

## Crystal structure of a new compound, $\text{CuZnCl}(\text{OH})_3$ , isostructural with botallackite

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### ABSTRACT

A new compound, ideally  $\text{CuZnCl}(\text{OH})_3$ , 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 [ $\text{Cu}_2\text{Cl}(\text{OH})_3$ ] with space group  $P2_1/m$  and unit-cell parameters  $a = 5.6883(5)$ ,  $b = 6.3908(6)$ ,  $c = 5.5248(5)$  Å,  $\beta = 90.832(2)^\circ$ ,  $V = 200.82(3)$  Å<sup>3</sup>. The crystal structure of  $\text{CuZnCl}(\text{OH})_3$ , 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  $\text{CuZnCl}(\text{OH})_3$  and botallackite is the complete replacement of  $\text{Cu}^{2+}$  in the highly angle-distorted M1 site by non-Jahn-Teller distorting  $\text{Zn}^{2+}$ . The  $\text{CuZnCl}(\text{OH})_3$  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  $\text{Cu}_2\text{Cl}(\text{OH})_3$  polymorphs, to the substitution of  $\text{Zn}^{2+}$  for  $\text{Cu}^{2+}$ , even in the presence of large excess of  $\text{Zn}^{2+}$ . Its discovery, along with the recently described new mineral iyoite,  $\text{CuMnCl}(\text{OH})_3$ , implies that more botallackite-type compounds or minerals with the chemical formula  $\text{CuMCl}(\text{OH})_3$  ( $M = \text{Ni}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Cd}^{2+}$ , and  $\text{Mg}^{2+}$ ) may be synthesized or found in nature.

**Keywords:**  $\text{CuZnCl}(\text{OH})_3$ , copper-zinc hydroxylchloride, botallackite, atacamite group, crystal structure, Raman spectroscopy