Synthese und Kristallstrukturen von Seltenerdmetall-Antimoniden des Palladiums

Synthesis and Crystal Structures of Antimonides of Rare-Earth Metals and Palladium

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The new compounds $Pr_3Pd_6Sb_5$ ($a = 13.442(3)$, $b = 4.442(1)$, $c = 9.994(2)$ Å), $Nd_3Pd_6Sb_5$ ($a = 13.412(3)$, $b = 4.431(1)$, $c = 9.962(2)$ Å), and $Gd_3Pd_6Sb_5$ ($a = 13.293(2)$, $b = 4.397(1)$, $c = 9.881(2)$ Å) are isotypic and crystallize with the $Ce_3Pd_6Sb_5$ type structure ($Pmmn$; $Z = 2$). The rare-earth metal atoms are arranged in form of three pseudo-body-centered subcells, whereas Pd and Sb atoms form a three-dimensional arrangement derived from the well-known $ThCr_2Si_2$ and $CaBe_2Ge_2$ structures. GdPdSb ($a = 4.566(1)$, $c = 7.444(1)$ Å) and DyPdSb ($a = 4.545(1)$, $c = 7.354(1)$ Å) crystallize with an ordered variant of the $CaIn_2$ type structure ($P6_3mc$; $Z = 2$), also called as LiGaGe type, with slightly puckered hexagon nets of Pd and Sb atoms, which trigonally coordinate each other. In this series a decreasing radius of the rare-earth metal allows a tetrahedral non-metal environment of the Pd atoms and accordingly ScPdSb ($a = 6.310(1)$ Å) forms the MgAgAs type structure ($F\bar{4}3m$; $Z = 4$), a filled variant of the sphalerite type. The antimonides were prepared by heating mixtures of the elements at 600 °C and subsequent annealing at 900 – 1100 °C. Their structures have been determined by single-crystal X-ray methods.

Key words: Antimonides, Rare-Earth Metals, Palladium, Crystal Structures