structure (solids and liquids)

D 2000

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AuTa14S2 - Centered (Au,Ta)13 Icosahedra Organized According to the Motif of a Cubic Close Packing. — Ta-rich phases AuxTa15-xS2 with 0.4 ¡ · ¡ 1.1 are prepared by melting appropriate mixtures of Ta1.35S2, Ta, and Au and subsequent annealing at 1700 K (sealed Mo-crucible, vacuum). Brittle crystals are obtained in the presence of I2 as chemical transport agent. The lattice parameters of the rhombohedral phases, which are isostructural with Pd15P2, decrease with increasing Au content. The structures are determined by powder XRD and confirmed by a crystal structure analysis of a twinned crystal of composition Au0.7Ta14.3S2 (space group R3, Z = 1). The structure is based on a cubic close packing of Ta12-icosahedra. Au preferentially occupies the centers of these polyhedra, the remaining Ta atoms occupy octahedral sites, and the sulfur atoms are located in tetrahedral sites. — (HARBRECHT, B.; WAGNER, V.; Z. Anorg. Allg. Chem. 620 (1994) 6, 969-976; Inst. Anorg. Chem., Univ., D-53121 Bonn, Germany; DE)