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Calculation of Coster-Kronig Enhancement Factors For $_{60}$Nd and $_{61}$Pm at Different Excitation Energies

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Coster-Kronig processes are radiationless in which an inner-shell vacancy is transferred from one subshell of an atom to another, both belonging to the same principal shell. Because of the effect of Coster-Kronig transition on L X-ray fluorescence cross sections, an increase in L X-ray intensity were calculated theoretically at different exciation energies for L_1, L_2 and L_3 subshells. These are called as Coster-Kronig enhancement factors and were represented as $\kappa_i(i = \alpha, \beta, l)$. These calculated values were compared with other experimental and theoretical values. Calculations showed that when the excitation energies were increased with respect to absorbtion edge energy, L X-ray fluorescence cross sections decrease while Coster-Kronig enhancement factors increase.

Key Words: X-Ray fluorescence, Coster-Kronig transitions, Enhancement factors.

INTRODUCTION

X-Ray fluorescence (XRF) cross-sections are of great importance in the fields of atomic, molecular and radiation physics. These values required for quantitative multi-element trace analysis using energy-dispersive X-ray fluorescence, dosimetric computations for health physics and industrial irradiation processing. In addition, these values provide an indirect check on physical parameters, such as L subshell ionization cross-sections, Coster-Kronig transition probabilities.

The X-ray fluorescence cross-section is defined as the product of corresponding photoelectric cross-section and fluorescence yield at a given excitation energy. But, 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 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].

A systematic study of L X-ray fluorescence cross-sections, L shell fluorescence yields, Coster-Kronig transitions and the effect of Coster-Kronig transitions for different elements as a function of incident photon energy has previously been undertaken[3-9]. Recently, the Coster-kronig enhancement factors have investigated both experimentally and theoretically for some elements. Öz *et al.*[10,11] have investigated theoretical and experimental Coster-Kronig enhancement factors of some elements with $66 \le Z \le 72$ and $74 \le Z \le 90$. In a previous work[12,13], we measured Coster-Kronig enhancement factors for Yb, Lu, Os and Pt elements and for Cs. Thakkar *et al.*[14] have investigated contribution of Coster-Kronig transfer to proton induced L subshell X-ray production cross-sections for direct and indirect vacancie.

In this paper, we studied calculation of coster-kronig enhancement factors for $_{60}$Nd and $_{61}$Pm at different excitation energies. 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_{Li}'s are the binding energies of the subshells, K is the ground shell and E is the excitation energy.

THEORETICAL

The theoretical values of L X-ray fluorescence cross sections are calculated from subshell photoionization cross section[15] (σ_i, i = 1,2,3), fluoresence yield[16] (ω_i, i = 1,2,3), Coster-Kronig transition probabilities[16] (f_{ij}, i = 1,2; j = 2,3) and radiative decay rates[17] (F_{ij}, i = 1,2,3 and j = α,β,γ,l).

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

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

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

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

The calculated L XRF cross-sections are given in Tables 1-3.

TABLE-1
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR $_{60}$Nd and $_{61}$Pm (ONLY WHEN L_3 SUBSHELL WAS EXCITED)

Element	E (keV)	σ_{L_α}	σ_{L_β}	σ_{L_l}
		Calcd.	Calcd.	Calcd.
$_{60}$Nd	6.244	7586.649	1329.043	295.344
	6.721	6327.653	1108.494	246.332
$_{61}$Pm	6.497	7658.432	1352.585	298.089
	7.012	6390.696	1129.202	249.089

TABLE-2
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR $_{60}$Nd and $_{61}$Pm (WHEN L_3 AND L_2 SUBSHELLS WERE EXCITED)

Element	E (keV)	σ_{L_α}	σ_{L_β}	σ_{L_l}	σ_{L_γ}
		Calcd.	Calcd.	Calcd.	Calcd.
$_{60}$Nd	6.725	6725.565	4338.321	261.822	618.468
	7.087	6043.189	3940.328	233.271	560.970
$_{61}$Pm	7.069	6725.473	4749.768	262.137	632.376
	7.388	6011.274	4418.237	234.300	575.037

TABLE-3
L XRF CROSS-SECTIONS (BARNS/ATOM) FOR $_{60}$Nd and $_{61}$Pm (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}
		Calcd.	Calcd.	Calcd.	Calcd.
$_{60}$Nd	8.000	4831.684	3919.085	188.094	657.401
	10.000	2627.764	2261.662	102.297	577.820
$_{61}$Pm	8.000	5400.216	4644.906	210.483	625.947
	10.00	2956.054	2706.276	121.632	576.021

Determination of coster-kronig enhancement factors: As mentioned before, Coster-Kronig transitions are non-radiative transitions. Because of the effect of Coster-Kronig transition on L X-ray fluorescence cross sections, an increase in L X-ray intensity were calculated theoretically at different excitation energies for L_1, L_2 and L_3 subshells. Enhancement factors (κ_i) can be calculated using the following equations[11].

$$\kappa_{L,\alpha} = \frac{\sigma_1(f_{13} + f_{12}f_{23}) + \sigma_2 f_{23} + \sigma_3}{\sigma_3} \quad (5)$$

$$\kappa_\beta = \frac{\sigma_1\omega_1 F_{1\beta} + (\sigma_1 f_{12} + \sigma_2)\omega_2 F_{2\beta} + [\sigma_3 + \sigma_2 f_{23} + \sigma_1(f_{13} + f_{12}f_{23})]\omega_3 F_{3\beta}}{\sigma_1\omega_1 F_{1\beta} + \sigma_2\omega_2 F_{2\beta} + \sigma_3\omega_3 F_{3\beta}} \quad (6)$$

Both the theoretical Coster-Kronig enhancement factors for $_{60}$Nd and $_{61}$Pm 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}).

TABLE-4
κ_{α_1} AND κ_{α_2} COSTER–KRONIG ENHANCEMENT FACTORS FOR $_{60}$Nd and $_{61}$Pm

Element	E (keV)	κ_{α_1}	E (keV)	κ_{α_2}
		Calcd.		Calcd.
$_{60}$Nd	6.775	1.086	8.000	1.209
	7.087	1.097	10.000	1.247
$_{61}$Pm	7.069	1.085	8.000	1.184
	7.388	1.088	10.000	1.310

TABLE-5
κ_{ℓ_1} AND κ_{ℓ_2} COSTER–KRONIG ENHANCEMENT FACTORS FOR $_{60}$Nd and $_{61}$Pm

Element	E (keV)	κ_{ℓ_1}	E (keV)	κ_{ℓ_2}
		Calcd.		Calcd.
$_{60}$Nd	6.775	1.086	8.000	1.209
	7.087	1.097	10.000	1.247
$_{61}$Pm	7.069	1.085	8.000	1.184
	7.388	1.088	10.000	1.310

TABLE-6
κ_{β_1} AND κ_{β_2} COSTER–KRONIG ENHANCEMENT FACTORS FOR $_{60}$Nd and $_{61}$Pm

Element	E (keV)	κ_{β_1}	E (keV)	κ_{β_2}
		Calcd.		Calcd.
$_{60}$Nd	6.775	1.022	8.000	1.112
	7.087	1.022	10.000	1.130
$_{61}$Pm	7.069	1.020	8.000	1.101
	7.388	1.022	10.000	1.120

RESULTS AND DISCUSSION

The values of Coster-Kronig enhancement factors for $_{60}$Nd and $_{61}$Pm determined theoretically using eqns. 5 and 6, 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 can be seen from Tables 1-3 that when the excitation energies were increased, L X-ray fluorescence cross sections decrease.

In the present work, the results indicate 8.5-9.7 % for theoretical value of κ_{α_1} and κ_{l_1} enhancement of the XRF cross-sections; 18.4-31.0 % for theoretical value of κ_{α_2} and κ_{l_2} enhancements of the XRF cross-sections; 2.0-2.2 % for theoretical value of κ_{β_1} the enhancement of the XRF cross-sections and 10.1-13.0 % 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.*[2]. Öz *et al.*[10,11] reported the measurements of Coster-Kronig enhancement factors of some elements in the atomic number range $66 \leq Z \leq 72$ and $74 \leq Z \leq 90$ using photoionization of method. The present values are generally in agreement with the studies of Öz *et al.*[10,11].

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. It can also be seen from Tables 1-6 that calculations showed that when the excitation energies were increased with respect to absorption edge energy, L X-ray fluorescence cross sections decrease while Coster-Kronig enhancement factors increase.

REFERENCES

1. J.L. Labar, *X-Ray Spectrom.*, **20**, 111 (1991).
2. A. Rani, N. Nath and S.N. Chaturvedi, *X-Ray Spectrom*., **18**, 77 (1989).
3. E. Öz, Y. Özdemir, N. Ekinci, M. Ertugrul, Y. Sahin and H. Erdogan, *Spectrochim. Acta*, **55B**, 1869 (2000).
4. E. Öz, N. Ekinci, Y. Özdemir, M. Ertugrul, Y. Sahin and H. Erdogan, *J. Phys. B: At. Mol. Opt. Phys*., **34**, 631 (2001).
5. A. Kaya and M. Ertugrul, *J. Electr. Spectrosc. Rel. Phenom.*, **130**, 111 (2003).
6. I. Han, L. Demir and M. Agbaba, *Radiat. Phys. Chem*., **76**, 1551 (2007).
7. M. Ertugrul, *Nucl. Instrum. Meth. B*, **119**, 345 (1996).
8. M. Ertugrul, *J. Electr. Spectrosc. Rel. Phenom*., **125**, 69 (2002).
9. S. Puri and N. Singh, *Radiat. Phys. Chem*., **75**, 2232 (2006).
10. E. Öz, N. Ekinci, M. Ertugrul and Y. Sahin, *X-Ray Spectrom*., **32**, 153 (2003).
11. E. Öz, Y. Sahin and M. Ertugrul, *Radiat. Phys. Chem*., **69**, 17 (2004).
12. R. Yilmaz, E. Öz, M. Tan, R. Durak, A.I. Demirel and Y. Sahin, *Radiat. Phys. Chem*., **78**, 318 (2009).
13. R. Yilmaz and K. Arici, *Asian J. Chem*., **22**, 5463 (2010).
14. R. Thakkar, N. Singh and K.L. Allawadhi, *Asian J. Chem*., **21**, S254 (2009).
15. J.H. Scofield, Lawrence Livermore Laboratory Report, California (1973).
16. M.O. Krause, *J. Phys. Chem. Ref. Data*, **8**, 307 (1979).
17. J.H. Scofield, *Atom. Data Nucl. Data Tables*, **14**, 121 (1974).