

Investigation of Chemical Effects on the Ly_{2,3} and Ly₄ X-ray Production Cross Sections for Some Compounds of ⁶⁶Dy at Photon Energies Close to L₁ Absorption-edge Energy

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Abstract : The radiative decay of Li(i=1-3) sub-shell vacancies produced through photoionization results in production of the characteristic emission spectrum comprising several X-ray lines, whereas non-radiative vacancy decay results in Auger electron spectrum. Accurate reliable data on the Li(i=1-3) sub-shell X-ray production (XRP) cross sections is of considerable importance for investigation of atomic inner-shell ionization processes as well as for quantitative elemental analysis of different types of samples employing the energy dispersive X-ray fluorescence (EDXRF) analysis technique. At incident photon energies in vicinity of the absorption edge energies of an element, the many body effects including the electron correlation, core relaxation, inter-channel coupling and post-collision interactions become significant in the photoionization of atomic inner-shells. Further, in case of compounds, the characteristic emission spectrum of the specific element is expected to get influenced by the chemical environment (coordination number, oxidation state, nature of ligand/functional groups attached to central atom, etc.). These chemical effects on L X-ray fluorescence parameters have been investigated by performing the measurements at incident photon energies much higher than the Li(i=1-3) sub-shell absorption edge energies using EDXRF spectrometers. In the present work, the cross sections for production of the L_k(k= γ _{2,3}, γ ₄) X-rays have been measured for some compounds of ⁶⁶Dy, namely, Dy₂O₃, Dy₂(CO₃)₃, Dy₂(SO₄)₃·8H₂O, DyI₂ and Dy metal by tuning the incident photon energies few eV above the L₁ absorption-edge energy in order to investigate the influence of chemical effects on these cross sections in presence of the many body effects which become significant at photon energies close to the absorption-edge energies. The present measurements have been performed under vacuum at the IAEA end-station of the X-ray fluorescence beam line (10.1L) of ELETTRA synchrotron radiation facility (Trieste, Italy) using self-supporting pressed pellet targets (1.3 cm diameter, nominal thicknesses ~ 176 mg/cm²) of ⁶⁶Dy compounds (procured from Sigma Aldrich) and a metallic foil of ⁶⁶Dy (nominal thickness ~ 3.9 mg/cm², procured from Good Fellow, UK). The present measured cross sections have been compared with theoretical values calculated using the Dirac-Hartree-Slater(DHS) model based fluorescence and Coster-Kronig yields, Dirac-Fock(DF) model based X-ray emission rates and two sets of L₁ sub-shell photoionization cross sections based on the non-relativistic Hartree-Fock-Slater(HFS) model and those deduced from the self-consistent Dirac-Hartree-Fock(DHF) model based total photoionization cross sections. The present measured XRP cross sections for ⁶⁶Dy as well as for its compounds for the L_{2,3} and L₄ X-rays, are found to be higher by ~14-36% than the two calculated set values. It is worth to be mentioned that L_{2,3} and L₄ X-ray lines are originated by filling up of the L₁ sub-shell vacancies by the outer sub-shell (N_{2,3} and O_{2,3}) electrons which are much more sensitive to the chemical environment around the central atom. The present observed differences between measured and theoretical values are expected due to combined influence of the many-body effects and the chemical effects.

Keywords : chemical effects, L X-ray production cross sections, Many body effects, Synchrotron radiation

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