

Synthesis, crystal structure and thermal expansion of gaufroyite-type borates: $\text{Sr}_3\text{Bi}(\text{YO})_3(\text{BO}_3)_4$, $\text{Sr}_2\text{CaBi}(\text{YO})_3(\text{BO}_3)_4$ and $\text{Sr}_2\text{BaBi}(\text{YO})_3(\text{BO}_3)_4$

Andrey P. Shablinskii^{1,*}, Lidiya G. Galafutnic¹, Rimma S. Bubnova^{1,2}, Stanislav K. Filatov²

¹Institute of Silicate Chemistry, Makarova Emb. 2, Saint-Petersburg, 199034 Russia

²Saint-Petersburg State University, University Emb. 7/9, Saint-Petersburg, 199034 Russia

* shablinskii.andrey@mail.ru

Borates are perspective materials for luminescent matrix due to the wide bandgap, relatively easy synthesis and high thermal stability.

The $\text{Sr}_3\text{Bi}(\text{YO})_3(\text{BO}_3)_4$, $\text{Sr}_2\text{CaBi}(\text{YO})_3(\text{BO}_3)_4$ and $\text{Sr}_2\text{BaBi}(\text{YO})_3(\text{BO}_3)_4$ compounds were synthesized via solid state reactions. Reagents, SrCO_3 (99.99%), CaCO_3 (99.99%), Y_2O_3 (99.99%), BaCO_3 (99.99%), Bi_2O_3 (99.99%) and H_3BO_3 (99.99%), in stoichiometric ratios, were mixed in an agate mortar and pestle. This mixture was ground for 45 min and placed in platinum crucibles. The powder was heated at 600 °C for 3 h in air to decompose the metal carbonate and boric acid. Then, the mixture was pressed into a pellet and heated at 300 °C for 5 h, 500 °C for another 5 h, then ground carefully, and finally fired at 950 °C for 24 h.

Crystal structure $\text{Sr}_3\text{Bi}(\text{YO})_3(\text{BO}_3)_4$ was first investigated in [1]. Unit cell parameters of $\text{Sr}_3\text{Bi}(\text{YO})_3(\text{BO}_3)_4$ are: $a = 10.697(2)$, $c = 6.7222(1)$ Å, $V = 666.2(2)$ Å³, space group $P6_3$. There are 10 crystallographically independent atoms in the asymmetric unit. Among them, the Bi and B1 atoms locate on the special sites, and Y and O atoms occupy the general sites. The Y atom is coordinated by seven O atoms to form a pentagonal bipyramid. These YO_7 polyhedra share edges to form a one-dimensional (1D) chain along the c direction. The chains are bridged by B_2O_3 groups through sharing vertex oxygen atoms to construct a three-dimensional (3D) framework, which affords two kinds of channels along the [001] direction. Sr atoms and isolated $\text{B}(1)\text{O}_3$ triangles are located in the larger channel. The $\text{B}(1)\text{O}_3$ triangles are surrounded by Sr atoms.

The thermal behavior of $\text{Sr}_3\text{Bi}(\text{YO})_3(\text{BO}_3)_4$, $\text{Sr}_2\text{CaBi}(\text{YO})_3(\text{BO}_3)_4$ and $\text{Sr}_2\text{BaBi}(\text{YO})_3(\text{BO}_3)_4$ compounds was studied using in situ high-temperature XRD in the range 25-800 °C by means of Rigaku Ultima IV powder X-Ray diffractometer ($\text{CuK}\alpha$) with a high-temperature camera. According to the principles of high temperature crystal chemistry [2] for borates with isolated triangle groups, thermal expansion of these borates is practically isotropic.

The studies have been supported Russian Foundation of Basic Researches project №18-29-12106. X-Ray diffraction experiments were performed at the X-Ray Diffraction Center Of Saint-Petersburg State University.

Gao J., Li S. $\text{BiSr}_3(\text{YO})_3(\text{BO}_3)_4$: a new gaufroyite-type rare earth borate with moderate SHG response. *Inorg. Chem.*, 2012, 51, 420-424.

Bubnova R., Filatov S. High-temperature borate crystal chemistry. *Z. Kristallogr.*, 2013, 228, 395-428.