Poster Presentations

[MS32-P08] Some new examples of high-temperature phases quenched at ambient coditions

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Crystal structures look sometimes unusual at ambient conditions since they were formed at high temperature and have the special structural features for ambient conditions. Among them there are glassforming borates discussed below. **BaNa*M*(BO3)2, *M* = Y, Sc**. Ba^{2+} and Na^{+} are very different in size. The crystal structure undergoes polymorphic transformation at 775 ^{o}C forming unit cell with *c*/2 parameter. There is an obvious reason for that: B, O and Sc atoms have two non-equivalent positions for each atom with the difference ≈0.5 *c;* Ba and Na have one position each divided also ≈ 0.5 *c*. Double decreasing of unit cell along *c* leads to the decreasing of quantity of non-equivalent B, O and Sc and disordering of Ba and Na over one crystallographic site. We see the obvious similarity: the low temperature phase is indeed just slightly distorted high temperature phase, prepared for the reverse transition. **$Ba_3Bi_2(BO_3)_4$.** Ba^{2+} and Bi^{3+} differ in size and electron shell configuration; Bi^{3+} has a lone electron pair. The compound could be obtained by cooling a melt. At high temperature Ba and Bi are statistically distributed over three different positions *M*1, *M*2 и *M*3. At room temperature thermal motions of atoms decreases and the atomic differences show sharply themselves. That leads to the ordering the structure: in low temperature modification we observe *M*1, *M*2 and *M*3 sites splitting with formation of Ba- and Bi-subpositions. **$BaBi_2OB_2O_6$.** Synthesis and structural behavior on cooling is similar to that of $Ba_3Bi_2(BO_3)_4$: splitting of cationic positions is about 0.4–0.6 Å, taking splitting into account decreases R-factor from 14 down to 2.5 %.

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