

Synthetic $\text{LiAlGe}_2\text{O}_6$: The first pyroxene with $P2_1/n$ symmetry

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ABSTRACT

The structure determination of synthetic $\text{LiAlGe}_2\text{O}_6$ [$Z = 4$, space group $P2_1/n$, $a = 9.8892(5)$, $b = 8.3929(5)$, $c = 5.3995(3)$ Å, $\beta = 110.646(3)^\circ$], is a new pyroxene structure-type, and represents the first structural example of $P2_1/n$ pyroxene symmetry. The crystal structure of the Ge-analog phase of spodumene was solved from single-crystal X-ray diffraction data by classical Patterson methods with a subsequent structure refinement converging to $R_1 = 0.0169$. The new $P2_1/n$ pyroxene polymorph was found to consist of a single S-type rotated tetrahedral chain type, which is—similar to ordered $P2/n$ omphacite—composed of alternating Ge1O_4 and Ge2O_4 tetrahedra located at two distinct sites within a single chain. This $(\text{Ge1Ge2O}_6)_n$ chain is S-rotated, strongly bent ($\text{O4-O2-O4} = 154.8^\circ$) compared to that of the $C2/c$ spodumene structure, and assumes angles comparable to those of the two chains of spodumene at 3.3 GPa within the $P2_1/c$ symmetry. As a consequence of the interplay between the M1 and M2 sites, the new polymorph reveals a larger angular distortion for the AlO_6 octahedra, and the Li coordination is reduced from sixfold to fivefold coordination. This establishes $\text{Li}^{[5]}\text{Al}^{[6]}(\text{Ge}^{[4]}\text{Ge}^{[4]}\text{O}_6)$ as the corresponding crystallochemical formula for the new $P2_1/n$ representative within the monoclinic (clino)pyroxene family.

Keywords: $\text{LiAlGe}_2\text{O}_6$, clinopyroxenes, $P2_1/n$, X-ray diffraction