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Quetzalcoatlite: A new octahedral-tetrahedral structure from a $2 \times 2 \times 40$ μm^3 crystal at the Advanced Photon Source-GSE-CARS Facility

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ABSTRACT

The structure of quetzalcoatlite, $Zn_6Cu_3(TeO_3)_2O_6(OH)_6(Ag_xPb_y)Cl_{x+2y}$, $x + y \leq 2$, $Z = 1$, was solved and refined using data collected at the Advanced Photon Source-GSE-CARS facility, using a $2 \times 2 \times 40$ μm^3 single crystal. The structure is trigonal, space group $P\bar{3}1m$, $a = 10.145(1)$, $c = 4.9925(9)$ Å, $V = 445.0(1)$ Å^3, and was refined to $R = 5.1$ for 395 unique observed reflections. $Te^{6+}O_6$ octahedra and Jahn-Teller distorted $Cu^{2+}O_4(OH)_2$ octahedra share edges to form layers parallel to (001), and $ZnO_2(OH)_2$ tetrahedra share vertices to form six-member rings parallel to (001). Layers of octahedra and tetrahedra alternate along *c*, and form a new framework structure by vertex sharing. Channels through the framework parallel to *c* are occupied by Ag, Pb, and Cl ions. Electron microprobe analysis revealed Ag and Cl overlooked in the original microchemical analysis. Up to one-third of the Ag was substituted by Pb, and a Pb-rich analog may exist.