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Rietveld analysis of dicalcium aluminate ($Ca_2Al_2O_5$)—A new high pressure phase with the Brownmillerite-type structure

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ABSTRACT

Dicalcium aluminate ($Ca_2Al_2O_5$) was prepared in a piston cylinder apparatus at 1250 °C and 2.5 GPa. The compound is orthorhombic with space group symmetry */2mb*, a = 5.2281(1) Å, b = 14.4686(2) Å, c = 5.4004(1) Å (Z = 4, D_{calc} = 3.481 g/cm^3), and belongs to the brownmillerite structure family. Main building units are (1) layers of perovskite type corner connected AlO_6-octahedra perpendicular to [010], and (2) zweier single chains of AlO_4-tetrahedra running parallel [100]. The alternate stacking of the layers and sheets of single chains results in a three dimensional network in which the calcium ions are incorporated for charge compensation. The present structure is the first example for an alkaline earth aluminate with zweier single chains of tetrahedra.