A Single Crystal Study of $RE_{14}Co_3In_3$ (RE = Y, Tb, Dy, Ho, Er)

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The rare earth-cobalt-indides $RE_{14}Co_3In_3$ (RE = Y, Tb, Dy, Ho, Er) were prepared in polycrystalline form from the elements by arc-melting. Small single crystals were grown through a special annealing sequence. The compounds were investigated on the basis of X-ray powder and single crystal data: $Lu_{14}Co_{2}In_{3}$ ($Gd_{14}Co_{3}In_{2,7}$) type, $P4_{2}/nmc$, Z=4, a=959.0(1), c=2319.1(5) pm, wR2 = 0.055, 2289 F^2 values, 65 variables for $Y_{13.90}Co_{2.99}In_{3.02}$, a = 953.8(1), c =2315.8(5) pm, wR2 = 0.108, 2357 F^2 values, 65 variables for Tb_{13.92}Co_{3.01}In_{2.92}, a = 949.24(3), c = 2296.5(1) pm, wR2 = 0.129, $2518 F^2$ values, 65 variables for Dy_{13.90}Co_{2.97}In_{2.95}, a = 946.3(1), c = 2289.0(5) pm, wR2 = 0.099, 2297 F^2 values, 64 variables for $Ho_{14}Co_{2.80}In_{2.89}$, and a =941.0(1), c = 2274.2(5) pm, wR2 = 0.140, 2450 F^2 values, 65 variables for Er_{13.83}Co_{2.88}In_{3.10}. All RE_{14} Co₃In₃ indides show a small degree of In/Co mixing (between 7 and 16% Co) on the 4cIn 1 site and defects on the 8g Co1 positions (between 84 and 95% Co). Except for the holmium compound, the $RE_{14}Co_3In_3$ intermetallics also reveal RE/In mixing on the 4c RE1 sites, leading to the refined compositions. The seven crystallographically independent RE sites have between 9 and 10 nearest RE neighbors. The RE₁₄Co₃In₃ structures consist of a complex intergrowth of rare earth based polyhedra. Both cobalt sites have a distorted trigonal-prismatic rare earth coordination. An interesting feature is the In2–In2 dumb-bell with an In2–In2 distance of 300 pm (for Ho₁₄Co_{2.80}In_{2.89}). The crystal chemistry of the $RE_{14}Co_3In_3$ indides is discussed.

Key words: Rare Earth Compounds, Intermetallics, Crystal Chemistry