Poster Presentations

[MS20-P10] High-Temperature Study of K- and Rb-Boroleucite Crystal Structures by Rietveld Method

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Leucite-like borosilicates take attention because of a wide range of substitutions and unusual thermal behaviour. Up to now three modifications of $KBSi_2O_6$ (cubic *I*-43*d* [1], Ia3d [2] and monoclinic $P2_1/a$ [3]) and cubic (I-43d) modification of $RbBSi_2O_6$ [4] determined with ANA type of three dimensional framework structure are known. Present study is focused on high-temperature structural investigation of cubic modifications of K- and Rbboroleucites.
High-temperature powder X-ray diffraction (HTPXRD) study has been performed in air in the temperature range 20-1000 °C. Crystal structures were refined using the Rietveld method (Topas program package). As it was noted recently by us [5] cubic $KBSi_2O_6$ structure undergoes reversible transformation into a lower symmetrical modification in the temperature range 300-500 °C. Present Rietveld refinement showed that over 300 °C cubic $KBSi_2O_6$ (I-43d) transforms reversibly into intermediate monoclinic modification which transforms later at 500 °C into Ia3d cubic phase. Thus the thermal polymorphic transformation of $KBSi_2O_6$ looks like: I-43d <-> P21/a <-> Ia3d. These three phases are very similar to each other and belong to ANA type of structure. Consequently the transformation has displacive character and occurs continuously without breaking bonds. In [2] continuous transformation from I-43d directly to Ia3d space group in the temperature range 565-700 °C has been reported for slightly hydrated $KBSi_2O_6$ boroleucite from Rietveld refinement of synchrotron powder diffraction data. According to HTPXRD data cubic $RbBSi_2O_6$ (I-43d) transforms over 300 °C directly into higher symmetrical Ia3d phase; Rietveld refinement of low- and high- temperature modifications at 25 and 400 °C are presented, respectively. Evolution of boroleucite structure under temperature and chemical composition changes is discussed.

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