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Potential host phase of aluminum and potassium in the Earth's lower mantle

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ABSTRACT

An Al-rich phase produced by phase transformation from a natural mid-oceanic ridge basalt under lower mantle conditions was studied by X-ray diffraction and analytical transmission electron microscopy. The phase, coexisting with silicate perovskites, the Ca-ferrite-structure phase, and stishovite, has hexagonal symmetry (space group $P6_3/m$) and the composition $[(M^+,Ca)_1(Mg,Fe)_2]_{\Sigma 3}(Al,Si)_{5.5–6.0}O_{12}$, where M = Na^+, K^+. The alkali-free phase with the complex solid solution, $[Ca_{0.79}Mg_{0.12}]_{\Sigma 0.91}[Mg]_{2.00}\,[Al_{4.09}Si_{1.48}]_{\Sigma 5.57}\square_{0.43}O_{12}$, has a unit cell with a = 8.765 (3) Å, c = 2.762 (3) Å, V = 183.7 (2) Å^3, Z = 1, a formula weight = 429.31, and a calculated density = 3.88 g/cm^3 at 0 GPa and 4.16 g/cm^3 at 23 GPa. This Al-rich phase is considered to be same as the hexagonal phases recently reported, and thus the hexagonal phases can potentially host alkali and alkali-earth elements in the lower mantle.