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Coexisting hydroxyl groups and H_2O molecules in minerals: A single-crystal neutron diffraction study of eosphorite, $MnAlPO_4(OH)_2 \cdot H_2O$

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Abstract

The crystal chemistry of eosphorite from Chamachhu (Skardu District, Baltistan, Pakistan) $[(Mn^{2+}_{0.94}Fe^{2+}_{0.06}Al_{0.01})_{\Sigma 1.01}AlPO_4(OH_{1.90}F_{0.10})_{\Sigma 2} \cdot H_2O$, $a = 6.9263(4)$, $b = 10.4356(8)$, $c = 13.5234(10)$ Å, $V = 977.5(1)$ Å^3, space group *Cmca*, $Z = 8$], has been reinvestigated by means of electron microprobe analysis in wavelength-dispersive mode and single-crystal neutron diffraction at 20 K. The anisotropic structural refinement has been performed with final agreement index $R_1 = 0.0381$ for 82 refined parameters and 860 unique reflections with $F_o > 4\sigma(F_o)$. The analysis of the difference-Fourier maps of the nuclear density allowed an unambiguous location of the H sites, the description of the H_2O molecule and the OH-group configuration, along with the hydrogen-bonding scheme. We can now describe the structure of eosphorite as built by $(Mn,Fe)O_4(OH,H_2O)_2$ and $AlO_2(OH)_2(OH,H_2O)_2$ octahedra, which both form chains running along [100]. The two types of chains are connected, via shared corners, to form a set of (100) sheets held together by P-tetrahedra (and hydrogen bonds) to form a three-dimensional framework. This material provides the rare opportunity to investigate the H-bond configuration of coexisting hydroxyl groups and H_2O molecules in minerals by single-crystal neutron diffraction.

Keywords: Eosphorite, crystal chemistry, single-crystal neutron diffraction, hydrogen bonding