

Structural Comparisons of Three Intermetallic Antimonide Families

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High quality single crystals of the ternary antimonides $LnNi_xSb_2$ ($Ln = Y, Gd - Er$; $x \approx 0.6$) and $LnNiSb_3$ ($Ln = Pr, Nd, Sm$) have been grown from an antimony flux. Their crystal structures have been characterized by single crystal X-ray diffraction experiments. The $LnNi_xSb_2$ compounds adopt the $HfCuSi_2$ structure type and crystallize in the tetragonal space group $P4/nmm$ with $Z = 2$ and lattice parameters of $a \approx 4.3 \text{ \AA}$, $c \approx 9.3 \text{ \AA}$, and $V \approx 170 \text{ \AA}^3$. These compounds are layered and consist of Ln -capped Sb square nets and Ni tetrahedral frameworks arranged in an anti-PbO fashion. The $LnNiSb_3$ compounds adopt the $CeNiSb_3$ structure type and crystallize in the orthorhombic space group, $Pbcm$ (No. 57), $Z = 12$, with lattice parameters $a \approx 12.5$, $b \approx 6.2$, $c \approx 18.4 \text{ \AA}$, and $V \approx 1400 \text{ \AA}^3$. Similar to the $LnNiSb_2$ compounds, these compounds are layered but consist of rare-earth atoms located above and below planes of nearly square, buckled Sb nets, however with layers of highly distorted edge- and face-sharing $NiSb_6$ octahedra. The structures of the $LnNi_xSb_2$ ($Ln = Y, Gd - Er$; $x \approx 0.6$) and $LnNiSb_3$ ($Ln = Pr, Nd, Sm$) compounds are similar to the structure of the simple binary phases $LnSb_2$ ($Ln = La, Nd, Sm, Gd-Er$). In an effort to correlate and elucidate the origin of the physical behavior observed, the structural units found within these three families will be compared.

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