

s11.m1.o5 Pentaborates and hexaborates crystal chemistry on the base of OD-theory.

E.L. Belokoneva, T.A. Korchemkina, O.V. Dimitrova.. *Moscow State University, Geology Department, 119899 Moscow Russia.*

Keywords: borate, OD-theory, genetic-structural classification.

Notes

The modern classification of borate minerals has been developed by Strunz¹. It follows the important rule suggested first by Christ and Clark² of selection of fundamental building blocks (FBB) before applying usual systematization in accordance with the degree of their condensation.

Dornberger-Schiff³ theory of OD structures inspects the symmetry of layers and symmetry relations between layers in the crystal structures. As she mentioned, such a method may be applied not only to layers, but also to structural "rods" or "blocks".

The FBB and the "block" in the OD-theory are the same. One may describe the symmetry of the aperiodic, 1D- and 2D-periodic units and their combinations via symmetry groupoids of different ranks, to predict non-existing structures and to suggest the modification of systematics.

In hexaborates one FBB $6(3\Delta+3T)$ is aperiodic in macallisterite, aksaite, rivadavite; condensed in 1D-periodic chain in aristarainite; 2D-periodic layers occur in tunnelite, nobleite, ginorite (strontioginorite, volkovite) and strontiorborite. The interlayer space varies and that determines the kind of pairs of adjacent layers and the division of structures into subgroups.

In pentaborates there are four FBB: $(1)5(4\Delta+1T)$, $(2)5(3\Delta+2T)$, $(3)5(2\Delta+3T)$, $(4)5(1\Delta+4T)$ with a similar topology. Their condensation gives three branches of structures: (1) sborgite (isolated), ammonioborite (sorogroup), lardellite (chain), RbB_5O_8 (framework); (2) ulexite (isolated), probertite and kaliborite (different chains), heidornite and tuzlaite (layers); (3) ezcurrite (chain), biringuccite, veatchite, volkovskite, new synthetic $LiBa_2[B_{10}O_{16}(OH)_3]$ and $Ba[B_5O_8(OH)]H_2O$ (polar layers) and gowerite, nasinite (non-polar layers); condensation of gowerite and nasinite layers lead to frameworks of hilgardites which are divided into two subgroups.

The higher degree of condensation correlates with the decrease of the amount of water in the structure and the increase of the temperature of crystallization of natural and hydrothermally synthesized phases. It correlates also with the dimension of ionic radii of the cations from Pb, Sr, Ca in frameworks and layers to Na, Mg in bands, chains, isolated units. Because of polytypic correlation many compounds are involved in joint mineral formation. The structural unity and variety in the group of minerals offer the tool for their classification. The approach developed here may be applied to tetra- and triborates. This work was supported by RFBS, project 98-03-32719. We are indebted to Prof. Tillmanns whose critical reading of Abstract improved the final version.

[1] Strunz H. "Classification of borate minerals", *Eur. J. Mineral.* (1997), 9: 225-232

[2] Christ C.L., Clark J.R. "A crystal - chemical classification of borate structures with emphasis on hydrated borates", *Phys. Chem. Minerals* (1977), 2: 59-87.

[3] Dornberger - Schiff K. "Grundzuege einer Theorie der OD-Structures aus Schichten", *Deuts. Acad. Wiss., Berlin, Abh., Kl. Chemie, Geologie und Biologie*, (1964), N3, 1-164.