

Finite and Infinite Chains of Heavy-Atom Clusters

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Discovered during the search for novel topological insulators^[1], we discovered new pseudo one-dimensional compounds. The reaction of Bi with Sn, Pt and BiI₃ above 300 °C yielded shiny, black, air insensitive crystals of the subiodide Sn[PtBi₆I₁₂] as well as the partially substituted (Sn_{0.7}Bi_{0.2}□_{0.1})[PtBi₆I₁₂]. Through extensive investigations into the synthetic pathway with the help of differential scanning calorimetry, the two compounds could be isolated and synthesized independently. The rhombohedral crystal structures consist of alternating cuboctahedral [PtBi₆I₁₂]²⁻ cluster anions and Sn²⁺ or Bi³⁺ cations in octahedral coordination between trigonal faces of two cuboctahedra. These concatenate them into linear chains, which makes Sn[PtBi₆I₁₂] an analogue to the compound Pb[PtBi₆I₁₂]^[2], while (Sn_{0.7}Bi_{0.2}□_{0.1})[PtBi₆I₁₂] with its vacant positions consists of finite strands. Additionally, the crystals' cube-like morphology originates from six weaker Bi⋯I inter-cluster bridges per cluster connecting the chains. Alternatively, the structure can be interpreted as an ordered defect variant of the NaCl structure type. The heavy elements show strong spin-orbit coupling. If this exceeds the width of the chemical band gap of the compound, a non-trivial topology can be expected.

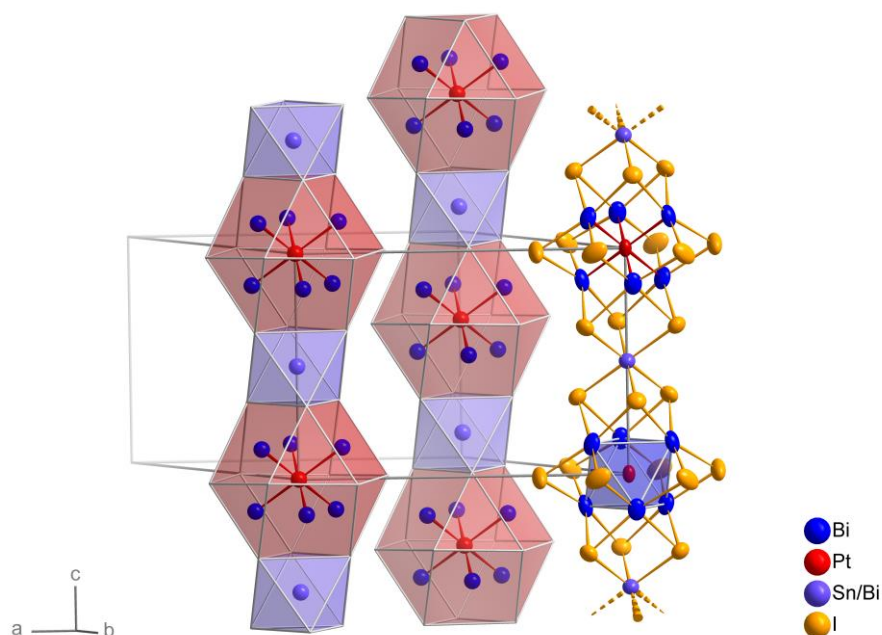


Figure 1 – Strands of (Sn_{0.7}Bi_{0.2}□_{0.1})[PtBi₆I₁₂] showcasing the different coordination environments.

[1] a) M. Z. Hasan, C. L. Kane, *Rev. Mod. Phys.* **2010**, *82*, 3045; b) Y. Ando, *J. Phys. Soc. Jpn.* **2013**, *82*.

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