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Crystal structure of phase X, a high pressure alkali-rich hydrous silicate and its anhydrous equivalent

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ABSTRACT

Phase X, ascribed by Luth (1995) to a hydrous K-rich silicate formed from the breakdown of K-amphibole at high pressures, was synthesized at 1250–1300 °C and 10–16 GPa in four different compositions: $Na_{1.78}(Mg_{1.89}Al_{0.13})Si_{2.02}O_7$ (anhydrous sodic phase X), $Na_{1.16}K_{0.01}(Mg_{1.89}Al_{0.14})Si_{2.02}O_7H_{0.65}$ (sodic phase X), $K_{1.85}Mg_{2.06}Si_{2.01}O_7$ (anhydrous phase X), and $K_{1.54}Mg_{1.93}Si_{1.89}O_7H_{1.04}$ (phase X). A general chemical formula for these phases can be expressed as $A_{2-x}M_2Si_2O_7H_x$, with A = K and/or Na, M = Mg and/or Al, and x = 0–1. Structure determination from single-crystal X-ray diffraction data shows that anhydrous sodic phase X is trigonal with space group $P\bar{3}1m$, whereas the other three have an identical structure with space group $P6_3cm$. Both $P\bar{3}1m$ and $P6_3cm$ structures are characterized by MgO_6 octahedral layers that are stacked along the **c** axis and inter-linked together by Si_2O_7 tetrahedral dimers and K or Na cations. Within the MgO_6 layers, each MgO_6 octahedron shares three edges with neighboring MgO_6 octahedra to form brucite-like layers with one out of three octahedral sites vacant. Large K or Na cations are situated right below and above each occupied octahedron in the MgO_6 layers, whereas the Si_2O_7 groups are located below and above each vacant octahedron in the layers. The two types of structures, however, differ in the relative orientation of MgO_6 octahedral layers, the coordination of K or Na, and the configuration of SiO_4 tetrahedral dimers. By comparison, the $Na_2Mg_2Si_2O_7$ phase synthesized by Gasparik and Litvin (1997) appears to have the stoichiometry identical to anhydrous sodic phase X. Hence, these two high-pressure phases are likely to possess the same structure, or at least are closely related to each other structurally.