Structure solution and electronic properties of the new offset hollandite $K_2Sn_3O_7$

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We present the compound $K_2Sn_3O_7$, a Sn^{4+}-containing oxide with a unique structure type among oxides. A combination of X-ray and neutron diffraction was essential to solve the structure of this compound from powder data. The compound is orthorhombic and reminiscent of an offset hollandite, where open channels hold a row of four K^+ per channel per cell. UV-visible spectroscopy indicates a wide band gap semiconductor, which is confirmed by first-principles electronic-structure calculations of band structures, densities of states, and optical properties. The continued discovery of new structure types in ternary tin oxides should remain a priority for the identification of prospective ion conductors and transparent conducting compounds.