

Crystal structure of a new compound, CuZnCl(OH)₃, isostructural with botallackite

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ABSTRACT

A new compound, ideally CuZnCl(OH)₃, was found on a metallic mining artifact of copper composition at the Rowley mine, Maricopa County, Arizona, U.S.A., and studied with electron microprobe analysis, single-crystal X-ray diffraction, and Raman spectroscopy. It is isostructural with botallackite [Cu₂Cl(OH)₃] with space group *P2₁/m* and unit-cell parameters $a = 5.6883(5)$, $b = 6.3908(6)$, $c = 5.5248(5)$ Å, $\beta = 90.832(2)^\circ$, $V = 200.82(3)$ Å³. The crystal structure of CuZnCl(OH)₃, refined to $R_1 = 0.018$, is characterized by brucite-type octahedral sheets made of two distinct and considerably distorted octahedra, M1 and M2, which are coordinated by (5OH + 1Cl) and (4OH + 2Cl), respectively. The octahedral sheets are parallel to (100) and connected by O–H···Cl hydrogen bonding. The major structural difference between CuZnCl(OH)₃ and botallackite is the complete replacement of Cu²⁺ in the highly angle-distorted M1 site by non-Jahn-Teller distorting Zn²⁺. The CuZnCl(OH)₃ compound represents the highest Zn content ever documented for the atacamite group of minerals, in conflict with all previous reports that botallackite (like atacamite) is the most resistant, of all copper hydroxylchloride Cu₂Cl(OH)₃ polymorphs, to the substitution of Zn²⁺ for Cu²⁺, even in the presence of large excess of Zn²⁺. Its discovery, along with the recently described new mineral iyoite, CuMnCl(OH)₃, implies that more botallackite-type compounds or minerals with the chemical formula CuMCl(OH)₃ ($M = \text{Ni}^{2+}, \text{Co}^{2+}, \text{Fe}^{2+}, \text{Mn}^{2+}, \text{Cd}^{2+}, \text{and Mg}^{2+}$) may be synthesized or found in nature.

Keywords: CuZnCl(OH)₃, copper-zinc hydroxylchloride, botallackite, atacamite group, crystal structure, Raman spectroscopy