Poster Presentations

[MS32-P09] What is "rigid unit" in borates?

Rimma Bubnova[1,2], Stanislav Filatov[2]

[1] Institute of the Silicate Chemistry of Acad.
Russ. Sci.199034, Makarov Emb. 2, Russia
[2] Geology Department, St.Petersburg State
University, 199034, University emb. 7/9,
St.Petersburg, Russia
E-mail: rimma_bubnova@mail.ru

Although the term «rigid boron-oxygen group» introduced by J. Krogh-Moe is used for a half of a century it has not been yet strongly defined. The relation of this sentence to the other crystal chemical terms like "fundamental building block", "structural module", "independent anionic unit" etc. is also discussed. Among inorganic compounds nearly ideal polyhedra (TO3 and TO4) whose configuration and bond lengths do not change under heating or pressure, are usually considered as rigid units. In borates rings formed by three polyherdra are charged normally to the rigid groups as well. Depending of polymerization type these rings could then form multiple rigid cyclic groups or modules. Approach to the definition of "rigid group" term present here is based on results of physical properties investigations, particularly thermal expansion anisotropy, and differs from standard geometrical approach for the separation building modules forming crystal structure. *Rigid groups* are essentially single cyclic triborate B-O rings and their combinations – *multiple cyclic groups formed by sharing of triborate rings via tetrahedra*. Among them there are double (tetra- and pentaborate groups) and triple rings (hexaborate groups) constructed from single rings by sharing tetrahedra. Fourfold ring formed by sharing four triple tetrahedral rings proposed by Bokii and Kravchenko in [2] has not been found jet in borates. For example, in $Na_8B_{12}O_{20}(OH)4$ structure [3], six single triborate rings combined into sixfold ring where every single ring has common tetrahedral with both neighbors. Further rising of rings' multiplicity leads to appearing of infinite chain from triborate rings sharing tetraherda (rigid group 1D [1]).

An example of combination of tetraborate groups by sharing tetrahedral is described in [1]. Kernite chain containing pentaborate groups sharing tetrahedron could also be considered as 1Drigid group. Character of kernite thermal expansion allows suggesting that the chains do not change their configuration with temperature [4] and just displace relative each other. The existing of rigid layers could also be suggested.

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