Crystal Structure and Magnetic Properties of the Novel Hollandite $\text{Ba}_{1.3}\text{Co}_{1.3}\text{Ti}_{6.7}\text{O}_{16}$

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Z. Naturforsch. 2011, 66b, 1097–1100; received September 20, 2011

Single crystals of the new barium hollandite $\text{Ba}_{1.3}\text{Co}_{1.3}\text{Ti}_{6.7}\text{O}_{16}$ were obtained from a $\text{BaCl}_2$ flux ($I^2/m, Z = 1, a = 9.9470(4), b = 2.9714(2), c = 10.2260(5)$ Å, $\beta = 90.906(2)^\circ$). In the crystal structure piles of Ba atoms are situated within a framework of edge- and vertex-sharing octahedra (Co,Ti)O$_6$. The composition was deduced from microprobe analyses, structure refinements and charge balance arguments in agreement with the observed magnetic properties. The temperature dependence of the magnetic susceptibility $\chi(T)$ of $\text{Ba}_{1.3}\text{Co}_{1.3}\text{Ti}_{6.7}\text{O}_{16}$ single crystals reveals paramagnetism down to 2 K. The value of the Co magnetic moment deduced from the Curie-Weiss law agrees well with the theoretical value of the high-spin state spin-only moment of $\mu_{\text{eff}} = 3.87\, \mu_B$ for Co$^{2+}$ ($S = 3/2$).

Key words: Hollandite, Cobaltate, Titanate