

New mineral tomiolloite: a unique microporous tellurite

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

SUPPLEMENTARY MATERIAL

Supplementary Table S1. Crystal structure refinement details for tomiolloite

Crystal data	
Ideal Chemical Formula	$(\text{Al}_{11}\text{Te}^{6+}_1)_{\Sigma 12}(\text{Te}^{4+}\text{O}_3)_5\text{O}_{3.14}(\text{OH})_{20.86}(\text{SO}_3)_{0.93}^*$
Crystal system, Space group	Hexagonal, $P6_3/m$
Temperature (K)	100(1)
a, c (Å)	13.3360(19), 11.604(2)
V (Å ³)	1787.3(6)
Z	2
Calculated density (g cm ⁻³)	3.272
Radiation type and wavelength (Å)	Synchrotron, $\lambda = 0.71096$
μ (mm ⁻¹)	5.297
Crystal dimensions (mm)	0.001 × 0.001 × 0.030
Reflections for cell refinement	2045, 2.27–20.00° 2 θ
Data Collection	
Crystal description	Transparent needle
Diffractometer	Dectris EigerX 16M
θ (°) range	2.488–32.070
Indices range of h, k, l	$h: \pm 19, k: \pm 17, l: \pm 16$
Absorption correction	Multi-scan SADABS (Bruker, 2001)
T_{\min}, T_{\max}	0.3673, 0.4644
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32626, 2021, 1643
R_{int}	0.0945
Data completeness to 25.242° θ (%)	98.2
Refinement	
Number of reflections, parameters, restraints	2021, 102, 2
$R_1[F^2 > 2\sigma(F^2)], R_1(\text{all})$	0.0650, 0.0808
$wR_2[F^2 > 2\sigma(F^2)], wR_2(\text{all})$	0.1655, 0.1784
$GoF(F^2)$	1.062
$\Delta\rho_{\min}, \Delta\rho_{\max}$ (e Å ⁻³)	-4.17, 5.14

*S and associated O sites refine to 0.93 of a SO₃ group due to the nature of structural data collection on thin needles, hence a small additional amount of OH (0.14 OH *pfu*) must be O for charge balance.