American Mineralogist, Volume 86, pages 927–931, 2001

The crystal structure of aravaipaite

ANTHONY R. KAMPF*

Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, U.S.A.

ABSTRACT

The crystal structure of aravaipaite, $Pb_3AlF_9 \cdot H_2O$, monoclinic, $P2_1/n$, a = 25.048(4), b = 5.8459(8), c = 5.6805(7) Å, β = 94.013(3)°, V = 829.7(2) Å^3, Z=4, was solved by direct methods and refined by full-matrix least-squares techniques to R = 0.049 for 1170 observed reflections [$F_o > 4\sigma(F_o)$] and R = 0.089 for all 1820 reflections collected using Mo$K\alpha$ X-radiation and a CCD-based detector. The structure of aravaipaite contains a square-packed layer of F atoms on either side of which are bonded Pb atoms in a fluorite (β-PbF_2)-type configuration. This layer parallel to {100} serves as a template to which on both sides are attached AlF_6 octahedra and $PbF_6(H_2O)_2$ polyhedra. The resulting thick slabs are connected via Pb-O-Pb and Al-F-Pb bonds. The two nonequivalent Pb atoms in the fluorite-type layer are each coordinated to 11 F atoms and exhibit typical lone-pair behavior.

Aravaipaite was originally reported to be triclinic. The structure analysis yielded the new monoclinic cell provided above and required the following revisions in the mineral's description. Morphology: forms {100} and {401}; lamellar on {100}. Twinning: polysynthetic on {100}. Cleavage: {100} perfect micaceous, {011} good, {010} and {001} fair. Density (calc.): 6.703 g/cm^3. Optical orientation: X = b; Z ∧ a = 24° in the obtuse angle β. A powder pattern calculated from the structure data is also provided.