# Zur Kenntnis eines Vanadyl-Oxocuprat-Phosphats $CaCu(VO)(PO_4)_2$ mit $Cu^{2+}$ auf Positionen der $VO^{2+}$-Ionen und einer kupferreicheren Phase $CaCu_{1,13}(VO)_{0,87}(PO_4)_2$

On an Vanadyl Oxocuprate Phosphate $CaCu(VO)(PO_4)_2$ Containing $Cu^{2+}$ at Positions of $VO^{2+}$ Ions and a Copper Rich Phase $CaCu_{1.13}(VO)_{0.87}(PO_4)_2$

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Calcium, Copper, Vanadyl-Phosphate, Crystal Structure

Single crystals of $CaCu(VO)(PO_4)_2$ (I) and $CaCu_{1.13}(VO)_{0.87}(PO_4)_2$ (II) have been prepared using solid state reactions in closed and evacuated quartz tubes. X-ray characterization led to orthorhombic symmetry, space group $D_{2h}^{16}$-Pnma, lattice constants *a*, *b*, *c* (I): 9.708(1), 9.603(1), 6.913(1) Å and (II): 9.700(1), 9.614(1), 6.896(1) Å, Z = 4. Strongly deformed $CaO_8$ cubes are connected by planar $CuO_4$ polygons or square $VO_{1+4}$ pyramids. Short V-O distances are features of $VO^{2+}$ groups. Two point positions are occupied in a disordered manner by $Cu^{2+}$ and $VO^{2+}$. The replacement of $Cu^{2+}$ by $VO^{2+}$ at one position depends on the ratio $VO^{2+}$ : $Cu^{2+}$ at the neighbouring position, since otherwise there would be collisions of the apical oxygen atoms of neighbouring $VO_{1+4}$ pyramids.

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