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Description and crystal structure of liversidgeite, $Zn_6(PO_4)_4 \cdot 7H_2O$, a new mineral from Broken Hill, New South Wales, Australia

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Abstract

Liversidgeite, ideally $Zn_6(PO_4)_4 \cdot 7H_2O$, is a new mineral from Block 14 Opencut, Broken Hill, New South Wales, Australia. The mineral occurs as white, thin, bladed crystals and as hemispherical aggregates of radiating crystals in cavities in sphalerite-galena ore. Associated minerals are anglesite, pyromorphite, greenockite, sulfur, and an unknown Zn phosphate sulfate. Individual crystals are up to 0.1 mm in length and 0.05 mm across. Liversidgeite is transparent to translucent, with a vitreous luster and a white streak. It is brittle with an irregular fracture, the Mohs hardness is ~3–3.5, and the observed and calculated densities are 3.21(2) and 3.28 g/cm^3, respectively. Chemical analysis by electron microprobe gave ZnO 54.62, MnO 0.49, PbO 0.18, P_2O_5 32.62, As_2O_5 0.65, SO_3 0.35, H_2O 14.04, total 102.95 wt%, with H_2O content derived from the refined crystal structure. The empirical formula calculated on the basis of 23 O atoms is $Pb_{0.01}(Zn_{5.86}Mn_{0.06})_{\Sigma 5.92}(P_{4.01}As_{0.05}S_{0.04})_{\Sigma 4.10}O_{16.20} \cdot 6.8H_2O$. Liversidgeite is triclinic, space group $P\bar{1}$, with $a = 8.299(1)$, $b = 9.616(1)$, $c = 12.175(1)$ Å, $\alpha = 71.68(1)$, $\beta = 82.02(1)$, $\gamma = 80.18(1)°$, $V = 905.1(2)$ Å^3 (single-crystal data), and $Z = 2$. The six strongest lines in the X-ray powder diffraction pattern are [*d*(Å), (*I*), (*hkl*)]: 8.438 (80) (011), 3.206 (60) (01$\bar{3}$), 2.967 (75) (2$\bar{1}$2, 114), 2.956 (75) (21$\bar{2}$), 2.550 (85) (233, 2$\bar{1}$3), 2.537 (100) (22$\bar{1}$, 01$\bar{4}$, 31$\bar{1}$). The crystal structure of liversidgeite was refined to an *R*1 index of 5.95% based on 3054 observed ($F_o > 4\sigma F_o$) reflections measured with Mo$K\alpha$ X-radiation. The structure is based on two distinct, infinite zigzag chains of edge-sharing $Zn\phi_6$ (ϕ = unspecified anion) octahedra that extend in the *a* direction. The chains link to each other via common corners and also via corner-sharing PO_4 tetrahedra, forming sheets parallel to the (011) plane. The sheets link via $[Zn_2\phi_8]$ dimeric building units, comprising edge-sharing $Zn\phi_5$ trigonal bipyramids and $Zn\phi_4$ tetrahedra, resulting in an open framework. Large ellipsoidal channels extend along the *a* direction and are occupied by interstitial H_2O groups and the H atoms of the H_2O groups that coordinate to the Zn cations. An extensive network of hydrogen bonds provides additional linkage between the sheets in the structure, via the interstitial H_2O groups. The topology of the liversidgeite structure is identical to that of synthetic, monoclinic $Zn_2Co_4(PO_4)_4(H_2O)_5 \cdot 2H_2O$.

Keywords: Liversidgeite, new mineral species, zinc phosphate, crystal structure, Broken Hill, New South Wales, Australia