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

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## ABSTRACT

Boralsilite, $Al_{16}B_6Si_2O_{37}$, is monoclinic, space group *C*2/*m*, with $a = 14.767(1)$, $b = 5.574(1)$, $c = 15.079(1)$ Å, $\beta = 91.96(1)°$, 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 ($Al_{18}B_4O_{33}$), and werdingite. These structures are all based on a backbone of chains of edge-sharing $AlO_6$ octahedra arranged parallel to *c* (≅ 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 $^{[5]}$Al1-Si, $^{[5]}$Al2-$^{[4]}$B2, $^{[5]}$Al3-$^{[3]}$B1, and $^{[5]}$Al4-$^{[3]}$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 $Al_{18}B_4O_{33}$. 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.