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Synchrotron X-ray diffraction study of the structure of shafranovskite, $K_2Na_3(Mn,Fe,Na)_4[Si_9(O,OH)_{27}](OH)_2 \cdot nH_2O$, a rare manganese phyllosilicate from the Kola peninsula, Russia

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Abstract

The structure of shafranovskite, ideally $K_2Na_3(Mn,Fe,Na)_4[Si_9(O,OH)_{27}](OH)_2 \cdot nH_2O$ (n ~ 2.33), a K-Na-manganese hydrous silicate from Kola peninsula, Russia, was studied using synchrotron X-ray radiation and a MAR345 image-plate detector at the Swiss-Norwegian beamline of the European Synchrotron Radiation Facility (ESRF, Grenoble, France). The structure [trigonal, space group $P31c$, a = 14.519(3), c = 21.062(6) Å, V = 3844.9(14) Å^3] was solved by direct methods and partially refined to $R_1 = 0.085$ ($wR_2 = 0.238$) on the basis of 2243 unique observed reflections ($|F_o| \geq 4\sigma_F$). Shafranovskite is a 2:1 hydrous phyllosilicate. Sheets of Mn and Na octahedra (***O*** sheets) are sandwiched between two silicate tetrahedral sheets ($\boldsymbol{T}_1$ and $\boldsymbol{T}_2$). The 2:1 layers are parallel to (001). The upper tetrahedral sheet $\boldsymbol{T}_1$ consists of isolated $[Si_{13}(O,OH)_{37}]$ islands composed of three six-membered rings. The octahedral sheet ***O*** consists of $Mn\varphi_6$, $Na1\varphi_6$, and $Na2\varphi_6$ octahedra (φ = O, OH, H_2O). This unit can be considered as a trioctahedral sheet with each 20th octahedron vacant. The lower tetrahedral sheet $\boldsymbol{T}_2$ consists of $[Si_{13}(O,OH)_{37}]$ islands linked into a sheet through an additional SiO_3OH tetrahedron. The Na3, K1, K2 atoms, and H_2O32 groups are between the 2:1 layers and provide their linkage along **c**.