The Solid Solution $TmNi_{1-x-y}In_{1+x}$

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The thulium nickel indide TmNiIn forms solid solutions $TmNi_{1-x-y}In_{1+x}$. Several samples have been prepared by arc-melting of the elements under argon. The structure of TmNiIn contains two crystallographically different nickel sites. The Ni1 atoms have a trigonal prismatic coordination by indium, while the Ni2 sites have six thulium neighbors in a trigonal prismatic arrangement. The Ni1 sites show defects in the solid solution, while the Ni2 sites have Ni2/In mixing with a maximal occupancy of 32 at.-% indium. The structures of three single crystals of solid solutions have been refined, leading to the compositions $TmNi_{0.88}In_{1.10}$ ($a = 747.06(7)$, $c = 367.8(1)$ pm, $wR2 = 0.0342$, 323 F^2 values, 16 variables), $TmNi_{0.80}In_{1.16}$ ($a = 752.94(7)$, $c = 366.5(1)$ pm, $wR2 = 0.0475$, 503 F^2 values, 16 variables), and $TmNi_{0.76}In_{1.21}$ ($a = 758.4(1)$, $c = 366.68(7)$ pm, $wR2 = 0.0949$, 226 F^2 values, 16 variables). The crystal chemical peculiarities and the differences in chemical bonding are briefly discussed.

Key words: Solid Solution, Crystal Structure, Solid State Synthesis