Conichalcite Revisited: Structural and Chemical Characterisation of a Sample from the Maria Catalina mine, Copiapó Province, Chile

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Conichalcite, $CaCu(OH)(AsO_4)$, commonly forms in the oxidation zone of copper ore bodies. It belongs to the adelite group that comprises eleven minerals and three synthetic compounds crystallising in $P2_12_12_1$ (the closely related descloizite group is characterised by space group *Pnma*). The general formula of this group is $M1M2(OH,O)[X(O_4,O_3OH)]$ ($M1$ = Na^+, Ca^{2+}, Pb^{2+}, Sr^{2+}; $M2$ = Mg^{2+}, Al^{3+}, $Mn^{2+,3+}$, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}; X = Si^{4+}, P^{5+}, V^{5+}, As^{5+}). The crystal structure of conichalcite was first determined by Qurashi and Barnes (1963), originally in *Pnma*, but with final refinement in $P2_12_12_1$ (a = 7.400, b = 5.842, c = 9.210 Å). Unit-cell parameters of the pure end-member were reported by Radcliffe and Simmons (1971) to be a = 7.393, b = 9.220, c = 5.830 Å.

A conichalcite sample with bright green chisel-shaped prisms from the Maria Catalina mine, Pampa Larga district, Copiapó Province, Chile, associated with kröhnkite, mansfieldite and baryte, was investigated by electron microprobe (EMP) analysis and single-crystal structure refinement (CCD area detector data, Mo$K\alpha$ radiation, 293 K, 2_{max} = 70°). The EMP analysis demonstrate a near-endmember composition, but with strong zoning of very minor impurity elements (Na, Sr, Zn, Mg, Al, P, S, Si). Most zones are less than 1 μm thick, and the precise chemical composition of each zone was not measurable.

The Maria Catalina sample crystallises in space group $P2_12_12_1$, with a = 7.404(2), b = 9.241(2), c = 5.831(1) Å, V = 398.96(14) Å^3, Z = 4. The refinement yielded $R1(F)$ = 0.0202, w$R2(F^2)$ = 0.0463 for 1739 unique reflections; for 1660 'observed reflections' with ${F_o}^2 > 4\sigma({F_o}^2)$ $R1(F)$ is 0.0183. The sample may show some slight racemic twinning (twin ratio 0.963(11):0.037). The combination of EMP analysis and crystal-structure refinement gave the empirical formula $Ca(Cu_{0.97}Zn_{0.02}Mg_{0.01})(OH)[(As_{0.97}P_{0.03})O_4)$.

In conichalcite from Maria Catalina, all atoms lie on general positions. This contradicts the model of Qurashi and Barnes (1963) in which the Cu atom is located on a special position (0, 0, 0.75), although the involved atomic shift is very small. [4+2]-coordinated Cu atoms form elongated square bipyramids (<Cu–(O,OH)> = 2.104 Å) that are interconnected by common edges to form chains parallel to [001]. Each AsO_4 tetrahedron (<As–O> = 1.692 Å) links two such chains into a three-dimensional framework. [8]-coordinated Ca^{2+} cations occupy the framework cavities; their coordination polyhedron is a slightly distorted square antiprism (<Ca–(O,OH)> = 2.512 Å). The hydrogen bond is medium strong (O5–H···O2 = 2.688(2) Å).

References

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