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Structure of a new Al-rich phase, $[K, Na]_{0.9}[Mg, Fe]_2[Mg, Fe, Al, Si]_6O_{12}$, synthesized at 24 GPa

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ABSTRACT

A new Al-rich phase, $[K_{0.56}Na_{0.32}][Ca_{0.04}Mg_{1.66}Fe^{2+}_{0.3}][Mg_{0.98}Fe^{3+}_{0.3}Al_{2.62}Si_{2.1}]O_{12}$, was synthesized at 24 GPa, 1700 °C, and its structure was determined by single-crystal X-ray diffraction. The unit cell is hexagonal, space group $P6_3/m$, a = 8.830(1), c = 2.779(1) Å, V = 187.65(5) Å^3, Z = 1, formula weight = 448.62, calculated density = 3.970 g/cm^3. The previously unknown structure consists of alkali- and vacancy-bearing M3 sites in tunnels along c, mostly Mg-bearing linear arrays of trigonal prismatic M2 sites, very unusual for mantle phases, and a framework of edge-linked distorted octahedral M1 sites filled mostly with Al and Si. The observed range of compositional variations and high density suggest complex solid solution behavior at the lower-mantle pressures similar to pyroxenes at the upper-mantle and majorite garnet at the transition-zone pressures. The stability of the Al-rich phase appears to expand to lower Al contents with increasing pressure, suggesting that a chondritic lower mantle could contain up to 24% of the new phase on the molecular basis.