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Crystal structure analysis of synthetic $Ca_4Fe_{1.5}Al_{17.67}O_{32}$: A high-pressure, spinel-related phase

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ABSTRACT

The compound $Ca_4Fe_{1.5}Al_{17.67}O_{32}$ was synthesized at 2.5 GPa and 1250 °C using a piston-cylinder apparatus. The crystal structure, determined from single-crystal X-ray diffraction data collected at 295 K (tetragonal, space group $I\bar{4}2d$, $a = 20.1847(14)$ Å, $c = 5.6203(6)$ Å, $V = 2289.83(3)$ Å^3, $Z = 4$) was refined to a final R-index of 0.024 for 1229 independent observed reflections and 130 parameters. The main building units comprising the compound are 11.8×7.2 Å wide spinel-type ribbons running parallel to [001], which are connected via corner-sharing $(Fe,Al)O_6$-octahedra. Additional linkage between the spinel units is provided by AlO_4-tetrahedra residing on the $\bar{4}$-axis as well as by Ca cations, in sevenfold coordination with oxygen attached to the spinel-like building units. Refinement of site occupancies reveals that the incorporation of Fe occurs at two of four octahedral and at two of three tetrahedral sites. Apparently, $Ca_4Fe_{1.5}Al_{17.67}O_{32}$ represents a new structure type exhibiting more pronounced structural modifications relative to the spinel aristotype compared with the so-called spinelloid structures. Furthermore, this synthetic compound contains Fe^{2+} in tetrahedral coordination, which is relatively uncommon among inorganic materials.