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High-Temperature Crystal Chemistry Of Danburite-Like Borosilicates

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Among unhydrous alkaline borosilicates $RB_2Si_2O_8$ (R = Ca, Sr, Ba) there are three naturally occurring members: danburite (Ca) (Dunbar, Machatschki, 1931), pekovite (Sr) and maleevite (Ba) (Pautov et al, 2004). Their orthorhombic structure consists of tetrahedral framework with boron and silicon orderly distributed in different tetrahedral sites. Almost all known unhydrous borosilicates are structurally similar to aluminosilicate relatives. Danburite structure type is topologically identical to that of paracelsian $RAl_2Si_2O_8$ (R = Sr, Ba), although the latter one represents pseudo-orthorhombic framework with monoclinity angle $\beta\sim$90.01°.

Present study is devoted to study of formation and high-temperature behavior particularly expansion, transitions, melting/decomposition for the danburite-like phases with the use of synthetic compounds. Polycrystalline maleevite, $BaB_2Si_2O_8$, mixed with sanbornite $BaSi_2O_5$, was obtained by slow cooling of stoichiometric melt from 1000 to 900 ° C for 2.5 hours. It is shown that $BaB_2Si_2O_8$ could not be obtained by solid-state reaction at 800, 900 and 950 ºC in a wide range of compositions. Synthetic pecovite, $SrB_2Si_2O_8$, mixed with insignificant amount of $SrSiO_3$,was obtained by solid state reactions at 900 ºC for 127 hours. For the $CaB_2Si_2O_8$the high-temperature XRD data for single crystal from (Sugiyama & Takéuchi, 1985) were used for calculation of thermal expansion coefficients. Thermal behavior of $RB_2Si_2O_8$ (R = Sr, Ba) was studied using high-temperature powder X-ray diffractometry and heat treatments. $BaB_2Si_2O_8$ and $SrB_2Si_2O_8$ were studied in the temperature range 30-900 ºC with temperature steps of 40 and 30 ºC respectively.

Comparative analysis of thermal expansion of Ca, Sr, Ba-compounds showed that the members of danburite group have relatively low average coefficient of volume thermal expansion ($23 \pm 3 \times 10^{-6}$ ºC^{-1}), closer to that of silicates (23×10^{-6} ºC^{-1}) than that of alkaline borosilicates (36×10^{-6} ºC^{-1}) (Bubnova & Filatov, 2008). The tendency of increasing the values of thermal expansion coefficients and the anisotropy of thermal expansion is observed with increasing cation size.

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