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The new mineral cuprozheshengite, $Pb_4CuZn_2(AsO_4)_2(PO_4)_2(OH)_2$, from Yunnan, China, with site-selective As-P substitution

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Abstract

Cuprozheshengite, $Pb_4CuZn_2(AsO_4)_2(PO_4)_2(OH)_2$, is a new mineral species from Yunnan, China. It occurs as sub-millimeter greenish-blue hemispherical aggregates of microscopic blade-like crystals on hemimorphite and is closely associated with veszelyite and galena. Cuprozheshengite is brittle with irregular fracture and has a Mohs hardness of 2½–3 and perfect cleavages on {011}. The calculated density is 5.91 g/cm^3. The empirical chemical formula of the holotype is $(Pb_{3.97}Na_{0.04}Ca_{0.01})_{\Sigma 4.02}Cu_{1.06}Zn_{2.09}(AsO_4)_2[(P_{0.84}As_{0.12}Si_{0.01})_{\Sigma 0.97}O_4]_2(OH)_2$ based on 18 O atoms per formula unit. Cuprozheshengite is triclinic, space group $P\overline{1}$, with unit-cell parameters $a = 4.7977(8)$, $b = 8.5789(8)$, $c = 10.3855(9)$ Å, $\alpha = 97.270(8)°$, $\beta = 101.902(12)°$, $\gamma = 91.495(11)°$, $V = 414.30(9)$ Å^3, and $Z = 1$. Cuprozheshengite is a member of dongchuanite group, whose general formula is $A_4{}^{VI}B^{IV}B_2(X1O_4)_2(X2O_4)_2(OH)_2$, where A is an interlayer cation with Pb being dominant; B are transition metals with two crystallographic positions, ^{IV}B has tetrahedral coordination and is fully occupied by Zn, while ^{VI}B has octahedral coordination and is dominated by Zn or Cu; $X1$ and $X2$ are cations with tetrahedral coordination, occupied by As and P. Like other dongchuanite group minerals, the structural framework of cuprozheshengite is composed of two heteropolyhedral columns along [100]. Type 1 columns comprise corner-linked $[^{IV}BO_4]$ and $[X2O_4]$ tetrahedra. Each tetrahedron is connected with three other tetrahedra in the columns. Type 2 columns have alternating $[^{VI}BO_4(OH)_2]$ octahedra with pairs of corner-connected $[X1O_4]$ tetrahedra. These two columns are connected by corner-sharing between $[^{IV}BO_4]$ and $[X1O_4]$ tetrahedra to form layers parallel to (011). Pb atoms occupy two independent sites between the layers. Cuprozheshengite is named as the copper analog of zheshengite. Single-crystal X-ray diffraction reveals that As and P order over the $X1$ and $X2$ sites, with As tending to occupy $X1$. Density functional theory (DFT) calculations confirm the occupancy propensity of As benefiting structural stability. The structural and stability studies of cuprozheshengite may have implications for local environmental governance. As a stable mineral in the water and elemental cycles after weathering, cuprozheshengite still has the potential to continually crystallize, fixing As into a stable crystalline waste form.

Keywords: Cuprozheshengite, dongchuanite group, new mineral, crystal structure, DFT calculations, As-P ordering