

Abstract Submitted
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Chemical Physics and Properties of ThPt₂ ANDREAS LEITHE-JASPER, MPI-CPfS Dresden, ROMAN GUMENIUK, MPI-CPfS Dresden and TU Bergakademie Freiberg, WALTER SCHNELLE, MICHAEL NICKLAS, YURI GRIN, MPI-CPfS Dresden — ThPt₂ crystallizes with a unique type of structure (space group $I4/mmm$, $a = 4.1569(2)$ Å, $c = 14.3678(6)$ Å, which belongs to the group of the close-packed tetragonal structures (Pearson symbol $tI12$). An analysis of the chemical bonding by the electron density/electron localizability approach reveals formation of two-dimensional platinum anions separated by the Th cations. Measurements of magnetic susceptibility, electrical resistivity and specific heat show ThPt₂ to be diamagnetic with good metallic conductivity ($\rho(300 K) \approx 8.5 \mu\Omega \text{ cm}$). The properties are in good agreement with the calculated electronic structure with a low DOS ($N(E_F) = 0.92$ states $\text{eV}^{-1} \text{ f.u.}^{-1}$). The stability of the compound with respect to other possible structural modifications was studied theoretically.

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