Condensed $[Ru_4Sn_6]$ Units in the Stannides $LnRu_4Sn_6$ (Ln = La, Pr, Nd, Sm, Gd) – Synthesis, Structure, and Chemical Bonding

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The stannides $LnRu_4Sn_6$ (Ln = La, Pr, Nd, Sm, Gd) were prepared by reaction of the elements in an arc-melting furnace and subsequent annealing at 1120 K. The praseodymium, the neodymium, and the samarium stannide were obtained for the first time. The $LnRu_4Sn_6$ stannides were investigated by X-ray diffraction both on powders and single crystals. They adopt the YRu_4Sn_6 type structure which was refined from single crystal X-ray data for the samarium and the gadolinium compound: *I*4̄2*m*, *a* = 686.1(1), *c* = 977.7(2) pm, *wR*2 = 0.0649, 483 F^2 values for $SmRu_4Sn_6$, and *a* = 685.2(1), *c* = 977.6(3) pm, *wR*2 = 0.0629, 554 F^2 values for $GdRu_4Sn_6$ with 19 variables for each refinement. The striking structural motif of these stannides are distorted $RuSn_6$ octahedra with Ru-Sn distances ranging from 257 to 278 pm. Four of such octahedra are condensed via common edges and faces forming $[Ru_4Sn_6]$ units which are packed in a tetragonal body-centered arrangement. The rare-earth atoms fill the voids between the $[Ru_4Sn_6]$ units. Based on an extended Hückel calculation, strong bonding interactions were found for the Ru-Sn and the various Sn-Sn contacts.