

ON THE EXISTENCE OF A NOVEL HIGH -PRESSURE  $\text{CaAl}_2\text{O}_4$  MODIFICATION

Lazic, B.<sup>1</sup>, Kahlenberg, V.<sup>1</sup>, Konzett, J.<sup>1</sup> & Kaindl, R.<sup>1</sup>

Institut für Mineralogie und Petrographie, Universität Innsbruck, Innrain 52, A-6020 Innsbruck, Austria  
 e-mail: Biljana.Lazic@uibk.ac.at

In the course of an ongoing research project on the high pressure crystal chemistry of alkaline earth aluminates a previously unknown  $\text{CaAl}_2\text{O}_4$  polymorph has been observed. Polycrystalline ceramic precursors have been prepared by solid state reactions using  $\text{Al}_2\text{O}_3$  and  $\text{CaCO}_3$  as starting materials. The subsequent high pressure experiment was conducted using an end-loaded piston cylinder press at 3.5 GPa and 1000°C with a run time of 51 hours. Several crystals could be recovered from the Pt-container and were characterised by single crystal X-ray diffraction and micro-Raman spectroscopy. The crystals showed twinning by pseudo-merohedry which was accounted for in the structure determination. Structure solution was accomplished by direct methods. Final least squares refinements converged to a residual of  $R_1 = 0.0343$ . The basic crystallographic data of the new compound are as follows: monoclinic symmetry, space group  $P2_1/m$  with two formula units per unit cell ( $a=5.5562(2)\text{Å}$ ,  $b=3.7627(1)\text{Å}$ ,  $c=7.0560(3)\text{Å}$ ,  $\beta=101.360(30)^\circ$ ,  $V=144.62\text{Å}^3$ ,  $D_{\text{calc}}=3.629\text{g/cm}^3$ ). The two main building units of the structure are: (1) layers of  $\text{AlO}_6$  – octahedra, connected to each other by edge sharing and (2) calcium atoms residing between these layers for charge compensation (Fig. 1). The alternate stacking of the octahedral layers and sheets of Ca atoms results in a three-dimensional network.

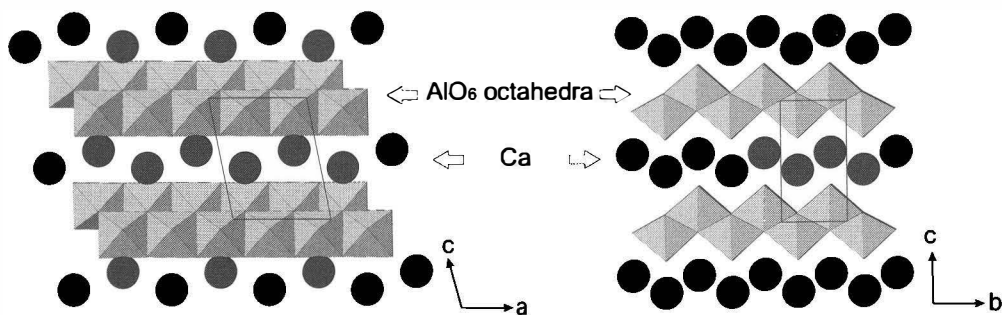


Fig. 1: Layers of  $\text{AlO}_6$ -octahedra and Ca atoms residing between the layers

From a structural point of view, the new HP-phase is closely related to boehmite ( $\gamma\text{-AlOOH}$ ). The octahedral building units in both compounds are identical. Differences arise from the connection between neighbouring layers. In case of boehmite linkage is provided by hydrogen bonding.