

Disordered distribution of Cu in the crystal structure of leightonite, $\text{K}_2\text{Ca}_2\text{Cu}(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$

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ABSTRACT

The crystal structure of leightonite, $\text{K}_2\text{Ca}_2\text{Cu}(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$, $C2/c$, $a = 11.654(2)$, $b = 7.497(1)$, $c = 10.097(1)$ Å; $\beta = 125.21(1)^\circ$, $V = 720.8(2)$ Å³, $Z = 2$ has been solved by direct methods and refined to $R = 3.90\%$ for 1564 $F_o > 4\sigma(F_o)$, using $\text{MoK}\alpha$ X-ray data from a crystal twinned on $\{20\bar{1}\}$. Structural sub-units $[\text{Ca}(\text{SO}_4)_2]^{2-}$ formed by one CaO_8 polyhedron and two opposite-sided SO_4 tetrahedra are linked by edge sharing. These sub-units are linked to each other by corner sharing to form a three-dimensional framework with channels, where the Cu atoms are located. The framework of CaO_8 polyhedra and SO_4 tetrahedra exhibits a perfect orthorhombic symmetry whereas the copper atoms located at the Cu1 and Cu2 sites are not equivalent because they have different partial occupancies (0.37 and 0.13, respectively). Both Cu1 and Cu2 are coordinated by O atoms to form two rhombically elongated octahedra (2 + 2 + 2 Jahn-Teller distortion). K and Ow are disordered on the same site. The crystal structure of leightonite closely resembles that of the triclinic polyhalite, $\text{K}_2\text{Ca}_2\text{Mg}(\text{SO}_4)_4 \cdot 2\text{H}_2\text{O}$, with the main difference being the different distribution of Cu in leightonite with respect to Mg in polyhalite.