Theoretical X-ray relative intensities at incident photon energies across the L_i(i=1-3) absorption edges for Yb

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Abstract

The intensity ratios, $I_{Lk}/I_{L\alpha1}$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_3, \beta_4, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ *and* $I_{Lj}/I_{L\alpha}$ *(j = β, γ) have been evaluated at incident photon energies across the* L_i*(i=1-3) absorption edge energies of* $_{70}$*Yb using theoretical data sets of different physical parameters, namely, the Dirac-Hartree-Slater (DHS) and the Dirac-Fock (DF) model based* L_i*(i=1-3) sub-shell photoionization cross sections, the DF model based X-ray emission rates, and the DHS model based fluorescence and Coster-Kronig yields in order to highlight the importance of electron exchange effects at photon energies in vicinity of the absorption edge energies.*

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1. Introduction

Accurate data on the relative intensities of different X-ray lines are of considerable importance for investigation of atomic inner-shell ionization processes as well as for a variety of applications including the quantitative elemental analysis of different types of samples using X-ray emission techniques (EDXRF and PIXE). The relative intensities of different X-ray lines can be deduced from the X-ray production (XRP) cross sections which, in turn, can be evaluated using theoretical data on physical parameters, namely, photoionization cross sections (PCS), fluorescence and Coster-Kronig (CK) yields and X-ray emission rates. Different sets of these physical parameters evaluated using the Dirac-Hartree-Slater (DHS) and Dirac-Fock (DF) models are available in literature [1]. In the DHS model, the potential is assumed to be equal for the initial and final states of the atom undergoing transitions. In the DF model, the potential is assumed to be different for initial and final states and hence electron exchange and overlap effects were included. In the present work, the L_i(i=1-3) sub-shell intensity ratios have been evaluated at incident photon energies just above (within 100 eV) the L_i edge energies of the Ytterbium (Z=70) using the DF model based PCS [2] for comparison with those calculated using the DHS model based PCS [3] in order to highlight the importance of electron exchange and overlap effects at photon energies in vicinity of the absorption edge energies.

2. Evaluation Procedure

The production cross sections (σ^X_{Lk}) for the L*k* $(k = l, \eta, \alpha_1, \alpha_2, \beta_1, \beta_{2,15}, \beta_{3,4}, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ X-rays at incident photon energy, E_{inc}, have been evaluated using the equations

$$\sigma^X_{Lk} = \sigma^\tau_{L_i} \omega_i F_{ik} \quad (1)$$

Where, F_{ik} (*i*=1-3) represents the fractional emission rate, ω_i (i=1-3) represents the Li sub-shell fluorescence yields and $\sigma^\tau_{L_i}$ denotes the total number of vacancies in the L_i(i=1-3) sub-shells including those transferred through the CK transitions and can be calculated using the equation

$$\sigma^\tau_{L_i} = \sigma^P_{L_i} + \sum_{k<i} \sigma^\tau_{L_k} f_{ki} \quad (2)$$

Where, $\sigma^P_{L_i}$ (i=1-3) represent the Li sub-shell photoionization cross sections and the f_{ki} are the Li sub-shell CK transitions probabilities. The intensity ratios, $I_{Lk}/I_{L\alpha1}$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_{3,4}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ and $I_{Lj}/I_{L\alpha}$ (j = β, γ) have been deduced from the L_k XRP cross sections using the equations,

$$I_{Lk}/I_{L\alpha1} = \sigma^X_{Lk}/\sigma^X_{La1} \quad (3)$$

In these evaluations, the DF model based X-ray emission rates [4], the DHS model based L_i(i=1-3) sub-shell fluorescence and Coster-Kronig yields [5] and two sets of the photoionization cross sections (PCS) based on the DHS [3] and the DF [2] models were used. The DHS model based photoionization cross sections [3] are available at selected incident photon energies across the L_i(i=1-3) absorption edge energies. These cross sections at required incident photon energies have been interpolated from the available limited data assuming a dependence of the form (aE^b).

3. Results and Discussion

The two sets of calculated intensity ratios, $I_{Lk}/I_{L\alpha1}$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_3, \beta_4, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ and $I_{Lj}/I_{L\alpha}$ (j = β, γ) for $_{70}$Yb are given in Tables 1 &

2. It may be mentioned that the DF model [2] based PCS in the considered photon energy range are lower than the DHS model [3] based values by ~14-27% for the L_1 sub-shell and by ~6-15% for the L_2 and the L_3 sub-shells. The X-ray intensity ratios, $I_{Lk}/I_{L\alpha1}$ $(k=\eta,\beta_1,\gamma_{1,5},\gamma_{6,8})$ evaluated using the DF model based PCS are found to be lower than those calculated using the DHS model based PCS values by 40-45%. Similarly, the ratios, $I_{Lk}/I_{L\alpha1}$ $(k=\beta_{3,4},\beta_{9,10},\gamma_{2,3},\gamma_4)$ evaluated using the DF model based PCS are lower than those evaluated using the DHS values by 40-48%. Therefore, the exchange and overlap effects are found to be significant, predominantly, in vicinity of the L_i sub-shell absorption edge energies.

References

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[4] J.L. Campbell and J.X. Wang, Atom. Data Nucl. Data Tables 43 (1989) 281.
[5] Sanjiv Puri, D. Mehta, B.Chand, N.Singh and P.N. Trehan, X-ray Spectrom. 22 (1993) 358.

Table 1: The intensity ratios, $I_{Lk}/I_{L\alpha1}(\text{DHS})$ $(k=l,\eta,\alpha_2,\beta_1,\beta_{2,15},\beta_3,\beta_4,\beta_{9,10},\gamma_{1,5},\gamma_{6,8},\gamma_{2,3},\gamma_4)$ and $I_{Lj}/I_{L\alpha}$ (j = β, γ), at incident photon energies across the L_i(i=1-3) sub-shell absorption edges of Yb.

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E (KeV)	$\frac{I_{Ll}}{I_{L\alpha_1}}$	$\frac{I_{L\alpha_2}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_{2,15}}}{I_{L\alpha_1}}$	$\frac{I_{L\eta}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_1}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{1,5}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{6,8}}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_3}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_4}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_{9,10}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{2,3}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_4}}{I_{L\alpha_1}}$	$\frac{I_{L\beta}}{I_{L\alpha}}$	$\frac{I_{L\gamma}}{I_{L\alpha}}$
8.996	0.049	0.113	0.201										0.193	
9.046	0.049	0.113	0.201										0.193	
9.991	0.049	0.113	0.201	0.021	0.778	0.152	0.0008						0.892	0.138
10.001	0.049	0.113	0.201	0.021	0.770	0.151	0.0008						0.884	0.136
10.031	0.049	0.113	0.201	0.021	0.771	0.151	0.0008						0.885	0.136
10.081	0.049	0.113	0.201	0.021	0.780	0.153	0.0008						0.894	0.138
10.500	0.049	0.113	0.201	0.021	0.785	0.154	0.0008	0.103	0.077	0.0049	0.046	0.0061	1.065	0.185
10.510	0.049	0.113	0.201	0.021	0.785	0.154	0.0008	0.104	0.078	0.0050	0.046	0.0061	1.067	0.186
10.540	0.049	0.113	0.201	0.021	0.786	0.154	0.0008	0.105	0.079	0.0050	0.047	0.0062	1.069	0.186
10.590	0.049	0.113	0.201	0.021	0.786	0.154	0.0008	0.106	0.080	0.0050	0.047	0.0062	1.071	0.187

Table 2: The intensity ratios, $I_{Lk}/I_{L\alpha1}(\text{DF})$ $(k=l,\eta,\alpha_2,\beta_1,\beta_{2,15},\beta_3,\beta_4,\beta_{9,10},\gamma_{1,5},\gamma_{6,8},\gamma_{2,3},\gamma_4)$ and $I_{Lj}/I_{L\alpha}$ (j = β, γ), at incident photon energies across the L_i(i=1-3) sub-shell absorption edges of Yb.

E (KeV)	$\frac{I_{Ll}}{I_{L\alpha_1}}$	$\frac{I_{L\alpha_2}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_{2,15}}}{I_{L\alpha_1}}$	$\frac{I_{L\eta}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_1}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{1,5}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{6,8}}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_3}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_4}}{I_{L\alpha_1}}$	$\frac{I_{L\beta_{9,10}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_{2,3}}}{I_{L\alpha_1}}$	$\frac{I_{L\gamma_4}}{I_{L\alpha_1}}$	$\frac{I_{L\beta}}{I_{L\alpha}}$	$\frac{I_{L\gamma}}{I_{L\alpha}}$
8.996	0.049	0.113	0.201										0.193	
9.046	0.049	0.113	0.201										0.193	
9.991	0.049	0.113	0.201	0.038	1.39	0.273	0.0015						1.446	0.247
10.001	0.049	0.113	0.201	0.036	1.31	0.257	0.0014						1.373	0.232
10.031	0.049	0.113	0.201	0.035	1.29	0.253	0.0014						1.355	0.229
10.081	0.049	0.113	0.201	0.037	1.36	0.266	0.0014						1.414	0.240
10.500	0.049	0.113	0.201	0.032	1.18	0.231	0.0012	0.174	0.130	0.0083	0.077	0.0102	1.531	0.287
10.510	0.049	0.113	0.201	0.032	1.17	0.228	0.0012	0.183	0.137	0.0087	0.081	0.0108	1.536	0.289
10.540	0.049	0.113	0.201	0.031	1.14	0.224	0.0012	0.197	0.148	0.0094	0.088	0.0116	1.540	0.292
10.590	0.049	0.113	0.201	0.031	1.12	0.219	0.0012	0.211	0.158	0.0100	0.094	0.0124	1.539	0.293