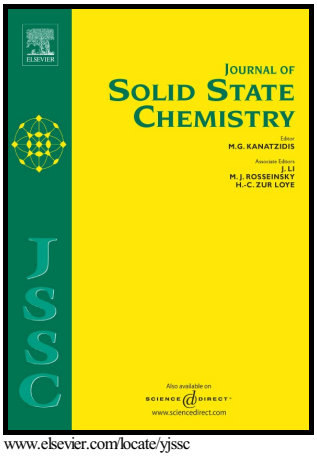

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Ternary palladium-indium-phosphorus and platinum-indium-phosphorus compounds based on the Cu_3Au-type: structure, bonding, and properties

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Abstract

Two metal-rich compounds, Pd_5InP and Pt_5InP, were synthesized as phase-pure powders using a high-temperature ampoule technique. According to the Rietveld analysis, they crystallize in the fairly rare Pd_5TlAs structure type (tetragonal system, *P4/mmm* space group, Pearson symbol tP7, with a = 3.9303(5) Å, c = 6.9269(1) Å, Z = 1, R_p = 0.029, R_b = 0.004 for Pd_5InP, and a = 3.9500(1) Å, c = 6.9814(3) Å, Z = 1, R_p = 0.034, R_b = 0.005 for Pt_5InP. For both compounds, main structural units are indium-centered $[TM_{12}In]$ cuboctahedra (TM=Pd, Pt), alternating along the c axis with $[TM_8P]$ rectangular prisms of the $PtHg_2$ type. DFT electronic structure calculations and magnetic measurements indicate 3D metallic conductivity and diamagnetic behavior for both compounds. According to the bonding analysis based on the electron localizability indicator topology and charge density, both compounds are intermetallic in nature and feature four-centered interactions of the 3TM+In type between the transition metal and indium atoms in their heterometallic fragments, complemented in the case of platinum by Pt-Pt pairwise interactions. Both compounds do not show any significant hydrogen uptake up to pressures of ca. 7 MPa and temperatures of 700 K.

Graphical abstract

Phase-pure metal-rich compounds, Pd_5InP and Pt_5InP, crystallizing in the Pd_5TlAs-type structure, are obtained by high-temperature ampoule route from transition metals and InP.