Synthesis and crystal structure of $Ba_3B_6Si_2O_{16}$

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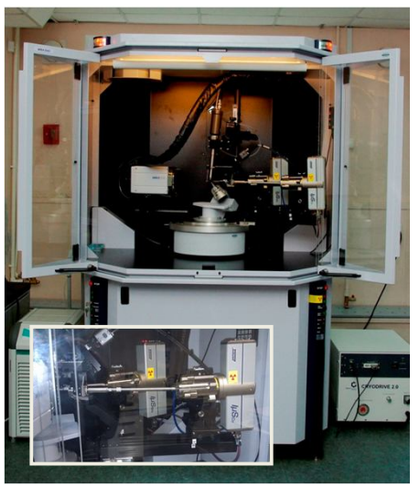
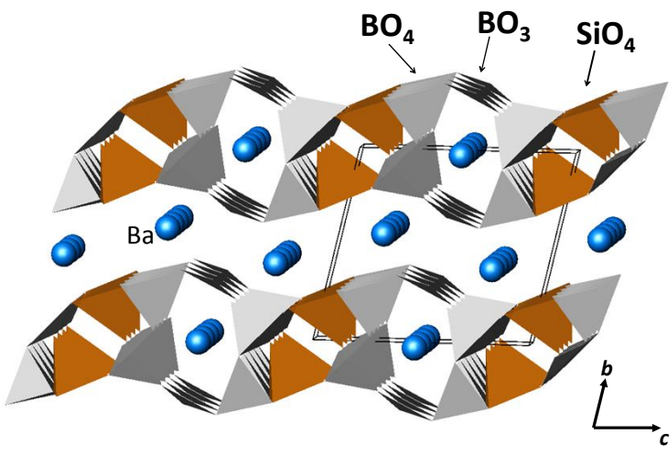
Single crystals of $Ba_3B_6Si_2O_{16}$ silicoborate were obtained by slow cooling a melt of stoichiometric composition. Crystal structure was determined by direct methods from X-ray single crystal diffractometry data (Bruker KAPPA APEX DUO, MoKa, CCD detector) using a small colorless plate. The structure consists of layered silicoborate anion formed by four crystallographically independent polyhedra: one BO_3 triangle, two BO_4 tetrahedra and one SiO_4 tetrahedron. Ba atoms occupy two different positions in the structure: one of them is inside the layer and another one between the layers. Silicoborate layers are located parallel to (010).





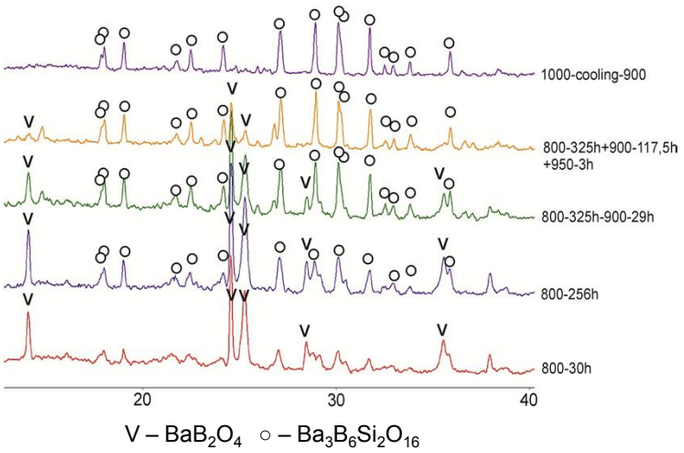
Crystal Structure

Triclinic, P-1
a = 5.0382(8) Å
b = 7.6574(12) Å
c = 8.5262(14) Å
α = 77.677(5) °
β = 77.879(5) °
γ = 86.324(5) °
R = 0.07 (2940 Refl.)
0.09 (3922 Refl.)

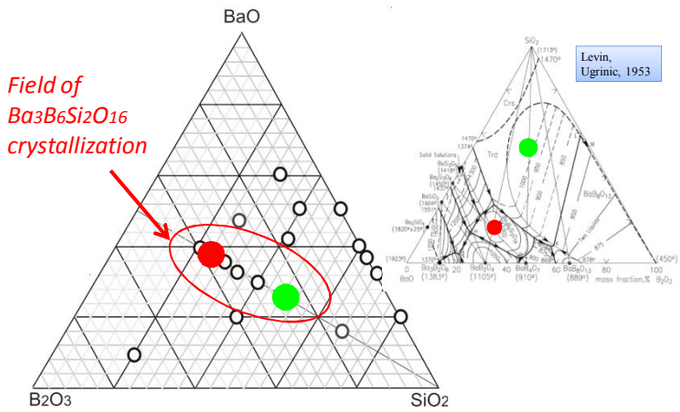
Phase Formation in BaO-B_2O_3-SiO_2 System

According to triangulation reported in (Levin, Ugrinic, 1953) $Ba_3B_6Si_2O_{16}$ is only one stable compound in the BaO-B_2O_3-SiO_2 ternary system. In a wide field of compositions near 3BaO x $3B_2O_3$ x $2SiO_2$ we obtained $Ba_3B_6Si_2O_{16}$ by solid state reaction at 800, 900 and 950 °C mixed with barium borates and/or silicates depending on the composition of initial mixture. Powder XRD data obtained by us for the pure $Ba_3B_6Si_2O_{16}$ synthesized by cooling a melt are in well agreement with the reported before in PDF database and with structural data presented here.

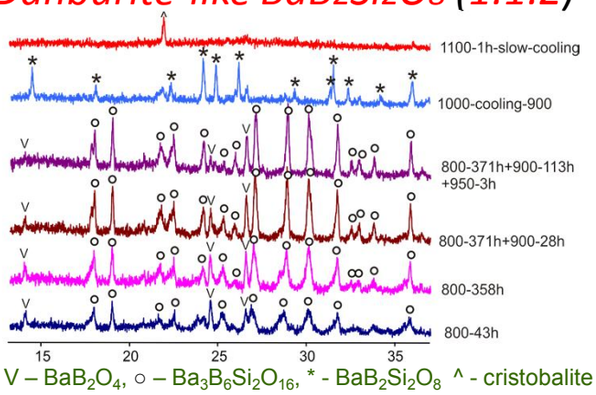
● *$Ba_3B_6Si_2O_{16}$ (3:3:2)*



V – BaB_2O_4 ○ – $Ba_3B_6Si_2O_{16}$



● *Danburite-like $BaB_2Si_2O_8$ (1:1:2)*



V – BaB_2O_4, ○ – $Ba_3B_6Si_2O_{16}$, * - $BaB_2Si_2O_8$ ^ - cristobalite

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