

Crystal structure of boralsilite and its relation to a family of borosaluminosilicates, sillimanite, and andalusite

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ABSTRACT

Boralsilite, $\text{Al}_{16}\text{B}_6\text{Si}_{37}\text{O}_{107}$, is monoclinic, space group $C2/m$, with $a = 14.767(1)$, $b = 5.574(1)$, $c = 15.079(1)$ Å, $\beta = 91.96(1)^\circ$, and $Z = 2$. The structure was solved with direct methods and refined to an unweighted residual of 0.026 using 1193 observed reflections. The structure is closely related to those of sillimanite, andalusite, grandidierite, synthetic aluminum borate ($\text{Al}_{18}\text{B}_4\text{O}_{33}$), and werdingite. These structures are all based on a backbone of chains of edge-sharing AlO_6 octahedra arranged parallel to c ($\cong 5.6$ Å) and at the vertices and center of a pseudo-tetragonal subcell having $a \cong b \cong 7.5$ Å. In the boralsilite structure, AlO_6 octahedral chains are cross-linked by Si_2O_7 disilicate groups, BO_4 tetrahedra, BO_3 triangles, and AlO_5 trigonal bipyramids. A given BO_4 or SiO_4 tetrahedron or BO_3 triangle shares two vertices with two adjacent AlO_6 octahedra of one chain and a third vertex with an octahedron vertex of an adjacent chain, thus cross-linking the AlO_6 octahedral chains. Further linkage is provided through vertex-sharing of AlO_5 trigonal bipyramids. These bipyramids alternate with B or Si polyhedra parallel to AlO_6 octahedral chains to form four kinds of cross-linking chains of polyhedra, with alternate atom pairs $^{[5]}\text{Al1-Si}$, $^{[5]}\text{Al2-}^{[4]}\text{B2}$, $^{[5]}\text{Al3-}^{[3]}\text{B1}$, and $^{[5]}\text{Al4-}^{[3]}\text{B3}$. The units which cross-link between chains of AlO_6 octahedra can alternatively be viewed as consisting of Si_2O_7 dimers, trimers of edge-sharing AlO_5 trigonal bipyramids (plus a B triangle and B tetrahedron), and dimers of edge-sharing AlO_5 trigonal bipyramids (plus B triangles and tetrahedra). Variations on these themes are found in the structures of sillimanite, andalusite, grandidierite, werdingite, mullite, and synthetic $\text{Al}_{18}\text{B}_4\text{O}_{33}$. The interchangeability and variety of the various interchain units appears to result in part from the flexibility produced by the ability of Al and B to assume a variety of coordinations by oxygen and from the potential for partial vacancy of some anion and cation sites.