

Structure

D 2000

DOI: 10.1002/chin.201205006

05- 006

**New Lanthanum-Stannide/Germanide:  $\text{La}_3\text{Sn}_{4.4}\text{Ge}_{0.6}$ ,  $\text{La}_3\text{Sn}_{3.1}\text{Ge}_{0.9}$  and  $\text{La}_9\text{Sn}_{6.7}\text{Ge}_{3.3}$ .** — The new title compounds are obtained from melts of the elements and characterized by single crystal XRD and FP-LAPW band structure calculations.  $\text{La}_3\text{Sn}_{4.4}\text{Ge}_{0.6}$  crystallizes in the tetragonal space group  $I4/mcm$  with  $Z = 4$  ( $\text{Ti}_4\text{PbTe}_3$ -type structure). The structure contains isolated  $(\text{Ge/Sn})^{4-}$  anions and heavily puckered  $4.8^2$ -nets of  $[\text{Sn}_4]^{4+}$  ions.  $\text{La}_3\text{Sn}_{3.1}\text{Ge}_{0.9}$  crystallizes in the orthorhombic space group  $Cmcm$  with  $Z = 4$  ( $\text{Er}_3\text{Ge}_4$ -type structure).  $\text{La}_9\text{Sn}_{6.7}\text{Ge}_{3.3}$  crystallizes with its own structure type in the tetragonal space group  $P4_2/nm$  with  $Z = 8$ . The structure contains isolated Sn and Ge atoms,  $[\text{Sn/Ge}]_2$  dumbbells, bent  $[\text{Sn}_3]$  trimers, planar four-membered  $[\text{Ge}_4]$  rings, and planar six-membered rings  $[\text{M}_6]$  (M: Sn, Ge). — (DUERR, I.; ROEHR\*, C.; Z. Naturforsch., B: Chem. Sci. 66 (2011) 10, 1015-1028 ; Inst. Anorg. Anal. Chem., Albert-Ludwigs-Univ., D-79104 Freiburg/Br., Germany; Ger., Abstr. Eng.) — W. Pewestorf