

## BaAlGaO<sub>4</sub> - A Stuffed Derivative of Tridymite

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Beamline(s): X3A1

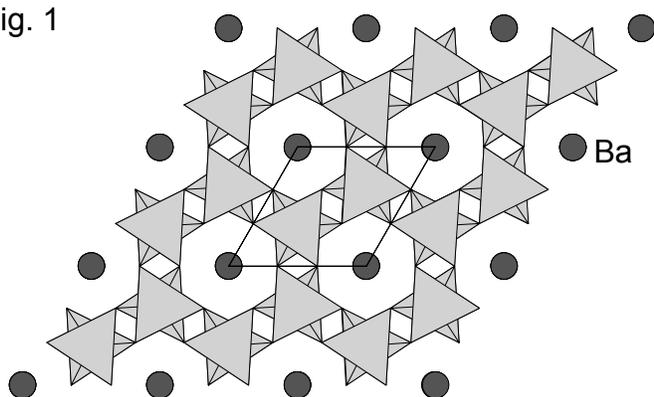
Single crystals of a barium aluminogallate with composition BaAlGaO<sub>4</sub> have been prepared by solid state reactions. The crystal structure of this compound has been investigated by single crystal diffraction techniques (space group P 6<sub>3</sub>22, a=5.279(1)Å, c=8.784(1)Å). The structure comprises hexagonal sheets of (Al,Ga)O<sub>4</sub>-tetrahedra arrayed in six-fold rings. Within a single ring the adjacent tetrahedra show an UDUDUD topology. The Al- and Ga-cations are statistically distributed among the centers of the tetrahedra. Successive sheets are stacked in an "ABAB..." sequence parallel to [001]. The resulting structure, illustrated in **Figure 1**, has wide channels parallel to [001] in which the Ba cations are incorporated for charge compensation. A 6<sub>3</sub>-axis runs through the center of each six-fold ring, and a triad axis passes through the center of each tetrahedron. In this model the T-O-T angle between neighboring sheets is therefore constrained to be 180°, which is energetically unfavorable [1]. Actually, the anisotropic displacement parameters of the bridging O-atom on the triad axis define an extremely oblate ellipsoid (**Figure 2a**). This angle is reduced to a more favorable value by off-centering of the apical oxygens, which then occupy three symmetrically equivalent split positions about the triad axis (**Figure 2b**).

The structure of BaAlGaO<sub>4</sub> can be regarded as a stuffed derivative of the SiO<sub>2</sub> modification tridymite, where the Si atoms have been replaced by Al / Ga and the Ba ions reside in voids of the tetrahedral framework.

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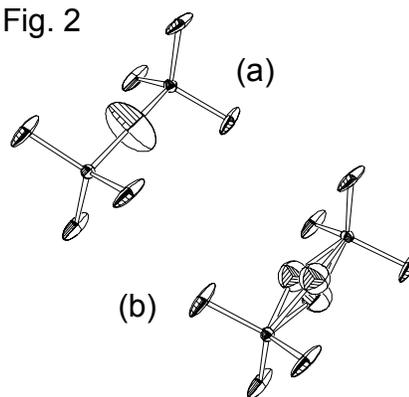
**References:** [1] F. Liebau, Structural chemistry of silicates, Springer Verlag, Berlin 1985.

Fig. 1



**Figure 1.** Projection of the crystal structure of BaAlGaO<sub>4</sub> parallel to [001].

Fig. 2



**Figure 2.** Side view of two adjacent (Al,Ga)O<sub>4</sub> tetrahedra belonging to neighboring layers. (a) Bridging apical O atom on the triad axis (b) Split position off the triad axis for bridging oxygen.