

Poster Presentations

[MS18-P15] **Polytypic modifications of huntite-like rare-earth aluminium and gallium borates $RM_3(BO_3)_4$, where $R = Y, Ce - Yb, M = Al, Ga$.** Elena Dobretsova^a, Kirill Boldyrev^b, Elena Borovikova^a

^a*Crystallography Department, Lomonosov's Moscow State University, Moscow, Russia* ()

^b*Institute of Spectroscopy RAS, Troitsk, Moscow, Russia*

e-mail: elena-dobrecova@yandex.ru

Anhydrous orthoborate crystals $RM_3(BO_3)_4$ ($R = Y, Ce - Yb, M = Al, Ga$) with very similar polytypic structures have been grown by flux method through spontaneous nucleation and characterized by infrared spectroscopy in a crystalline state. The dependence of the realized borate space group from the sort of R- and M-atoms was revealed. They can be considered as multifunctional materials having device potential due to their good thermal and chemical stability and a possibility of wide isomorphous substitutions. Most of them belong to the huntite structure type $CaMg_3(CO_3)_4$ with sp. gr. *R32* [2], some of aluminium borates also have monoclinic modifications with sp.gr. *C2/c*.

In the structures of both modifications three kinds of coordination polyhedra are present: trigonal prisms for RO_6 , octahedra for MO_6 , and two types of planar triangular BO_3 groups.

A comparison of these structures proves their polytypic nature [1]. In each of them it is possible to distinguish two different types of layers, identical for two modifications. In the rhombohedral polytype layers of the first type with prisms are multiplied around layers of the second type by two-fold axes, whereas in the monoclinic modification by centres of symmetry. Methods of vibrational spectroscopy coupled with factor group analysis were applied in order to understand the peculiarities of the structures of the borates $RM_3(BO_3)_4$.

Factor group analysis for the compounds, crystallizing in the space groups *R32* and *C2/c*,

which are the polytypes with the very similar structures, has been performed. The differences observed in the spectra have been explained by the differences of symmetry.

The assignment for the stretching and bending vibrations of BO_3^{3-} groups and external modes has been made. The external modes include the translational modes of R^{3+} , M^{3+} , and BO_3^{3-} ions, and the BO_3^{3-} librations. The dependence of the realized borate space group from the type of rare-earth atom was revealed. The main differences are observed in the region of asymmetrical stretching vibrations of BO_3^{3-} units. The borates with rare-earth elements Pr – Nd form the monoclinic structures. The borates $SmAl_3(BO_3)_4$ and $NdAl_3(BO_3)_4$ have been obtained in two modifications. The borates $RA_3(BO_3)_4$, where $R = Y, Gd - Yb$ crystallize in sp.gr. *R32*. The formation of aluminium borates with large cations La and Ce do not occur. The borates $RGa(BO_3)_4$ crystallize in rhombohedral modification irrespective of the type of rare-earth atoms.

[1] Belokoneva E.L., Timchenko T.I. (1983). *Sov. Phys. Crystallogr.*, **28**, 65

[2] Mills A.D. (1962). *Inorgan. Chem.*, **1**, 960.

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