
CALCULATION OF THE B-O TRIANGLE TO B-O TETRAHEDRON RATIO IN BORATES

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The ratio of the numbers of BO$_3$ triangles and BO$_4$ tetrahedra which make up an anion complex is frequently used for the identification of the so-called fundamental building blocks. Assuming the following bonding model this ratio can be calculated in advance from the borate composition. A covariantly bound anion complex extends weak ionic bonds towards the cations. To complete its octet each O forms two covalent bonds either with 2B or 1B+1H. The B atoms, which have no preference for triangular or tetrahedral O coordination, adopt a mixing ratio, expressed by (1), where all O atoms can have the proper number of B-O-B and/or B-O-H bonds.

\[ \%\Delta = 4 - A/C'. (2 - \%OH) \]

where \( A/C' \) is the ratio of the number of anions (O and/or OH) of the anion complex to the number of central atoms (B). \( \%OH \) is the ratio of the number of OH groups bound to a central atom to the total number of O atoms bound to a central atom. Eq. (1) is valid in a restricted composition range where lie one quarter of all borates. 222 of these borates had been tested with eq. (1) and an agreement was found for 85% of them. A detailed account is in print with Z. Kristallogr.

Keywords: BORATES, TRIANGLE TO TETRAHEDRON RATIO, BO$_3$ TO BO$_4$ RATIO


MONOCLINIC SUPERSTRUCTURE OF SrMgF$_4$ WITH PEROVSKITE-TYPE SLABS

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Crystals of Ce-doped SrMgF$_4$ have been found to have a monoclinic P1$_1$2$_1$ structure with doubled a and tripled c lengths with respect to the orthorhombic Cmcm structure previously reported in the literature. The perovskite-type slabs, composed of corner-sharing MgF$_6$ octahedra and Sr atoms, are stacked along the b axis. The six crystallographically independent MgF$_6$ octahedra are rotated so as to provide long periodicities along a and c. The coordination numbers and bond distances around six crystallographically independent Sr atoms are slightly different in each case. Although there are no constraints among the positional parameters of the six independent Sr atoms in P1$_1$2$_1$, they align almost on a plane perpendicular to a. The Mg1F$_6$, Mg4F$_6$, Mg2F$_6$, and Mg3F$_6$, and Mg3F$_6$ and Mg6F$_6$ octahedra are pairwise related by these pseudo-mirror planes defined by the Sr atoms. These local mirror planes are thought to originate at the high temperature phase transition from the Cmcm archetype.

Keywords: INORGANIC FERROELECTRIC STRUCTURE


CRYSTAL STRUCTURES OF PHASES IN THE SYSTEM CaO-K$_2$O-P$_2$O$_5$

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There are a number of elements constituting the condensed phases formed during combustion and gasification of biomass fuels. In addition to the traditionally studied major ash forming elements (Ca, K, Na, Si), a significant amount of P is contained in many biomass fuels and sludges. However, reliable identification tools such in terms of powder X-ray diffraction (XRD) patterns for many ash species containing P are lacking. To remedy this situation structural investigations for a number of phases in the system CaO-K$_2$O-P$_2$O$_5$ has been initiated. The situation is complicated by the fact that many ternary compounds in the system shows several structurally close-related phase modifications. A combination of single-crystal high-temperature structures, high-temperature powder diffraction and Rietveld techniques are used to clarify the intricate phase relations.

The crystal structures of Ca$_3$K$_4$P$_6$O$_{17}$ and Ca$_5$K$_3$(PO$_4$)$_2$, formed from high-temperature melts, have been determined using single-crystal X-ray diffractionmetry. Ca$_4$K$_3$P$_5$O$_{17}$ crystallizes in a monoclinic space-group P21/n with the well parameters: \( a=9.8170(2) \) Å, \( b=5.6750(1) \) Å, \( c=13.3030(3) \) Å and \( \beta=104.218(1) \). Ca$_5$K$_3$(PO$_4$)$_2$ crystallizes in the trigonal space-group R3c with the cell parameters (hexagonal axes): \( a=10.4636(1) \) Å and \( c=37.2493(1) \) Å. Calculated and experimental powder XRD pattern for the different phase modifications of the structures will be presented.

Keywords: PHOSPHATE, HIGH-TEMPERATURE STRUCTURE, XRD PATTERN