

The Modulated Structure of SrAuSn₂

Saeid Esmailzadeh^a, Rolf-Dieter Hoffmann^b, and Rainer Pöttgen^b

^a Department of Inorganic Chemistry, Arrhenius Laboratory, Stockholm University,
SE-106 91 Stockholm, Sweden

^b Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster,
Corrensstraße 36, D-48149 Münster, Germany

Reprint requests to R. Pöttgen. E-mail: pottgen@uni-muenster.de

Z. Naturforsch. **59b**, 1451 – 1457 (2004); received August 24, 2004

Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

The ternary stannide SrAuSn₂ was synthesized by induction melting of the elements under an argon atmosphere in a sealed niobium ampoule in a water-cooled sample chamber of a high-frequency furnace. The structure of SrAuSn₂ was investigated by X-ray powder and single crystal diffraction. It was found to be favourable to describe as a commensurately modulated structure. The 3+1 dimensional superspace group symmetry $P : Cmc m(\alpha, 0, 0) : 0s0$ with the unit cell dimensions $a = 460.20(14)$, $b = 2038.8(8)$, $c = 460.34(19)$ pm and the modulation wave vector $\mathbf{q} = 1/4 [100]^*$. The Sn1 atoms were those with the strongest modulation while the rest of the atoms showed rather small deviations from the average structure. The SrAuSn₂ structure is closely related to the CeNiSi₂ type. Geometrically these structures are built up from distorted ThCr₂Si₂ and AlB₂ slabs. The gold atoms are located in the ThCr₂Si₂ slab. They have a distorted square pyramidal tin coordination at Au–Sn distances ranging from 266 to 294 pm. These pyramids are condensed *via* common edges forming two-dimensional layers. The latter are condensed *via* the Sn1 atoms within the AlB₂ slabs that form one-dimensional zigzag chains with Sn1–Sn1 distances ranging from 282 to 288 pm. These chains show the strong modulations. Together, the gold and tin atoms build up a three-dimensional [AuSn₂] network, in which the strontium atoms fill distorted hexagonal channels.

Key words: Stannide, Crystal Structure, Modulated Structure