Synthesis and Crystal Structure of $\text{Zr}_5\text{Rh}_2\text{In}_4$ and $\text{Hf}_5\text{Rh}_2\text{In}_4$
– New Ternary Indides with $\text{Lu}_5\text{Ni}_2\text{In}_4$ Type Structure

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Dedicated to Professor Albrecht Mewis on the occasion of his 60th birthday

Z. Naturforsch. 57 b, 1353–1358 (2002); received August 2, 2002

Indium, Crystal Structure, Zirconium, Hafnium, Rhodium

The ternary indides $\text{Zr}_5\text{Rh}_2\text{In}_4$ and $\text{Hf}_5\text{Rh}_2\text{In}_4$ were synthesized by high-frequency melting of the elements in glassy carbon crucibles in a water-cooled sample chamber. Both compounds have been investigated by X-ray diffraction on powders and single crystals: $\text{Lu}_5\text{Ni}_2\text{In}_4$ type, $Pbam$, $a = 1739.8(2)$, $b = 758.3(1)$, $c = 337.42(5)$ pm, $wR^2 = 0.0420$, 1015 $F^2$ values for $\text{Zr}_5\text{Rh}_2\text{In}_4$, and $a = 1732.1(3)$, $b = 757.5(2)$, $c = 333.36(7)$ pm, $wR^2 = 0.0534$, 739 $F^2$ values for $\text{Hf}_5\text{Rh}_2\text{In}_4$ with 36 variables per refinement. The structures contain three crystallographically different zirconium (hafnium) sites with coordination numbers 12, 14, and 16. Striking structural motifs are distorted rhodium-centered trigonal prisms formed by the zirconium (hafnium) atoms and CuAu related distorted cubes of zirconium (hafnium) and indium atoms. The shortest interatomic distances occur for Zr-Rh and Hf-Rh followed by Rh-In. Chemical bonding in these intermetallics is briefly discussed.