

Ternary Scandium-rich Indides $\text{Sc}_{50}\text{T}_{13}\text{In}_3$ and $\text{Sc}_{50}\text{Rh}_{13}\text{In}_3\text{O}_y$ ($T = \text{Rh}, \text{Ir}; y \approx 8$) – Synthesis and Crystal Structure

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New intermetallic compounds $\text{Sc}_{50}\text{Rh}_{13.3}\text{In}_{2.7}$ and $\text{Sc}_{50}\text{Ir}_{13.6}\text{In}_{2.4}$ and the suboxides $\text{Sc}_{49.2}\text{Rh}_{13}\text{In}_{3.8}\text{O}_{8.8}$ and $\text{Sc}_{49.2}\text{Rh}_{13.7}\text{In}_{2.8}\text{O}_{8.0}$ were synthesized from the elements or with Sc_2O_3 as an oxygen source, respectively, in sealed tantalum tubes in a water-cooled sample chamber of an induction furnace. They crystallize with a new cubic structure type, space group $Fm\bar{3}$, $a = 1772.5(6)$ pm, $wR2 = 0.032$, 1111 F^2 values, 34 variables for $\text{Sc}_{50}\text{Rh}_{13.3}\text{In}_{2.7}$, $a = 1766.5(6)$ pm, $wR2 = 0.041$, 745 F^2 values, 34 variables for $\text{Sc}_{50}\text{Ir}_{13.6}\text{In}_{2.4}$, $a = 1764.4(2)$ pm, $wR2 = 0.044$, 690 F^2 values, 41 variables for $\text{Sc}_{49.2}\text{Rh}_{13}\text{In}_{3.8}\text{O}_{8.8}$, and $a = 1761.5(6)$ pm, $wR2 = 0.054$, 740 F^2 values, 42 variables for $\text{Sc}_{49.2}\text{Rh}_{13.7}\text{In}_{2.8}\text{O}_{8.0}$. The main structural motifs are rhodium-centered indium cubes in an *fcc* like arrangement in which the octahedral and tetrahedral voids are filled by $\text{In}_2\text{Sc}_{12}$ and InSc_{12} icosahedra, respectively, resembling a Li_3Bi -like structure. The Rh1 (Ir1) and Sc4 atoms lie between these polyhedral units. The oxygen atoms partially fill Sc_6 octahedra in $\text{Sc}_{49.2}\text{Rh}_{13}\text{In}_{3.8}\text{O}_{8.8}$ and $\text{Sc}_{49.2}\text{Rh}_{13.7}\text{In}_{2.8}\text{O}_{8.0}$ with Sc–O distances of 214–230 pm. These octahedra are condensed *via* common edges and faces, encapsulating the $\text{In}_2\text{Sc}_{12}$ icosahedra. Due to the high scandium content one observes strong Sc–Sc bonding with Sc–Sc distances ranging from 303 to 362 pm in $\text{Sc}_{49.2}\text{Rh}_{13}\text{In}_{3.8}\text{O}_{8.8}$. The shortest distances occur for Sc–Rh (267–295 pm). The crystal chemical relationship with the Li_3Bi -related suboxide $\text{Ti}_{12}\text{Sn}_3\text{O}_{10}$ is discussed.

Key words: Scandium, Intermetallics, Suboxides, Crystal Structure