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The crystal structure of ramdohrite, $Pb_{5.9}Fe_{0.1}Mn_{0.1}In_{0.1}Cd_{0.2}Ag_{2.8}Sb_{10.8}S_{24}$: A new refinement

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Abstract

The crystal structure of ramdohrite, $Pb_{5.9}Fe_{0.1}Mn_{0.1}In_{0.1}Cd_{0.2}Ag_{2.8}Sb_{10.8}S_{24}$, from the Chocaya mine, Potosí, Bolivia, determined by Makovicky and Mumme from film data in 1983, was refined from single-crystal diffractometer data to the R value 0.060, based on 5230 reflections [$I > 2\sigma(I)$] from a twinned crystal. Lattice parameters are a = 8.7348(3), b = 13.0543(4), c = 19.3117(6) Å, and β = 90.179(2)°, space group $P2_1/n$.

Two bicapped trigonal prismatic sites of lead bridge and unite adjacent $(311)_{PbS}$ slabs. These slabs contain five distinct coordination pyramids of Sb with trapezoidal cross sections, a mixed and disordered Sb-Ag-Cd-(Pb) site, refined as 0.39 Sb + 0.61 Ag, a pure Ag site with a very open, irregular tetrahedral coordination, and an octahedral site occupied by Pb. The $(311)_{PbS}$ slabs contain large lone electron pair micelles formed by four distinct antimony sites in alternation with small such micelles formed by a single Sb site. The geometric arrangement of these slabs is not based on crankshaft chains of short, strong Me-S bonds but on a chess-board arrangement of (predominantly) Sb pairs that share two common S atoms via short bonds. Relationships to, and differenced from, fizelyite and uchucchacuaite are described and discussed.

Keywords: Ramdohrite, crystal structure, fizelyite-andorite series, Pb-Ag-Sb sulfosalt