MS13-P02

New borates with similar structures and different properties – acentric nonlinear optical $KGd[B_6O_{10}(OH)_2]$ and centrosymmetric $KHo[B_6O_{10}(OH)_2]$

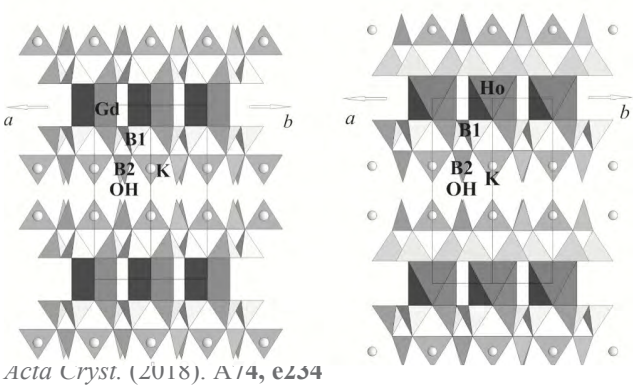
Anastasiia Topnikova[1], Elena Belokoneva[1], Olga Dimitrova[1], Anatoliy Volkov[1], Sergey Stefanovich[2]

1. Department of Crystallography, Geological Faculty, Lomonosov Moscow State University, Moscow, Russia
2. Department of Chemical Technology and New Materials, Chemical Faculty, Lomonosov Moscow State University, Moscow, Russia

email: nastya_zorina@rambler.ru

Single crystals of two new borates, $KGd[B_6O_{10}(OH)_2]$ and $KHo[B_6O_{10}(OH)_2]$ [1], have been synthesized under hydrothermal conditions in complicate borosilicate and borate systems at different pH-values. The syntheses were performed at the temperature 270-290 °C under pressure of 70-100 atm. Both structures are similar in unit cell but differ in symmetry. The first borate is found to be acentric (sp.gr. *P*-62*m*), the second is centrosymmetric (sp.gr. *P*-31*m*) (Fig.1). The same anionic radical of new type in both borates is characterized as polyborate layer composed of tetrahedrons (T) in a form of mica-like layer added by triangles (Δ). Crystal chemical formula of new layer is $[B_6O_{10}(OH)_2]^{4-}{}_{\infty\infty}$ because B2-triangles hold statistically only two positions attributable to the four tetrahedra, notation is 6:$[4T + 2\Delta]_{\infty\infty}$, or three on a ring of six tetrahedra, $[6T + 3\Delta]_{\infty\infty}$. Multiplication of the layers by symmetry is differently produced in the structures: by mirror plane in K, Gd-borate or the inversion center in K, Ho-borate. Two polar layers are attached to top and bottom of GdO_6 trigonal prisms and HoO_6 octahedrons, correspondingly. K- and B-triangles positions are statistically occupied in both structures. Disorder along c* in acentric $KGd[B_6O_{10}(OH)_2]$ and overlapping of K- and B2-positions in its interlayer space may be eliminated in larger cell with tripled period along *c*-axis and resulting polar structure of $P3_1$ symmetry. In centrosymmetric $KHo[B_6O_{10}(OH)_2]$, which also has disorder along c* axes and tripling of cell, K- and B2-positions holds the inversion center symmetry. Despite of the almost complete structural identity, new acentric K, Gd-borate clearly demonstrates second-order nonlinear optical activity (SHG response up to 45 SiO_2 units) in contrast to centrosymmetric K, Ho-borate. We suppose that key of properties explanation is in the acentric structure of K, Gd-borate and polar ordering in this crystal.

The reported study was funded by RFBR according to the research project № 18-35-00645.



References:

[1] Belokoneva, E. L., Topnikova, A. P., Stefanovich, S. Yu, Dobretsova, E. A., Volkov, A. S., Dimitrova, O. V. (2015). Solid State Scien., 46, 43-48.

Keywords: structures, borates, symmetry