Tobias A. Teichtmeister and Hubert Huppertz*

The crystal structure of Tb₃B₅O₁₁(OH)₂

Abstract

Tb₃B₅O₁₁(OH)₂, orthorhombic, Pnna (no. 52), a = 4.4471(1) Å, b = 13.0934(4) Å, c = 13.9055(3) Å, V = 809.68(4) Å³, Z = 4, Rᵣ(F) = 0.0260, wRᵣ(F²) = 0.0556, T = 301(1) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

Tb₃B₅O₁₁(OH)₂ was obtained as a side phase during related experiments, investigating the system Tb₄O₇–CuO–B₂O₃. Small colorless crystals were found within the blue main product, which was obtained after the following procedure. Tb₄O₇ (0.06 mmol, Auer–Remy KG, 99.9 %), CuO (0.11 mmol, ChemPur, 99 %), and B₂O₃ (0.46 mmol, Alfa...
2 Experimental details

Refinements of the crystal structure were carried out in space group $Pnna$ (no. 52). Bond valence sums indicated protonation of the O7 atom. As a direct consequence of the symmetry of the crystal structure, a split-site H7a and H7b with occupation factors 0.5 each is necessary for a reasonable description of the hydrogen atoms. Interatomic OH-distances were fixed at 0.83 Å using DFIX records. Two reflections were omitted from the refinement due to their high deviation.

3 Comment

Terbium is the second lanthanoid displaying a structure type recently reported for Nd$_3$B$_5$O$_{11}$(OH)$_2$ [8]. The crystal structure consists of a three-dimensional framework of corner-sharing [BO$_4$] tetrahedra forming corrugated 10- and 14-membered rings in the $bc$-plane, and eight-membered rings in the $ac$-plane. Different coordination numbers are observed for the two crystallographically different Tb-sites (Tb1: $CN$ = 10; Tb2: $CN$ = 8). The H7-split-site can be interpreted as a hydroxide-group, forming a hydrogen-bond to another O7 atom, acting as the acceptor.

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