

Crystal structure of tooeleite, $\text{Fe}_6(\text{AsO}_3)_4\text{SO}_4(\text{OH})_4 \cdot 4\text{H}_2\text{O}$, a new iron arsenite oxyhydroxy-sulfate mineral relevant to acid mine drainage

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ABSTRACT

The crystal structure of tooeleite, $\text{Fe}_6(\text{AsO}_3)_4(\text{SO}_4)(\text{OH})_4 \cdot 4\text{H}_2\text{O}$, has been solved from high-resolution synchrotron XRD powder data recorded on a sample from Tooele county, Utah. The structure is monoclinic, space group $C2/m$, $a = 8.9575(1)$, $b = 6.4238(1)$, $c = 9.7912(1)$ Å, $\beta = 96.032(1)^\circ$, $V = 560.27(3)$ Å³, $d_{\text{calc}} = 3.16$ g/cm³. The structure was solved by direct methods and atomic positions, site occupancies, and isotropic displacement parameters were refined by the Rietveld method. The AsO_3 pyramids bond to FeO_6 octahedra by both edge- and corner-linkage, forming layers that intercalate SO_4 groups. Assignment of structural H_2O and OH groups were done from bond-valence analysis. Tooeleite is the only arsenite-sulfate mineral known and has been recently identified as the main constituent of stromatolite-like deposits in the Carnoulès acid mine, Gard, France.

Keywords: Crystal structure, tooeleite, XRD data, synchrotron powder diffraction, new minerals, geomicrobiology, acid mine drainage