The crystal structure of pararobertsite and its relationship to mitridatite

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ABSTRACT

The crystal structure of pararobertsite, $Ca_2(H_2O)_2[Mn_3^{3+}O_2(PO_4)_3] \cdot H_2O$, $P2_1/c$, $a = 8.814(4)$, $b = 13.233(5)$, $c = 11.056(4)$ Å, $\beta = 101.184(7)°$, $V = 1265.0(9)$ Å^3, $Z = 4$ has been solved by direct methods and refined to $R = 0.042$ for 1319 $F_o > 4\sigma$ (F_o) using Mo$K\alpha$ X-ray data. In the structure of pararobertsite, Z-shaped edge-sharing chains of $Mn^{3+}O_6$ octahedra link to one another via shared O vertices and PO_4 tetrahedra to form a compact sheet of composition $^2_\infty[Mn_3^{3+}O_2(PO_4)_3]^{4-}$ oriented parallel to {100}. The space between the compact sheets is filled with a thick open assemblage of $CaO_5(H_2O)_2$ polyhedra and isolated water molecules. The structure bears strong similarities to the mitridatite (Fe^{3+}) structure and, therefore, to its robertsite (Mn^{3+}) isotype.