

## Structure of New Rare-Earth Borates $\text{Ln}[\text{B}_6\text{O}_9(\text{OH})_3]$ and its Relation to Boracites

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The crystal structures of rare-earth borates  $\text{Ln}[\text{B}_6\text{O}_9(\text{OH})_3]$ ,  $\text{Ln}=\text{Sm-Lu}$ , synthesized under hydrothermal conditions, are solved in the space group  $R3c$  ( $\text{Ln}=\text{Ho}$ ,  $a$  8.385(9),  $c$  20.71(4),  $R$  = 29%, and  $\text{Ln}=\text{Gd}$ ,  $a$  8.410(4),  $c$  20.72(1),  $R$  = 4.8%). New borates belong to hexaborate group. The polar anionic framework consists of fundamental building blocks FBB  $[3\text{T}+3\Delta]$ : six-membered rings of regularly alternating  $(\text{BO}_4)$ -tetrahedra and  $(\text{BO}_3)$ -triangles. Atoms of  $\text{Ln}$  and  $\text{H}$  are located in wide channels along threefold axis.  $\text{Ln}$ -borates have the closest structural relation to synthetic boracite  $\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$  with the same FBB [1].

Structural relationship between all boracite modifications can be revealed, if to pay attention to clusters of four hexaborate blocks of two types  $[6\text{T}]$  or  $[3\text{T}+3\Delta]$ . In the cubic boracites  $\text{M}_3\text{B}_7\text{O}_{13}\text{Cl}$  ( $\text{M} = \text{Mg, Fe}$ ) [2] and many synthetic analogues four blocks  $[6\text{T}]$  are linked via vertices. The trigonal and orthorhombic distortion [3] is caused by increase one of B-O bond and corresponding decrease of B coordination from tetrahedron to triangle. In the cubic  $\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$  such clusters consist of four blocks  $[3\text{T}+3\Delta]$ . In the trigonal  $\text{Ln}[\text{B}_6\text{O}_9(\text{OH})_3]$ , in comparison with  $\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$ , there is one B-atom less, what leads to destruction of such clusters with keeping single six-membered rings.

[1] Jeitschko W., Bither T.A., Bierstedt P.E., *Acta Cryst.*, 1977, **B33**, 2767. [2] Sueno S., Clark J.R., Papike J.J., Konnert J.A., *Am. Mineral.*, 1973, **58**, 691. [3] Dowty E., Clark J.R., *Z. Kristallogr.*, 1973, **138**, 64.

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