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The crystal structure and cation ordering of Phase-X-$(K_{1-x-n})_2(Mg_{1-n}[Al,Cr]_n)_2Si_2O_7H_{2x}$: A potential K- and H-bearing phase in the mantle*

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ABSTRACT

Phase-X, a potassium di-magnesium acid disilicate, is a high-pressure synthetic compound—a potential K-bearing silicate in the mantle—with space group $P6_3cm$ (no. 185), $a = b = 5.028(2)$ Å, $c = 13.216(3)$ Å, $V = 289.34$ Å^3, $Z = 2$. The structure has been determined with 1521 CCD measured intensities and refined by the least-square method to $R = 0.0187$. The structure is built up of octahedral MgO sheets and layers containing disilicate groups, Si_2O_7, (with distinct Si1 and Si2 tetrahedra linked by the apical O2 atom) alternating along the **c** axis. The octahedral sheet is based on a hexagonal closest-packed array of two layers of non-equivalent O atoms, O1 and O3; two-thirds of all edge-sharing M octahedra are filled. Within the framework of the Si_2O_7 groups are channel structures parallel to [100], [010], and [110] that contain K atoms disordered in the middle of a large trigonal cavity (the A site). The FTIR spectrum in the OH stretching region shows a sharp peak at 3602 cm^{-1} due to OH^- ordered in one anion site; the position of hydrogen, which operates in a charge-balancing substitution for the partial occupancy of the A site $(K_{1-x}\square_x)^A \leftrightarrow H_x\square_{1-x})^H$, is undetermined. Densification in phase-X is affected by the greater compression of the empty octahedra in the octahedral layer and by constraining the trigonal A cavity containing the K atom to the size of the Si_2O_7 disilicate group. This dense packing contributes to the relatively high zero-pressure calculated density of 3.38 g/cm^3.