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Crystal structure of $CaMg_2Al_6O_{12}$, a new Al-rich high pressure form

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ABSTRACT

The crystal structure of $CaMg_2Al_6O_{12}$, a new high-pressure phase synthesized at 21.8 GPa and 1200 °C using a multi-anvil apparatus, was solved by a newly developed structure program and refined by Rietveld analysis of the powder X-ray diffraction profile. The structure is hexagonal with cell constants $a = 8.7616(2)$ and $c = 2.7850(1)$ Å, and space group $P6_3/m$. The structure of this phase contains double chains of edge shared AlO_6 octahedra running along the c axis. Three double chains share corners to form sixfold positions in which octahedrally coordinated Mg atoms reside. The large Ca atoms are randomly distributed at ninefold sites with half-occupancy in the hexagonal tunnel. Previously reported Al-rich silicate phases could possibly have the same structure. This structure could thus qualify as one of the possible major host phases for aluminum in the lower mantle.