2}$, $B_{L_2} < E < B_{L_1}$ and $B_{L_1} < E < B_K$, where the L_1, L_2, L_3 are the subshells, B_{L_i}'s are the binding energies of the subshells, K is the ground shell and E is the excitation energy.

THEORETICAL CALCULATIONS

In this work, the theoretical L XRF cross-section are calculated by using following equations[14]

$$\sigma_{L\ell} = [\sigma_1(f_{13} + f_{12}f_{23}) + \sigma_2 f_{23} + \sigma_3]\omega_3 F_{3l} \tag{1}$$

$$\sigma_{L\alpha} = [\sigma_1(f_{13} + f_{12}f_{23}) + \sigma_2 f_{23} + \sigma_3]\omega_3 F_{3\alpha} \tag{2}$$

$$\sigma_{L\beta} = \sigma_1\omega_1 F_{1\beta} + (\sigma_1 f_{12} + \sigma_2)\omega_2 F_{2\beta} + [\sigma_3 + \sigma_2 f_{23} + \sigma_1(f_{13} + f_{12}f_{23})]\omega_3 F_{3\beta} \tag{3}$$

$$\sigma_{L\gamma} = \sigma_1\omega_1 F_{1\gamma} + (\sigma_2 + \sigma_1 f_{12})\omega_2 F_{2\gamma} \tag{4}$$

where σ_1, σ_2 and σ_3 are the photoionization cross-sections of the subshells L_1, L_2 and L_3, respectively[17]. ω_1, ω_2 and ω_3 are the corresponding subshell fluorescence yields[18]. f_{12}, f_{13} and f_{23} are the Coster-Kronig transition probabilities[18]. The X-ray emission rates for the filling of L-shell vacancies ($F_{ij} = F_{3\alpha}$, $F_{3\ell}$, $F_{3\beta}$, $F_{2\beta}$, $F_{2\gamma}$, $F_{1\beta}$, $F_{1\gamma}$), calculated with Hartree-Slater theory, are taken from Scofield[19], for example, $F_{3\alpha}$ value is given following relations[2].

$$F_{3\alpha} = \frac{\Gamma_3(M_4 - L_3) + \Gamma_3(M_5 - L_3)}{\Gamma_3} \tag{5}$$

where $\Gamma_3(M_4 - L_3)$ and $\Gamma_3(M_5 - L_3)$ are the partial radiative transition rates and Γ_3 is the total radiative transition rate of L_3 subshell[19].

Dertermination of Coster-Kronig enhancement factors: As mentioned before, It is known that the Coster-Kronig transitions are non-radiative transitions. L XRF cross sections can be calculated for the elements following equations[14]

$$\sigma_{L\ell} = \sigma_3 \omega_3 F_{3l} \tag{6}$$

$$\sigma_{L\alpha} = \sigma_3 \omega_3 F_{3\alpha} \tag{7}$$

$$\sigma_{L\beta} = \sigma_1 \omega_1 F_{1\beta} + \sigma_2 \omega_2 F_{2\beta} + \sigma_3 \omega_3 F_{3\beta} \tag{8}$$

$$\sigma_{L\gamma} = \sigma_1 \omega_1 F_{1\gamma} + \sigma_2 \omega_2 F_{2\lambda} \tag{9}$$

However, in fact Coster-Kronig transitions are present. For this situation, L XRF cross-section were evaluated using the eqns. 1-4.

Theoretical Coster-Kronig enhancement factors (κ) can be calculated using the following equations[14].

$$\kappa_{1,\alpha} = \frac{\sigma_1(f_{13} + f_{12}f_{23}) + \sigma_2 f_{23} + \sigma_3}{\sigma_3} \tag{10}$$

$$\kappa_\beta = \frac{\sigma_1 \omega_1 F_{1\beta} + (\sigma_1 f_{12} + \sigma_2)\omega_2 F_{2\beta} + [\sigma_3 + \sigma_2 f_{23} + \sigma_1(f_{13} + f_{12}f_{23})]\omega_3 F_{3\beta}}{\sigma_1 \omega_1 F_{1\beta} + \sigma_2 \omega_2 F_{2\beta} + \sigma_3 \omega_3 F_{3\beta}} \tag{11}$$

Both the theoretical Coster-Kronig enhancement factors for $_{55}$Cs are given in Tables 4-6 (In these tables, when L_3 and L_2 were excited, Coster-Kronig enhancement factors were represented to κ_{i_1}; when L_3, L_2 and L_1 were excited, Coster-Kronig enhancement factors were represented by κ_{i_2}).

RESULTS AND DISCUSSION

The L subshell XRF cross-sections were calculated using eqns. 1-4 and related data have been given in Tables 1-3. The values of Coster-Kronig enhancement factors for ^{55}Cs determined theoretically using eqns. 10 and 11, are listed in Tables 4-6. It is observed that the presence of non-radiative transitions cause changes in the X-ray intensities, thus it must be taken into account in quantative XRF. It is known that the non-radiative transitions compete with radiative transitions and they together determine both the absolute and the relative intensities of generated X-rays[14].

TABLE-1
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR ^{55}Cs
(ONLY WHEN L_3 SUBSHELL WAS EXCITED)

Element	E (keV)	α_{L_α}	α_{L_β}	α_{L_ℓ}
		Calculated	Calculated	Calculated
$_{55}$Cs	5.041	7228.981	1164.319	269.357

TABLE-2
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR ^{55}Cs
(WHEN L_3 AND L_2 SUBSHELLS WERE EXCITED)

Element	E (keV)	σ_{L_α}	σ_{L_β}	σ_{L_ℓ}	σ_{L_γ}
		Calculated	Calculated	Calculated	Calculated
$_{55}$Cs	5.401	6598.574	4424.229	245.860	544.888

TABLE-3
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR ^{55}Cs
(WHEN L_3, L_2 AND L_1 SUBSHELLS WERE EXCITED)

Element	E (keV)	σ_{L_α}	σ_{L_β}	σ_{L_ℓ}	σ_{L_γ}
		Calculated	Calculated	Calculated	Calculated
$_{55}$Cs	5.725	6206.257	5083.159	231.242	740.786

TABLE-4
κ_{α_1} AND κ_{α_2} COSTER-KRONIG ENHANCEMENT FACTORS FOR ^{55}Cs

Element	E (keV)	κ_{α_1}	E (keV)	κ_{α_2}
		Calculated		Calculated
$_{55}$Cs	5.401	1.085	5.725	1.184

TABLE-5
κ_{ℓ_1} AND κ_{ℓ_2} COSTER-KRONIG ENHANCEMENT FACTORS FOR ^{55}Cs

Element	E (keV)	κ_{ℓ_1}	E (keV)	κ_{ℓ_2}
		Calculated		Calculated
$_{55}$Cs	5.401	1.085	5.725	1.184

TABLE-6
κ_{β_1} AND κ_{β_2} COSTER-KRONIG ENHANCEMENT FACTORS FOR ^{55}Cs

Element	E (keV)	κ_{β_1}	E (keV)	κ_{β_2}
		Calculated		Calculated
$_{55}$Cs	5.401	1.021	5.725	1.101

In the present work, the results indicate 8.5 % for theoretical value of κ_{α_1} enhancement of the XRF cross-sections; 18.4 % for theoretical value of κ_{α_2} enhancements of the XRF cross-sections; 8.5 % for theoretical value of κ_{ℓ_1} enhancement of the XRF cross-sections; 18.4 % for theoretical value of κ_{ℓ_2} the XRF cross-sections; 2.1 % for theoretical value of κ_{β_1} the enhancement of the XRF cross-sections and 10.1 % for theoretical value of κ_{β_2} enhancement of the XRF cross-sections. Enhancements up to 65 % in the XRF cross-sections were reported by Rani *et al.*[1]. Recently, Oz *et al.*[14,15] reported the measurements of Coster-Kronig enhancement factors of some elements in the atomic number range $74 \leq Z \leq 90$ and $74 \leq Z \leq 90$ using photoionization of method. As a result of a study done by Oz *et al.*[14,15], the theoretical κ_{α_1}, κ_{ℓ_1} Coster-Kronig enhancement factors were reported as 8-9 % and up to 4-6 % for experimental; up to 20-30 % for theoretical κ_{α_2}, κ_{ℓ_2} and up to 14-20 % for experimental. In adidition, the theoretical κ_{β_1} Coster-

Kronig enhancement factors were reported as 2 %, 9-11 % for κ_{β_2} and up to 1-2 % for experimental κ_{β_1}, 8-10 % for κ_{β_2}. The present values are generally in agreement with the studies done by Oz *et al.*[14,15]. Consequently, it can be seen from Tables 4-6 that the intensities of the L_β lines arising from Coster-Kronig transitions are smaller than that for L_α and L_ℓ.

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