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Veatchite: Structural relationships of the three polytypes

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ABSTRACT

Crystal structures of the three polytypes of veatchite, $Sr_2B_{11}O_{16}(OH)_5 \cdot H_2O$, are determined by X-ray, single-crystal studies. The polytypes are: veatchite-1*A*, triclinic space group $P\overline{1}$, with a = 6.6378(6), b = 6.7387(6), c = 20.982(2) Å, α = 87.860(1), β = 82.696(12), γ = 60.476(1)°, V = 809.7(2) Å^3; veatchite-1*M,* monoclinic space group $P2_1$, with a = 6.7127(4), b = 20.704(1), c = 6.6272(4) Å, β = 119.209(1)°, V = 805.4(2) Å^3; and veatchite-2*M,*monoclinic space group *Cc* with a = 6.6070(3), b = 11.7125(5), c = 20.6848(9) Å, β = 91.998(1)°, V = 1599.7(2) Å^3. The crystal structures have two layer types with similar fundamental building blocks: **A** layer FBB = 3Δ2□:<Δ2□>-<2Δ□> and **B** layer FBB = 3Δ2□,1Δ:<Δ2□>-<2Δ□>,Δ (Grice et al. 1999). Unique in this FBB is the lone polyhedron with triangular coordination, which consists of a neutrally charged $[B(OH)_3]$ group. Layering has a directional component and depending on layer sequence the symmetry may be centrosymmetric or non-centrosymmetric. Related layered borate structures, biringuccite, nasinite, gowerite, and volkovskite, are compared. Observations indicate that veatchite-1*A* is the low-temperature and low-pressure polytype, veatchite-1*M* the high-temperature polytype, and veatchite-2*M* the moderate temperature and higher pressure polytype.

Keywords: Veatchite, crystal structures, polytype, borate, fundamental building block