

The new mineral tomiolloite, $\text{Al}_{12}(\text{Te}^{4+}\text{O}_3)_5[(\text{SO}_3)_{0.5}(\text{SO}_4)_{0.5}](\text{OH})_{24}$: A unique microporous tellurite structure

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ABSTRACT

Tomiolloite (IMA2021-019) is a new aluminum tellurite sulfite-sulfate mineral discovered at the Bambolla mine, Moctezuma, Sonora, Mexico, a well-known tellurium (Te) mineral locality. Tomiolloite forms roughly spherical clusters of crystals comprised of very thin, needle-like crystals (1 μm diameter, ~ 40 μm length) around a core of small, stubbier, broken crystals. Tomiolloite is generally found growing on tellurite or quartz. The strongest powder X-ray diffraction lines are [d_{obs} \AA (I_{obs}) (hkl)]: 11.667 (89) (100), 8.240 (38) (101), 4.107 (29) (202,211,121), 3.223 (100) (203,302,130), and 2.905 (37) (213,123,222,400). The empirical formula of tomiolloite, as determined by electron microprobe analysis, is $(\text{Al}_{10.64}\text{Te}_{1.01}\text{Fe}_{0.31}^{3+}\text{Zn}_{0.04})_{\Sigma 12}(\text{Te}_{3.00}^{4+}\text{Pb}_{0.02})_{\Sigma 5.02}(\text{S}_{0.49}^{4+}\text{S}_{0.49}^{6+}\text{Si}_{0.02})_{\Sigma 1.00}\text{O}_{21.53}[(\text{OH})_{20.86}\text{Cl}_{0.11}]_{\Sigma 20.97}$, which is simplified to the ideal formula $\text{Al}_{12}(\text{Te}^{4+}\text{O}_3)_5[(\text{SO}_3)_{0.5}(\text{SO}_4)_{0.5}](\text{OH})_{24}$. Significant Te^{6+} substitution for Al^{3+} is observed in tomiolloite, verified by X-ray photoelectron spectroscopy and crystal-structure analysis. The structure of tomiolloite was determined using synchrotron single-crystal X-ray diffraction, showing that tomiolloite is hexagonal and crystallizes in the space-group $P6_3/m$, with the unit-cell parameters $a = 13.3360(19)$ \AA , $c = 11.604(2)$ \AA , $V = 1787.3(6)$ \AA^3 , and $Z = 2$. Tomiolloite has a unique microporous framework structure, which bears a slight similarity to that of zemannite, but it has a much larger cavity diameter (8.85 \AA). The framework is built from edge-sharing $M\phi_6$ octahedra ($M = \text{Al}^{3+}$ and Te^{6+}), Te^{4+}O_3 trigonal pyramids, and Te^{4+}O_4 disphenoids. $M\phi_6$ octahedra edge-share to form crankshaft-shaped chains along c , with Te^{4+}O_n polyhedra filling notches in the crankshafts and providing linkages between adjacent chains. The framework has an overall positive charge, which is balanced by the presence of both sulfite (SO_3^{2-}) trigonal pyramids and sulfate (SO_4^{2-}) tetrahedra in the channels.

Keywords: New mineral, crystal structure, tellurium oxysalt, microporous, synchrotron radiation, X-ray diffraction, Moctezuma, Sonora, Mexico; Microporous materials: crystal-chemistry, properties, and utilizations