

## The crystal structure of ingersonite, $\text{Ca}_3\text{Mn}^{2+}\text{Sb}_4^{5+}\text{O}_{14}$ , and its relationships with pyrochlore

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### ABSTRACT

The crystal structure of ingersonite,  $[\text{Ca}_{2.93}\text{Mn}_{1.06}^{2+}\text{Fe}_{0.01}^{2+}][\text{Sb}_{3.95}^{5+}\text{Mg}_{0.05}]\text{F}_{0.15}\text{O}_{13.85}$ , has been solved and refined in the space group  $P3_121$  [ $a = 7.282(2)$ ,  $c = 17.604(4)$  Å,  $V = 808.4(3)$  Å<sup>3</sup>,  $Z = 3$ ] to  $R = 2.32\%$  for 2219  $F_o > 4\sigma(F_o)$  using  $\text{MoK}\alpha$  X-ray data.

The structure of ingersonite is isostructural with the synthetic weberite-3*T* polytype and related to the pyrochlore structure type. Both ingersonite and pyrochlore structures can be described as a sequence of pairs of polyhedral layers (named *M* and *N*), stacked along [111] and [001], respectively. In terms of the cation sites, *M* and *N* layers have general formula  $\text{AB}_3$  and  $\text{A}_3\text{B}$ , respectively, where B are the octahedral cations forming the  $\text{B}_2\text{X}_6$  framework of the pyrochlore structure and A are the larger, interstitial cations forming eightfold polyhedra in pyrochlore.

In ingersonite, the *M* layers occur at  $z \sim 1/6$ ,  $1/2$ , and  $5/6$ : The B octahedra are occupied by  $\text{Sb}^{5+}$  and share corners to form a pseudo-hexagonal tungsten bronze (HTB) motif with the A position occupied by octahedral  $\text{Mn}^{2+}$  at the center of the pseudo-hexagonal rings. *N* layers occur at  $z \sim 0$ ,  $1/3$ , and  $2/3$ , with A = Ca and B =  $\text{Sb}^{5+}$ : Isolated B octahedra share 6 edges with 6 eightfold A polyhedra, to form a continuous sheet similar to the analogous layer in pyrochlore. The stacking of successive pairs of *M* and *N* layers in ingersonite is the same as in pyrochlore. Nonetheless, a difference in the relative position between *M* and *N* layers in ingersonite and pyrochlore is observed. The crystal-chemical relationships with other pyrochlore-related minerals are outlined.

**Keywords:** Ingersonite, crystal structure, chemical data, weberite-3*T* polytype, pyrochlore-related structure, X-ray diffraction data