

The Crystal Structure of Clinoatacamite and the Quest for Paratacamite

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Pure $\text{Cu}_2(\text{OH})_3\text{Cl}$ is known to occur in the form of the three polymorphs atacamite, botallackite and clinoatacamite. While atacamite is orthorhombic the other two polymorphs are monoclinic. A rhombohedral structure type of $\text{Cu}_2(\text{OH})_3\text{Cl}$ has been described as paratacamite, but it is now assumed that this rhombohedral polymorph of $\text{Cu}_2(\text{OH})_3\text{Cl}$ has to be stabilized by partial substitution of Zn or Ni for Cu. The respective end members $\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$ and $\text{Cu}_3\text{Ni}(\text{OH})_6\text{Cl}_2$ are now known as the minerals herbertsmithite and gillardite.

The mineral clinoatacamite occurs as a corrosion product of copper and has also attracted attention for its unusual magnetic properties (Zheng et al. 2005). Here we report single crystal structure refinements of two clinoatacamite samples from the Sierra Gorda district in Northern Chile. Both samples show evidence of twinning, albeit with different twin laws. Microprobe analysis confirms the stoichiometry of clinoatacamite with only 0.014mol% Ni and 0.029mol% Zn substituting for Cu in the two samples respectively. Starting with the structure model of clinoatacamite described by Grice et al. (1996) the Zn-bearing sample refines to $R1=0.04$, with all hydrogen atoms located. The Ni-bearing sample refines to an even better R-value ($R1=0.033$) on the basis of the same structure model. However, long exposure X-ray diffraction images show evidence of additional weak diffraction maxima in this sample. The volume of the resulting unit-cell is fourfold compared to the unit cell of clinoatacamite. Based on possible models for this superstructure of clinoatacamite, the systematics of polymorphism in the $\text{Cu}_2(\text{OH})_3\text{Cl}$ -group of minerals is reassessed.

References

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