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Elyite, $Pb_4Cu(SO_4)O_2(OH)_4 \cdot H_2O$: Crystal structure and new data

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ABSTRACT

The crystal structure of elyite, $Pb_4Cu(SO_4)O_2(OH)_4 \cdot H_2O$, a = 14.233(2), b = 11.532(1), c = 14.611(2) Å, β = 100.45(1)°, V = 2358.4(5) Å^3, Z = 8, was solved by direct methods and refined in space group $P2_1/c$ to $R1$ = 3.64% and w$R2$ = 5.10% for the 5861 independent reflections. Data were collected on a tiny untwinned crystal fragment with a four-circle diffractometer (Mo$K\alpha$ radiation, CCD area detector). The structure contains eight unique Pb atoms, two isolated Cu atoms in planar fourfold-coordination (<Cu-O> = 1.933, 1.927 Å) and two isolated, almost ideal SO_4 tetrahedra. All anions coordinating Cu are OH groups. Two H_2O molecules are weakly bound to Pb atoms. The Pb atoms show highly variable coordinations due to variable stereochemical activities of the Pb^{2+} lone electron pairs. The connectivity of the structure is based on Pb-O polyhedra which are closely linked by common O ligands to form rod-like structure elements parallel to the b axis. The structure framework is held together by sharing ligands with CuO_4 squares and SO_4 tetrahedra. The CuO_4 squares can be considered as struts connecting the Pb-O rods along the c axis and, intermittently, along the a axis. A complex hydrogen bond system provides additional strengthening. The non-merohedral twinning parallel to {100} reported previously is explained by the presence of a pseudo-mirror plane in the structure. Comparisons are drawn with the structures of the related Pb-Cu-sulfates chenite, $Pb_4Cu(SO_4)_2(OH)_6$, and linarite, $PbCu(SO_4)(OH)_2$. The violet color of elyite and other Cu compounds might be related to the planar fourfold-coordination of Cu.