

Order-disorder, Polytypes and Twinning in the Crystal Structure of Vurroite

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Vurroite, ideally $\text{Pb}_{20}\text{Sn}_2(\text{Bi,As})_{22}\text{S}_{54}\text{Cl}_6$, is a complex mineral type, where the two minor chemical components, Sn and Cl, act as essential constituents together with Pb, Bi, As and S [1, 2]. X-ray single crystal data on vurroite strongly indicate an orthorhombic F-centred symmetry [1, 3]. In this study the crystal structure of vurroite is interpreted as an OD structure belonging to the category III of OD structures composed of equivalent layers [4]. The application of the OD procedures allowed the derivation of the OD-groupoid family (λ and σ operations), as well as the MDO (Maximum Degree of Order) structures. The layer symmetry (λ) is $A(2)mm$, the interlayer symmetry (σ) consists of a glide plane $n_{1/2,1/2}$ and two-fold screw axes parallel to [010] and [001] with the translation components $\frac{1}{4}b$ and $\frac{1}{4}c$, respectively. For this OD family two MDO polytypes exist. The former has monoclinic symmetry, $C12/c1$, whereas the latter is monoclinic, $P12/c1$. The OD treatment of the crystal structure of vurroite allowed to prove that the true symmetry of this mineral is monoclinic and that the apparent orthorhombic symmetry observed for the X-ray pattern of the measured crystal is due to a twinning phenomenon.

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