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Schubnelite, $[Fe^{3+}(V^{5+}O_4)(H_2O)]$, a novel heteropolyhedral framework mineral

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ABSTRACT

Schubnelite from the U deposit of Mounana, Gabon, crystallizes in space group $P\bar{1}$ with a = 5.466(1), b = 5.675(2), c = 6.610(1) Å, α =101.02(1), β = 95.10(1), γ = 107.31(1)°, and V = 189.8(2) $Å^3$. The structure of schubnelite $[Fe^{3+}(V^{5+}O_4)(H_2O)]$ contains isolated (VO_4) tetrahedra and edge-sharing $(Fe\phi_6)$ octahedra (φ = unspecified anion) and is isostructural with $[M(TO_4)(H_2O)]$ compounds with M = Mg,Mn and T = Mo,W. The topology of the schubnelite framework can be described as an arrangement of mutually orthogonal 6^3 and 4^4 nets. The fundamental building block (FBB) of the schubnelite structure does not occur in any other $M^{[6]}T^{[4]}\phi$ mineral. Many stoichiometrically similar compounds $[M(TO_4)(H_2O)]$ crystallize in the kieserite structure-type, including the synthetic compounds $V^{3+}(PO_4)(H_2O)$ and $Mn^{3+}(PO_4)(H_2O)$. The kieserite arrangement has a $^{[6]}M^{3+}$-(H_2O)-$^{[6]}M^{3+}$ bridge. Both $V^{3+}(3d^2)$ and $Mn^{3+}(3d^4)$ have electronic degeneracies that drive spontaneous distortions resulting in satisfaction of the incident bond-valence requirements around the bridging H_2O group. For Fe^{3+} $(3d^5)$ in schubnelite, there is no electronic degeneracy and hence no spontaneous local distortion of the environment around the Fe^{3+} cation. Hence, an Fe^{3+}-(H_2O)-Fe^{3+} bridge cannot form and schubnelite is forced to crystallize in a different arrangement.