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LETTER

Synthesis and crystal structure of $Li_{0.52}Mg_{0.96}Sc_{0.52}Si_2O_6$ orthopyroxene

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ABSTRACT

$Li_{0.52}Mg_{0.96}Sc_{0.52}Si_2O_6$ orthopyroxene was synthesized by the flux method and its structure studied with single-crystal X-ray diffraction. The crystal is orthorhombic with space group *Pbca* and unit-cell parameters $a = 18.259(5)$, $b = 8.883(2)$, $c = 5.271(1)$ Å, and $V = 854.9(3)$ Å^3. The structure refinement shows that the M1 and M2 sites are occupied by (0.48 Mg + 0.52 Sc) and (0.48 Mg + 0.52 Li), respectively. While the O3-O3-O3 kinking angle (165.40°) of the silicate tetrahedral A chain appears to be normal when compared with reported data, the kinking angle (151.92°) of the B chain is the largest of all orthopyroxenes examined at ambient conditions. This is the first orthopyroxene structure that contains more than 50% trivalent and monovalent cations in the M1 and M2 sites, respectively, and displays a kinking angle of the tetrahedral B chain that is greater than 150°. Our study demonstrates the stability of the new pyroxene structure type predicted by Pannhorst (1979) at room temperature.

Keywords: $Li_{0.52}Mg_{0.96}Sc_{0.52}Si_2O_6$, orthopyroxene, crystal structure, X-ray diffraction