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Chemical effect on the atomic and molecular cross sections of some Ce compounds near the K edge

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Abstract:

The absorption of X-rays in materials has been an important topic in the field of radiation physics and chemistry. X-ray absorption parameters such as mass attenuation coefficient, atomic, molecular and electronic cross sections, effective atomic number and electron density are important in the field of interaction of X-rays with matter. These parameters should be known accurately, since the interaction of X-ray with matter has wide application fields such as atomic, molecular and radiation physics, X-ray fluorescence surface chemical analysis, cancer therapy, dosimetric computations for health physics and space explanation.

In this study, the atomic and molecular cross sections were determined using the experimental total mass attenuation coefficients near the K edge in X-ray energy range from 31.817 to 51.698 keV for Ce_2O_3, $Ce(OH)_4$, $Ce(SO_4)_2$ and $CeCl_3.7H_2O$ compounds. The measurements were performed in a transmission geometry using the $K\alpha_2$, $K\alpha_1$, $K\beta_1$ and $K\beta_2$ X-rays from the different secondary source targets excited by the 59.54 keV photons from an annular Am-241 source. The energy gap, ionization energy, electron affinity and global electrophilicity values of oxide, sulphate, chloride and hydroxide ions were calculated utilizing the density functional theory (DFT/B3LYP). The experimental results of atomic and molecular cross sections were discussed based on these parameters. Also, the results were compared with the theoretical calculations.

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