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XPS structure and chemical bond nature in Cs2PuO2Cl4

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The quantitative analysis of the x-ray photoelectron spectral (XPS) structure of Cs2PuO2Cl4 single crustal containing the plutonyl group PuO22+ was done in the valence electrons binding energy range 0 - ˜35 eV taking into account binding energies and spectral structures of the core electronic levels (˜35 - 1250 eV) and the relativistic calculation data for the PuO2Cl42- (D4h) cluster reflecting plutonium close environment in Cs2PuO2Cl4. The experimental data suggest that the many-body processes and the multiplet splitting contribute to the valence XPS structure significantly less than the outer (0 - ˜15 eV) and the inner (˜15 - ˜35 eV) valence molecular orbitals formation does. The filled Pu 5f electronic states were shown to appear in the valence band of Cs2PuO2Cl4. The atomic Pu 6p electronic orbitals were shown to participate in formation of both inner and outer valence molecular orbitals (bands). The most part in the inner valence molecular orbitals formation were found to take the filled Pu 6p3/2 and O 2s, Cl 3s atomic shells. The composition and the sequent order of such orbitals in Cs2PuO2Cl4 were established in the binding energy range 0 - ˜35 eV. The obtained experimental and calculation data allowed for the first time a quantitative scheme of the molecular orbitals for Cs2PuO2Cl4. This scheme is essential and fundamental for understanding of the chemical bonding nature in Cs2PuO2Cl4 and for interpretation of the fine structures of other x-ray spectra.

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