Crystal structures and topology of two copper arsenates: zdenekite and mahnertite Natalia V. Zubkova[a], Dmitry Yu. Pushcharovsky[a], Simon J. Teat[b], Elizabeth J. Maclean[b], Halil Sarp[c], *[a]Geology Department, Moscow State University, 119992, Moscow Russia, [b]CCLRC Daresbury Laboratory, Daresbury, Warrington Cheshire WA4 4AD, UK, [c]Departement de Mineralogie du Museum d'Histoire naturelle de Geneve, 1, route de Malagnou, CH-1208 Geneve, Switzerland.* E-mail: nata_zubkova@rambler.ru

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Two copper arsenates - zdenekite, $NaPbCu_5(AsO_4)_4Cl{\cdot}5H_2O$, (sp. gr. $P2_1/n$, a=10.023(7) b=19.55(1) c=10.023(6) Å, β=90.02(1)°, Z=4, R = 0.096) and mahnertite, ideally $(Na,Ca)Cu_3[AsO_4]_2{\cdot}Cl{\cdot}5H_2O$, (sp. gr. $I4/mmm$, a = 10.037(1), c = 23.739(1) Å, Z = 8, R = 0.049) were discovered at Cap Garon mine, Var, France [1,2] and there single crystals were selected for X-ray study. The data were collected using a Bruker AXS SMART CCD area detector diffractometer on station 9.8 of the SRS Daresbury [3]. The most specific features of the crystal structures of zdenekite and mahnertite are identical sheets (0 1 0) for zdenekite and (0 0 1) for mahnertite. The sheets consist of clusters formed by four Cu-pyramids, which have one common vertice (Cl) and share edges. In both structures the AsO_4 tetrahedra are linked to each cluster of four Cu-polyhedra (four tetrahedra below and four tetrahedra above). Each tetrahedron shares two vertices with two Cu-polyhedra of one cluster and one vertex with a Cu-polyhedron from the adjacent cluster. The fourth vertex of each AsO_4 tetrahedron is linked to the Cu-pentahedron, which does not belong to clusters. Like the Cu-pentahedra considered above, the latter copper polyhedron is also a pentahedron and represents a distorted tetragonal pyramid. However, the latter copper atom is co-ordinated (along with four oxygen atoms) either by Cl atoms or by the water molecule statistically distributed in Cl(2) sites (in mahnertite) and by water molecule (in zdenekite) and oriented toward the interlayer space. All the oxygen atoms in this tetragonal pyramid are located in its base and simultaneously serve as vertices of the AsO_4 tetrahedra. In mahnertite mirror planes m parallel to (0 0 1) pass through the apical Cl atoms (partially substituted by H_2O molecules) of these pyramids providing the linkage between polyhedral sheets adjacent along [0 0 1]. As a result in mahnertite the heterogeneous framework is formed. In the structure of zdenekite each sheet can be described as a tetragonal one but the neighbouring sheets are shifted and the symmetry of zdenekite is lowered to monoclinic. In the structure of mahnertite the large voids of the framework accommodate Na,Ca-octahedra, water molecules and Cu atoms with partial occupancy factor. In zdenekite Na- and Pb-polyhedra and water molecules are located in the interlayer space. As a conclusion it can be emphasised that both mahnertite and zdenekite contain the new type of mixed polyhedral sheets, which are characterized by the different mode of stacking. Another alternation of the similar modules and consequently another polytypism can be also revealed in the future in chemically related mineral species.

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