

Structure and Properties of the Stannides CeAuSn, Ce₃Rh₄Sn₁₃, and Ce₃Ir₄Sn₁₃

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Intermetallic Compounds, Cerium, Mössbauer Spectra

CeAuSn, Ce₃Rh₄Sn₁₃, and Ce₃Ir₄Sn₁₃ were prepared by reaction of the elements in an arc-melting furnace and subsequent annealing at 970 K for two weeks. The three stannides were investigated by X-ray powder and single crystal techniques. CeAuSn crystallizes with the NdPtSb type, space group $P6_3mc$: $a = 472.7(2)$, $c = 771.6(3)$ pm, $wR2 = 0.0230$, 208 F^2 values, 11 variable parameters, and $BASF = 0.40(2)$. The gold and tin atoms form a pronounced two-dimensional [AuSn] polyanion which consists of slightly puckered Au₃Sn₃ hexagons. ¹¹⁹Sn Mössbauer data at 78 K show one signal at an isomer shift of $\delta = 1.90(7)$ mm/s subjected to unresolved quadrupole splitting of $\Delta E_Q = 0.55(2)$ mm/s. Ce₃Rh₄Sn₁₃ and Ce₃Ir₄Sn₁₃ adopt the cubic Yb₃Rh₄Sn₁₃ type structure, space group $Pm\bar{3}n$: $a = 970.51(3)$ pm, $wR2 = 0.0721$, 267 F^2 values (Ce₃Rh₄Sn₁₃) and $a = 972.29(6)$ pm, $wR2 = 0.0850$, 267 F^2 values (Ce₃Ir₄Sn₁₃) with 14 variable parameters for each refinement. Striking structural motifs in Ce₃Rh₄Sn₁₃ are condensed distorted trigonal [RhSn₆] prisms with Rh-Sn distances of 266 pm. The polyhedral network leaves two different cages which are occupied by cerium (6c position) and tin (2a position) atoms. The Sn2 atoms show occupancy parameters of only 92% (Ce₃Rh₄Sn₁₃) and 76% (Ce₃Ir₄Sn₁₃) and an extremely large displacement parameter indicating a rattling of these atoms within the icosahedral Sn₁₂ cages. Magnetic susceptibility measurements of Ce₃Rh₄Sn₁₃ show paramagnetic behavior down to 2 K with an experimental magnetic moment of 2.45(2) μ_B /Ce. No magnetic ordering is observed. Magnetization measurements show a moment of 0.78(2) μ_B /Ce at 2 K and 5.5 T. Resistivity data reveal only a very weak temperature dependence. The two crystallographically different tin sites are resolved in the ¹¹⁹Sn Mössbauer spectrum which shows a signal at $\delta = 2.12(1)$ mm/s subject to quadrupole splitting of 1.54(1) mm/s, superimposed by a singlet at $\delta = 2.47(1)$ mm/s. The Seebeck coefficient of Ce₃Rh₄Sn₁₃ is within a few $\mu V/K$ of zero over the temperature range of 10 - 300 K.