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Comparison of the homeomorphic crystal structures of Pb(Fe,Mn) (VO_4) (OH) = čechite and $PbCu(AsO_4)$ (OH) = duftite

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Čechite, $Pb(Fe,Mn)(VO_4)(OH)$ */1/*: a = 7.605(3), b = 9.435(4), c = 6.099(2) Å; space group Pnam; Z = 4; R = 0.043 for 931 reflections and $2\delta \leq 80°$. Crystals from the type locality Vraniče, near Přibram, Czecho-Slovakia. - Duftite, $PbCu(AsO_4)(OH)$ */2-4/*: a = 7.788(3), b = 9.223(3), c = 6.001(2) Å; space group $P2_12_12_1$; Z = 4, R = 0.052 for 639 reflections and $2\delta \leq 60°$. Hydrothermal synthesized crystals.

The minerals čechite and duftite are members of the descloizite resp. adelite group */5/*. The crystal structures of these homeomorphic mineral groups are strongly related to each other.

In both compounds the Pb atoms are (9) coordinated to O atoms: <Pb-O> is 2.76 Å (čechite) and 2.75 Å (duftite). The atoms (Fe,Mn) and Cu are (6) coordinated: In čechite the $(Fe,Mn)O_6$ octahedron shows less distortion, (Fe,Mn)-O varies from 2.02 to 2.20 Å, <(Fe,Mn)-O> = 2.13 Å. On the contrary in duftite the CuO_6 "octahedron" is strongly distorted: Cu-O = 1.91, 1.94, 2.10, 2.11, 2.29, 2.35 Å, <Cu-O> = 2.12 Å. The V and As atoms are as usual tetrahedrally coordinated by O atoms: <V-O> = 1.73, <As-O> = 1.69 Å.

The $(Fe,Mn)O_6$ resp. CuO_6 "octahedra" are linked by common O-O edges (2.71 to 2.97 Å) to chains parallel to (001). A network is formed by the interconnection with Pb atoms, hydrogen bonds, and vanadate resp. arsenate tetrahedra. As a reason for the different space groups of the two title compounds the deformation of the CuO_6 polyhedron, caused by the electron configuration of the Cu(II) atom (JAHN-TELLER effect), is assumed.

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