American Mineralogist, Volume 85, pages 231–235, 2000

The crystal structure of gearksutite, $CaAlF_4(OH)\cdot H_2O$

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ABSTRACT

The discovery of unusually well-crystallized samples of gearksutite allowed determination of its crystal structure. The crystals belong to space group $P\bar{1}$, a = 4.940(1), b = 6.810(1), c = 6.978(1) Å; α = 101.12(1), β = 94.86(1), γ = 110.07(1)°; V = 213.43(6) Å^3; Z = 2. The structure consists of layers of eightfold-coordinated calcium polyhedra connected through pairs of $[Al_2F_8(OH)_2]$ octahedra which are oriented identically, similar to those observed in other hydroxyl aluminum fluorides. A comparison with other minerals of similar composition is made. The structure data allowed us to reliably index the powder pattern and to show that the reflection intensities are strongly affected by preferred orientation.