MS14-P125 - LATE | AN OCCURRENCE OF THE ACENTRIC DISTORTION DUE TO Ag^{+}/Bi^{3+} ORDERING IN THE $AgBi_2B_5O_{11}$ BORATE

Volkov, Sergey (Grebenshchikov Institute of the Silicate Chemistry of the Russian Academy of Sciences, Saint-Petesburg, RUS); Bubnova, Rimma (Grebenshchikov Institute of the Silicate Chemistry of the Russian Academy of Sciences, Saint Peterburg, RUS); Krzhizhanovskaya, Maria (Department of Crystallography, Saint Petersburg State University, Saint-Petersburg, RUS); Charkin, Dmitri (Department of Chemistry, Lomonosov Moscow State University, Moscow, RUS); Stefanovich, Sergey (Department of Chemistry, Lomonosov Moscow State University,, Moscow, RUS); Povolotskiy, Alexey (Institute of Chemistry, Saint Petersburg State University, Saint-Petersburg, RUS)

The first silver bismuth borate, $AgBi_2B_5O_{11}$ has been synthesized and its crystal structure was characterized by a single-crystal X-ray diffraction. Crystal structure is orthorhombic, sp.gr. $Pna2_1$ and based on isolated B_5O_{10} pentaborate groups. Its structure is derived from that of centrosymmetric $Bi_3B_5O_{12}$ by ordered substitution of one Bi^{3+} ion for Ag^{+}, which results in the disappearance of the mirror plane and inversion centre. Second harmonic generation (SHG) measurements confirm the acentric crystal structure. Thermal expansion of this borate was studied by high-temperature X-ray powder diffraction in the 20–550 °C temperature range. It is strongly anisotropic: α_a = 20.4(2), α_b = 7.8(2), α_c = 3.1(1) × 10^{-6} °C^{-1} at 200 °C. The new compound was also characterized by thermal analysis, DFT calculations, vibrational and UV–Vis–NIR spectroscopy.

The optical measurements were performed at the Centre for Optical and Laser Materials Research, Research Park, Saint Petersburg State University. Powder X-ray diffraction experiments were performed at the Centre for X-ray Diffraction Studies, Research Park, Saint Petersburg State University. This work was financially supported by the Russian Science Foundation through the grant 18-73-00176.