THE THEORETICAL ANALYSIS OF THE X-RAY ABSORPTION SPECTRUM AT THE OXYGEN K-EDGE FOR $Cs_2UO_2Cl_4$

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The soft X-ray spectrum of Denning and co-workers for the high-lying excited levels at the oxygen K-edge for $Cs_2UO_2Cl_4$ was studied theoretically. We performed calculation with uranyl as the free ion and with uranyl as an ion embedded in crystal. The calculations in the crystalline environment were done using a crystal model. At the level of theory used, localized and delocalized hole description gives different results so we computed both sets of values. An important part of the investigation is the states near and well above the ionization threshold of oxygen 1s orbital. All calculations were performed using the COLUMBUS suite of programs. Correlation-consistent polarized double-zeta basis sets were used. The relativistic effects were treated through an implementation of the 68-electron relativistic effective core potentials (RECPs).