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Li(i=1-3) sub-shell X-ray Relative Intensities for some Elements

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The intensity ratios, $I_{Lk}/I_{L\alpha 1}$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_3, \beta_4, \beta_{5,7}, \beta_6, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ have been evaluated for some elements with 36≤Z≤92 at incident photon energies ranging $E_{L1} < E_{inc} \le 200\ keV$ using currently considered to be more reliable theoretical data sets of different physical parameters, namely, the RHFS model based Li(i=1-3) sub-shell photoionisation cross sections, the DF model based X-ray emission rates and the DHS model based fluorescence and Coster-Kronig yields. The important features pertaining to dependence of the calculated intensity ratios on the incident photon energy and atomic number (Z) have been discussed.

INTRODUCTION

Accurate data on the relative intensities of resolved L X-ray components for different elements at different incident photon energies are important for investigation of atomic inner-shell photoionisation 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 L X-ray relative intensities can be deduced from the X-ray production (XRP) cross sections which, in turn, can be evaluated using physical parameters, namely, photoionisation cross sections, fluorescence and Coster-Kronig (CK) yields, and X-ray emission rates. A thorough literature search revealed the non-availability of any tabulation of theoretical intensity ratios for the resolved L X-ray components produced following photoionisation.

In the present work, the L X-ray intensity ratios, $I_{Lk}/I_{L\alpha 1}$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_{3,4}, \beta_{5,7}, \beta_6, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ have been evaluated for some elements with 36≤Z≤92 at incident photon energies ranging E_{L1}<E_{inc}<200 keV using currently considered to be more reliable theoretical sets of different physical parameters in order to understand their dependence on incident photon energy and atomic number. At incident photon energies above the K-shell ionization thresholds of an element, the contribution to the production of different L X-ray lines due to the additional Li(i=1-3) sub-shell vacancies created following decay of the primary K-shell vacancies have also been included in the present calculations.

COMPUTATIONAL PROCEDURE AND DISCUSSIONS

The L*k* $(k = l, \eta, \alpha_1, \alpha_2, \beta_1, \beta_{2,15}, \beta_{3,4}, \beta_{5,7}, \beta_6, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ XRP cross sections (σ_{Lk}^{X}) for some elements with 36≤Z≤92 at incident photon energies ranging $E_{L1}<E_{inc}<200$ keV have been evaluated using the equations

$$\sigma_{Lk}^{X} = \sigma_{L_i}^{\tau} \omega_i F_{ik} \qquad (1)$$

where F_{ik} (*i*=1-3) represents the fractional emission rate for the L*k* [*k* = □$_{3}$,□$_{4}$,□$_{9,10}$, □$_{2,3}$, □$_{4}$ (for *i*=1); *k* = □$_{1}$, η,□$_{1,5}$, □$_{6,8}$ for (for *i*=2); *k* = *l*□□□□□ for *i*□□□] groups of X-rays and □$_i$(*i*=1-3) represents the Li sub-shell fluorescence yields. The $\sigma_{L_i}^{\tau}$ denote the total number of vacancies in the Li(i=1-3) sub-shells including those transferred through the CK transitions and can be calculated using the equation

$$\sigma_{L_k}^{\tau} = \sigma_{L_i}^{P} + \sum_{k<i} \sigma_{L_k}^{\tau} f_{ki} \qquad (2)$$

where $\sigma_{L_i}^{P}$ (i=1-5) represent the Li sub-shell photoionisation cross sections and the f_{ki} are the Li sub-shell CK transitions probabilities. For the evaluation of L*k* XRP cross sections, the DF model based X-ray emission rates[1], the RHFS model based photoionisation cross sections[2] and the DHS model based Li(i=1-3) sub-shell fluorescence and Coster-Kronig yields[3], were used in Eq. (1) and (2). At incident photon energies above the K-shell ionisation threshold energy (E_K) of an element ($E_K < E_{inc}<200$ keV), the number of additional Li(i=1-3) sub-shell vacancies (N_{Li}) created following decay of a primary K-shell vacancy have been calculated using relation

$$N_{Li} = \sigma_K^{P} \eta_{KL_i}, \ (i=1\text{-}3) \qquad (3)$$

where σ_K^{P} represents the K-shell photoionisation cross section at a given incident photon energy and the η_{KL_i} (*i*=1-3) represent the probability for production of the Li(i=1-3) sub-shell vacancies following decay of a primary K-shell vacancy. At these incident photon energies, the L*k* XRP cross sections have been calculated using Eqs. (1) and (2) by replacing $\sigma_{L_i}^{P}$ (*i*=1-3) with ($\sigma_{L_i}^{P}$ +N_{KLi}), where the number, N_{KLi}, have been evaluated using the RHFS model based photoionisation cross sections [2] and the DHS model based vacancy transfer probabilities, η_{KL_i} (*i*=1-3),[4] in Eq. (3). The intensity ratios, $I_{Lk}/I_{L\alpha1}(thr.)$ $(k = l, \eta, \alpha_2, \beta_1, \beta_{2,15}, \beta_{3,4}, \beta_{5,7}, \beta_6, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$, have been deduced from the L*k* XRP cross sections using the relation

$$\frac{I_{Lk}}{I_{L\alpha1}} = \frac{\sigma_{Lk}^{X}}{\sigma_{L\alpha1}^{X}} \qquad (4)$$

The present calculated intensity ratios,
$I_{Lk}/I_{L\alpha1}(thr.)$ $(k = l, \alpha_2, \beta_{2,15}, \beta_{5,7}, \beta_6)$ exhibited dependence on the atomic

number (Z) and for a given element these ratios are found to be independent of the incident photon energy. It may be noted that all these X-ray components including L□$_1$, originate following decay of the L_3 sub-shell vacancies. Therefore, these ratios depend only on the X-ray emission rates and are independent of the Li(i=1-3) sub-shell fluorescence and CK yields and the photoionisation cross sections.

The intensity ratios, $I_{Lk} / I_{L\alpha1}(thr.)$, for $(k = \eta, \beta_1, \beta_3, \beta_4, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ X-ray components exhibited dependence on both, the incident photon energy as well as atomic number (Z). It may be noted that the (Lη, L□$_1$, L□$_{1,5}$, L□$_{6,8}$) and the (L□$_{3,4}$, L□$_{9,10}$, L□$_{2,3,4}$) X-ray components, respectively, originate following decay of the L_2 and L_1 sub-shell vacancies. For a given element, the calculated ratios for $Lk(k = \eta, \beta_1, \beta_3, \beta_4, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ X-ray components were found to vary smoothly with the incident photon energy for $E_{inc.}<E_K$, and exhibited an abrupt significant decrease at E_{inc} just above the K-shell ionization threshold energy (E_K) and thereafter again varies smoothly with photon energy. A typical plot depicting the variation of $I_{Lk} / I_{L\alpha1}(thr.)$ (k=□□□ with the incident photon energy for $_{70}$Yb is shown in Figure 1.

The intensity ratios, $I_{Lk} / I_{L\alpha1}(thr.)$, for $(k = \eta, \beta_1, \beta_3, \beta_4, \beta_{9,10}, \gamma_{1,5}, \gamma_{6,8}, \gamma_{2,3}, \gamma_4)$ X-ray components, also exhibited abrupt jumps in their values in vicinity of the elements where cut-off/onset of certain intense CK transitions are located. For example, the L_1-$L_3M_{4,5}$ CK transitions are not allowed energetically for elements with 50≤Z≤74[5], which causes significant change in the values of L_1 sub-shell fluorescence (□$_1$) and CK (f_{13}) yields and hence intensity ratios for X-ray components originating following decay of L_1 sub-shell vacancies. A typical plot depicting the variation of ratios, $I_{Lk} / I_{L\alpha1}(thr.)$ for (k = □originating from the L_1 sub-shell and □□originating from the L_2 sub-shell evaluated at 20 keV incident photon energy with the atomic number (Z) is shown in Figure 2. It may be mentioned that the general trends depicted in figures (1) and (2) were found to be same for other investigated elements in the atomic region 36≤Z≤92.

The intensity ratios, $I_{Lk} / I_{L\alpha1}(camp)$, deduced using the Li(i=1-3) sub-shell fluorescence and CK yields tabulated by Campbell[6,7] are compared with the $I_{Lk} / I_{L\alpha1}(thr.)$ values in Fig. (1) and Fig. (2). The ratios, $I_{Lk} / I_{L\alpha1}(camp)$ (k=□□□ are found to be higher than the $I_{Lk} / I_{L\alpha1}(thr.)$ values by up to 15%. Similar differences were observed in case of other L_2 and L_3 sub-shell X-ray components. It may be emphasized here that the □$_i$ and f_{ij} yields recommended by Campbell[6,7] bear large uncertainties ~15-30%.

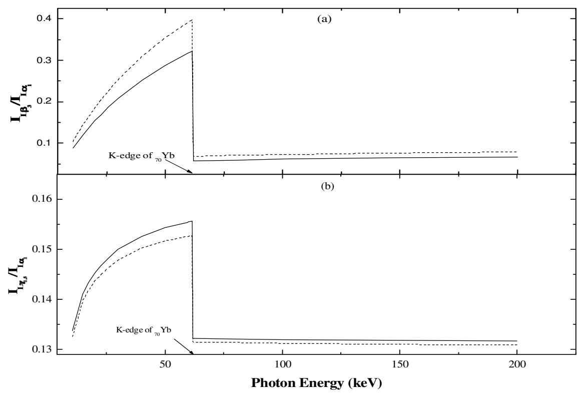

Fig 1: Plot of intensity ratios, $I_{Lk} / I_{L\alpha 1}$ (*k*=□*3* and □*1,5*), for $_{70}$Yb as a function of incident photon energy. The solid lines corresponds to the DHS values and dotted lines represent the intensity ratios calculated using Li(i=1-3) sub-shell fluorescence and CK yields recommended by Campbell [6,7].

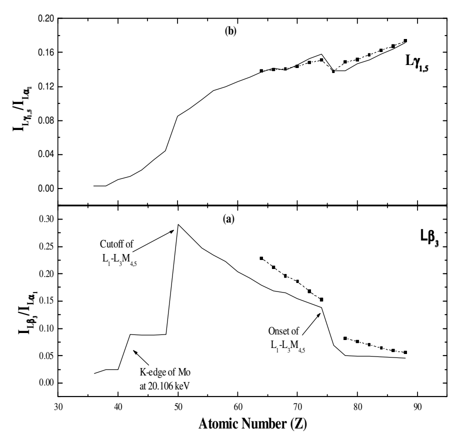

Figure 2: Plot of intensity ratios, $I_{Lk} / I_{L\alpha 1}$ (k=□$_3$ and □$_{1,5}$), at 20 keV incident photon energy as a function of atomic number (Z) . The solid lines corresponds to the DHS values and dotted lines with symbols represent the intensity ratios calculated using Li(i=1-3) sub-shell fluorescence and CK yields recommended by Campbell[6,7]

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