THEORETICAL CALCULATIONS FOR THE HIGH-LYING EXCITED AUTOIONIZING LEVELS 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 autoionizing levels at the oxygen K-edge for $Cs_2UO_2Cl_4$ is studied theoretically in an effort to explain the nature of the excited levels. An interesting feature is the intense polarized band well above the ionization threshold with an excitation energy of approx. 555 eV. This suggests a relatively long-lived autoionizing excited state. Based on the fact that sharp autoionizing resonances can be attributed to the occupation of an orbital with a high angular momentum, the 5g excited state has been suggested and we carried out self-consistent field (SCF) calculations (without spin-orbit) and single-excitation configuration interaction (CI) calculations(with spin-orbit). A 68-electron relativistic effective core potential was used on the uranium atom. Correlation-consistent polarized double-zeta basis sets were used. We calculated a number of states based on the uranium 5g orbitals and the energies obtained are very close to the experimental results.