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The crystal structure of namibite, $Cu(BiO)_2VO_4(OH)$, and revision of its symmetry

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ABSTRACT

The crystal structure of namibite, $Cu(BiO)_2VO_4(OH)$ [triclinic, space group $P\overline{1}$, $a = 6.210(1)$, $b = 7.398(1)$, $c = 7.471(1)$ Å, $\alpha = 90.10(1)$, $\beta = 108.73(1)$, $\gamma = 107.47(1)^\circ$, $V = 308.22(8)$ Å^3, $Z = 2$] was determined using single-crystal X-ray diffraction data. The refinement, based on 2140 unique reflections with $F_o > 4\sigma(F_o)$, gave $R1 = 3.61\%$. The structure determination showed namibite to be triclinic-pseudomonoclinic; the previously reported *C*-centered monoclinic cell is a pseudocell. The structure contains two unique Bi atoms, with nine Bi-O bonds between 2.17 and 3.39 Å. The Bi coordinations show some stereochemical influence of the lone pair of electrons on Bi^{3+}. A three-dimensional network is formed by linkages of Bi-O polyhedra to one slightly distorted $V^{5+}O_4$ tetrahedron that decorates chains of corner-sharing CuO_6 polyhedra extending parallel to the *b* axis. The CuO_6 polyhedra show the Jahn-Teller-distorted [4+2]-coordination of Cu^{2+}. Layers of Bi atoms parallel to (100) alternate with layers of parallel heteropolyhedral $[Cu(VO_4)O_2(OH)]$ chains. According to bond-valence calculations and geometrical considerations, the H atom of the OH group is probably involved in disordered or trifurcated H bonding. The structure of namibite represents a slightly distorted ordered variant of the monoclinic structure of brendelite, $(Bi,Pb)_2(Fe^{3+},Fe^{2+})O_2(OH)(PO_4)$. Further relations to synthetic $Cu_3Bi_4V_2O_{14}$, to the 7 Å chain-structure phosphates and sulfates, and to linarite are outlined.