

Crystal structure of mahnertite

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Abstract: Mahnertite, $(\text{Na}_{0.88}\text{Ca}_{0.12})\text{Cu}_{2.75}[\text{AsO}_4]_2\text{Cl}_{0.62}\cdot 3.63 \text{H}_2\text{O}$, $M = 565.17$, is tetragonal, with space group $I4/mmm$, $a = 10.037(1)$, $c = 23.739(1)$ Å, $V = 2391.5(4)$ Å³, $Z = 8$, $\rho_o = 3.32$, $\rho_c = 3.14$ g/cm³, $\mu = 9.78$ mm⁻¹. The crystal structure of mahnertite was solved and refined against data collected at the Daresbury Synchrotron Radiation Source, using a $20 \times 20 \times 2$ µm³ single crystal, $\lambda = 0.6898$ Å, $F(000) = 2150$, $R = 0.049$ for 639 reflections with $I > 2\sigma(I)$. The structure consists of sheets parallel to (001), which comprise two symmetrically independent distorted Cu 5-vertex square pyramids $\text{Cu}\phi_5$ ($\phi = \text{O}$, Cl or H₂O) as well as AsO₄ tetrahedra. Four Cu ϕ_5 pyramids located around the 4-fold axis share edges to form clusters linked by AsO₄ tetrahedra. The sheets are linked by the common apical vertex of the Cu(2) ϕ_5 polyhedra. As a result, a heterogeneous framework is formed. (Na,Ca) atoms, additional Cu(3) cations and H₂O molecules are located in the interlayers. The mineral is structurally related to zdenekite, NaPbCu₅(AsO₄)₄Cl·5H₂O.

Key-words: mahnertite, crystal structure, arsenate.

Introduction

The sodium copper arsenate mahnertite, ideally $(\text{Na,Ca})\text{Cu}_3[\text{AsO}_4]_2\text{Cl}\cdot 5\text{H}_2\text{O}$, was discovered in the Cap Garonne mine, Var, France (Sarp, 1996) and approved by the CNMMN of IMA before publication. The preliminary X-ray diffraction study of mahnertite (powder diagram and precession photos) (Sarp, 1996) revealed that the mineral is tetragonal with $a = 10.085$, $c = 23.836$ Å, space group $P4_22_12$, $Z = 8$. The results of the electron microprobe analysis led to the chemical formula $\text{Na}_{0.90}\text{K}_{0.05}\text{Ca}_{0.23}\text{Cu}_{2.79}(\text{AsO}_4)_{2.07}\text{Cl}_{0.81}\cdot 4.91\text{H}_2\text{O}$. Crystals of mahnertite are thin square plates, which form aggregates or spherules (0.2 mm in diameter). The crystal structure of mahnertite remained undetermined primarily because, due to the small size and plate-like shape of the crystals, data collection by conventional single crystal X-ray diffraction was not possible. However, the single crystal diffraction facility on the UK Synchrotron Radiation Source (SRS) at the Daresbury Laboratory is designed for measuring diffraction from small crystals (Wang, 2003). A study of the structural properties of mahnertite has therefore been carried out using synchrotron radiation and the results of this work are reported below.

Experimental

A single crystal with dimensions $20 \times 20 \times 2$ µm³ was used for the structure determination at room temperature. The small dimensions of the crystal were a result of the difficulty in separating out a single crystal from the aggregate of thin square plates which made up the sample from the Cap Garonne mine. The data were collected at $\lambda = 0.6898$ Å using a Bruker AXS SMART 1K CCD area detector diffractometer on station 9.8 of the SRS (Cernik *et al.*, 1997). The data were collected using a single 180° ω -rotation, corrected for absorption using the program SADABS (Sheldrick, 1997a) and processed (Clegg *et al.*, 1998) to yield refined tetragonal cell constants of $a = 10.037(1)$, $c = 23.739(1)$ Å, $V = 2391.5(4)$ Å³. The systematic absences indicated a I -centred cell. The details of the crystal data and of the data collection are summarised in Table 1.

SHELXTL (Sheldrick, 2000) and SHELX-97 (Sheldrick, 1997b) yielded solution by direct methods and refinement of the crystal structure by using 3947 reflections merged to 792 independent reflections (space group $I4/mmm$), of which 639 reflections have $I > 2\sigma(I)$ ($R_{\text{int}} = 0.052$). A first structure model was obtained in space

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Table 1. Crystal data, structure solution and refinement for mahnertite.

Chemical formula	(Na _{0.88} Ca _{0.12})Cu _{2.75} (AsO ₄) ₂ Cl _{0.62} ·3.63H ₂ O
Molecular weight	565.17
Temperature	293(2) K
Radiation and wavelength	synchrotron, 0.6898 Å
Crystal system, space group	tetragonal, <i>I4/mmm</i>
Unit cell dimensions	<i>a</i> = 10.037(1) Å <i>c</i> = 23.739(1) Å <i>V</i> = 2391.5(4) Å ³
Z	8
Density (calc.)	3.14 g/cm ³
Absorption coefficient μ	9.78 mm ⁻¹
<i>F</i> (000)	2150
Reflections for cell refinement	2083 (2 θ range 5.57 - 58.76°)
Crystal colour	dark green
Crystal size	0.02 × 0.02 × 0.002 mm ³
Data collection method	Bruker SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	2.14 to 29.38°
Index ranges	-13 ≤ <i>h</i> ≤ 9, -9 ≤ <i>k</i> ≤ 13, -22 ≤ <i>l</i> ≤ 21
Intensity decay	10%
Reflections collected	3947
Independent reflections	792 (<i>R</i> _{int} = 0.052)
Reflections with <i>I</i> > 2 σ (<i>I</i>)	639
Absorption correction	multi-scan
Max. and min. transmission	0.94 and 0.55
Structure solution	direct methods
Refinement method	full-matrix least-squares on <i>F</i> ²
Weighting parameters <i>a</i> , <i>b</i>	0.0822, 22.6201
Number of refined parameters	70
Final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> 1 = 0.049, <i>wR</i> 2 = 0.124
<i>R</i> indices (all data)	<i>R</i> 1 = 0.065, <i>wR</i> 2 = 0.136
Goodness-of-fit on <i>F</i> ²	1.079
Largest diff. peak and hole	2.99 and -1.51 e/Å ³

Table 2. Final positional and displacement parameters (Å²) for mahnertite.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
As	0.20754(5)	0.20754(5)	0.32286(5)	0.0143(4)
Cu(1)	0.5	0.2707(1)	0.28092(6)	0.0164(4)
Cu(2)	0.0	0.0	0.3783(1)	0.0201(7)
Cu(3)*	0.184(1)	0.184(1)	0.4556(8)	0.047(4)
Na _{0.88} Ca _{0.12}	0.5	0.0	0.3700(3)	0.025(1)
O(1)	0.3704(4)	0.1708(5)	0.3235(3)	0.023(1)
O(2)	0.1400(4)	0.1400(4)	0.2634(3)	0.015(2)
O(3)	0.1370(4)	0.1370(4)	0.3794(4)	0.022(2)
W(1)	0.340(2)	0.0	0.4443(7)	0.16(1)
W(2)*	0.5	0.31(1)	0.451(5)	0.17(5)**
W(3)*	0.5	0.23(1)	0.441(5)	0.15(4)**
W(4)*	0.626(8)	0.305(8)	0.449(3)	0.09(3)**
Cl(1)	0.5	0.5	0.3433(3)	0.026(1)
Cl(2)=Cl _{0.5} W _{0.5}	0.0	0.0	0.5	0.028(3)

* Occupancy coefficients for Cu(3) = 0.125, W(2) = W(3) = 0.25 and W(4) = 0.125 were fixed during the refinement
**Isotropic displacement parameters

The equivalent isotropic displacement parameters for cations, anions and W(1) water molecule were converted (Fischer & Tillmanns, 1988) from the anisotropic parameters ($U_{eq} = 1/3(U_{11} + U_{22} + U_{33})$).

group *I4*. The programme PLATON (Spek, 2003) was used to search for higher symmetry and, based on this, the space group *I4mm* was chosen. However, based on the close values of *R*_{int}, the centrosymmetric space group *I4/mmm*

Table 3. Selected interatomic distances (Å) for mahnertite.

As – O(1)	1.676(4) x 2	Cu(2) – O(3)	1.944(6) x 4
– O(2)	1.706(7)	av.	1.944
– O(3)	1.674(8)	– Cl(2)=Cl _{0.5} W _{0.5}	2.889(3)
av.	1.683		
O(2) – O(1)	2.734(7) x 2	Cu(3) – O(3)	1.93(2)
O(3) – O(1)	2.714(7) x 2	– W(4)	2.26(9)
O(1) – O(1)	2.833(9)	– W(1)	2.43(1) x 2
O(2) – O(3)	2.75(1)	– Cl(2)=Cl _{0.5} W _{0.5}	2.82(1)
av.	2.746		
Cu(1) – O(1)	1.928(5) x 2	(Na,Ca) – O(1)	2.420(6) x 4
– O(2)	1.971(4) x 2	– W(1)	2.39(2) x 2
av.	1.950	av.	2.41
– Cl(1)	2.737(4)		

was equally possible. The corresponding refinement in both space groups resulted in essentially the same preliminary values of R -factors (~ 0.09). In the refinement in the acentric space group the possibility of inversion twinning was taken into account by refining the batch scale factor: this parameter refined to a value of 50:50 indicating that either the structure is a 50:50 twin or a centre of symmetry has been omitted from the space group elements. The similar R -factors in the centric and acentric space groups as well as the more reasonable interatomic distances and atomic displacement parameters indicate that $I4/mmm$ is the true space group. Thus, the real symmetry of mahnertite revealed on the basis of three dimensional set of reflections became higher in respect to the space group $P4_22_12$ reported in its first description (Sarp, 1996). However, all systematic absences in the latter space group ($h00$: $h = 2n + 1$; $00l$: $l = 2n + 1$) were also observed in the three-dimensional set of reflections due to the I -centred cell. A small peak located in the difference Fourier map during the refinement was modelled as a partially occupied Cu(3) site, giving a final occupancy with sensible displacement parameter; with the assumption of occupancy on this site, the content of Cu in the cell (2.75 *apfu*) became close to that determined from electron microprobe analysis (2.79 *apfu*). The (Na,Ca) position was found in the difference Fourier map and was identified assuming the standard interatomic distances between these cations and O atoms. Its electron content confirmed the Na/Ca ratio found by electron microprobe analysis. Other residual electron density peaks were found and modelled as disordered water molecules. Three of the sites (W(2), W(3) and W(4)) are characterised by partial occupancies. The relatively high isotropic displacement parameters of these molecules as well as anisotropic displacement parameters and U_{eq} of the W(1) water molecule indicate that they are disordered over several sites, which are very close together. Since no new chemical information would be obtained by modelling this disorder, it was decided to leave them with relatively high U_{iso}/U_{eq} and without splitting.

The final difference Fourier map contained the following residual peaks: $\Delta\rho_{max} = +2.99 \text{ e}/\text{\AA}^3$, $\Delta\rho_{min} = -1.51 \text{ e}/\text{\AA}^3$. The atomic co-ordinates, displacement param-

eters and selected interatomic distances are given in Tables 2 and 3. Calculation of the sum of the bond strengths of the anions (Brese & O'Keeffe, 1991) allowed the assignment of O and H₂O to oxygen positions and indicated statistical replacement of Cl atoms by H₂O molecules in Cl(2) sites (Table 4). The largest deviations of the bond valence sums from being ideal were observed for Cl(1) and Cl(2) = (Cl,H₂O) which form the longest distances with Cu(1) and Cu(2), respectively. Due to the partial occupancies of the non-bonded water molecules, mahnertite can be considered as a mineral with some structural disorder and its general formula, mainly in accordance with electron microprobe analysis, is as follows: (Na_{0.88}Ca_{0.12})Cu_{2.75}[AsO₄]₂Cl_{0.62}·3.63H₂O ($Z = 8$). The density calculated on the basis of the structural formula, 3.14 g/cm³, essentially matches the experimental density of 3.32 g/cm³.

The intensity calculations (Yvon *et al.*, 1977) for mahnertite (Table 5) demonstrated a general agreement of the strongest reflections in the X-ray powder diffraction data despite some discrepancies between I_{obs} and I_{calc} . This difference can be attributed to a preferred orientation of the plate-like crystallites with the thickness of several micrometers. We can add that the observed values of intensity in the powder pattern were estimated visually. The figures were drawn using the program ATOMS3.2 (Dowty, 1995).

Discussion

The most specific feature of the mahnertite structure are sheets parallel to (001) (Fig. 1), which comprise two (Cu(1) and Cu(2)) symmetrically independent distorted Cu 5-vertex square pyramids (Cu ϕ_5), where ϕ is an unspecified ligand (O, Cl, H₂O) as well as AsO₄ tetrahedra. These sheets are identical to those recently found in monoclinic-pseudotetragonal zdenekite, NaPbCu₅(AsO₄)₄Cl·5H₂O (space group $P2_1/n$, $a = 10.023(7)$, $b = 19.55(1)$, $c = 10.023(6)$ Å, $\beta = 90.02(1)^\circ$; Zubkova *et al.*, 2003) and, consequently, the a_{tet} - and b_{tet} -parameters in both structures are almost the same. The bases of both inequivalent Cu pyramids are formed by four O atoms (average distance: 1.950 and 1.944 Å, respectively) whereas their

Table 4. Bond-valence calculations for mahnertite (the atoms with full occupancies are considered).

	As		Cu(1)		Cu(2)		(Na,Ca)	Σ	
O(1)	<i>1.28 x2</i>	1.28	<i>0.51 x2</i>	0.51			<i>0.20 x4</i>	0.20	1.99
O(2)	1.18		0.45 x2						2.08
O(3)	1.29				<i>0.49 x4</i>	0.49			1.78
W(1)							<i>0.22 x2</i>	0.22	0.22
Cl(1)			<i>0.14</i>	0.14 x4					0.56
Cl(2)=Cl _{0.5} W _{0.5}					<i>0.07</i>	0.07 x2			0.14
Σ	5.03		2.06		2.03		1.24		

Parameters taken from Brese & O'Keeffe (1991). Contribution to the balance of cations is in italics.

Table 5. X-ray powder diffraction data of mahnertite*.

<i>h k l</i>	<i>d_{calc}</i>	<i>d_{obs}</i>	<i>I_{calc}</i>	<i>I_{obs}</i>	<i>h k l</i>	<i>d_{calc}</i>	<i>d_{obs}</i>	<i>I_{calc}</i>	<i>I_{obs}</i>
0 0 2	11.870	11.90	100	100	424	2.099	2.110	1	5
1 0 1	9.245	9.29	7	60	501	2.000	2.009	1	5
1 1 0	7.097	7.132	5	50	0012	1.978	1.981	1	10
1 1 2	6.091	6.110	1	5	503	1.946		1	
2 0 0	5.019	5.046	4	60	2111	1.945}	1.953	1}	10
2 0 2	4.622	4.641	8	40	512	1.942		1	
1 0 5	4.292	4.307	3	15	435	1.849		1	
0 0 6	3.957	3.974	2	10		}	1.857	}	10
2 2 0	3.549	3.566	1	10	2012	1.840		1	
2 2 2	3.400	3.411	<1	<5	523	1.814	1.824	2	5
3 0 1	3.313	3.327	1	10	428	1.790	1.799	2	<5
1 0 7	3.213	3.232	2	5	440	1.774	1.783	2	10
2 0 6	3.107		4		442	1.755	1.765	1	5
3 0 3	3.082	3.098	10	80	525	1.735		1	
2 2 4	3.046	3.061	11	70	2212	1.728}	1.740	1}	10
0 0 8	2.967	2.982	2	<5	507	1.728		1	
3 2 1	2.765	2.780	5	35	600	1.673	1.682	1	10
1 1 8	2.738		1		2014	1.606		1	
3 0 5	2.735	2.749	4	20	509	1.597	1.606	2	10
2 2 6	2.642	2.652	8	35	536	1.578		1	
3 2 3	2.626	2.637	5	20	622	1.573	1.582	1	5
2 0 8	2.554	2.568	6	20	624	1.533	1.540	1	10
4 0 0	2.509	2.521	3	15	2214	1.530		1	
3 1 6	2.476		1		529	1.522	1.529	2	10
4 0 2	2.455	2.464	1	5		}			
3 2 5	2.401	2.411	4	15	4 1 3	2.327		<1	
3 3 0	2.366	2.383	1	<5	3 3 2	2.320	2.331	<1	<5
4 1 3	2.327		<1		2 1 9	2.274	2.284	4	20
3 3 2	2.320		<1		4 1 5	2.166		1	
2 1 9	2.274	2.284	4	20	327	2.152	2.169	1	10
4 1 5	2.166		1			}			
327	2.152	2.169	1	10					

* XRD pattern recorded with a Gandolfi camera (CuK α 1 radiation) (Sarp, 1996); *d_{calc}* and *I_{calc}* calculated using the program LAZY PULVERIX (Yvon et al., 1977)

apical fifth vertices accommodate Cl (Cl or H₂O in the Cl(2) site) at much longer distances (2.737, 2.889 Å). According to Effenberger (1988), the Cu^{[2+]₅} tetragonal

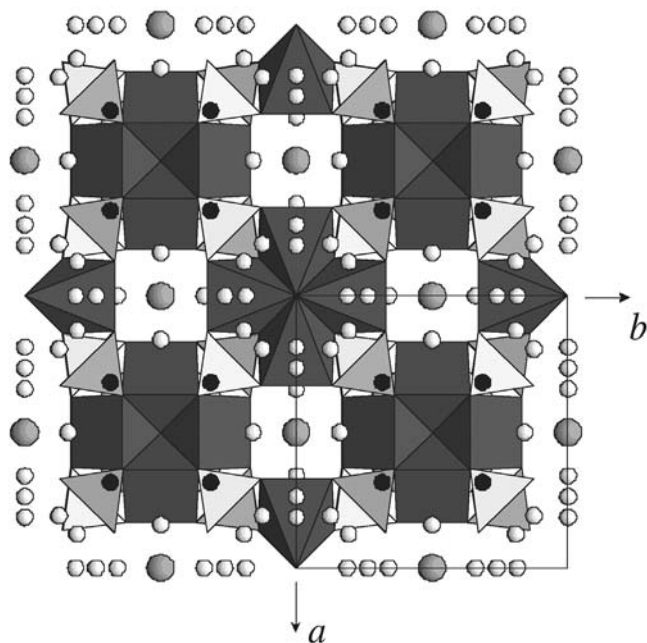


Fig. 1. The (001) sheets in the crystal structure of mahnertite. Cu-polyhedra for Cu(1) and Cu(2) cations and AsO_4 tetrahedra are shown in dark and light grey respectively. Cu(3) atoms are shown as small black circles. Water molecules and Na, Ca positions are shown as small and big grey circles respectively.

pyramids differ in the displacement of the copper atom with respect to the square base. This displacement can be characterized by the O–Cu–O angles formed by the O atoms located in the bases of the pyramids. In mahnertite these angles are close to 180° (175.6° and 178.5° for $\text{Cu}(1)\phi_5$ and $\text{Cu}(2)\phi_5$, respectively). This circumstance allows us to consider the copper atom in this pentahedron as being located approximately in the plane of the square base.

Four $\text{Cu}(1)\phi_5$ pyramids located around the 4-fold axes share edges to form clusters similar to those discovered in zdenekite (Zubkova *et al.*, 2003). Similar to mahnertite, in all $\text{Cu}\phi_5$ pentahedra of the zdenekite structure the Cu–Cl distance exceeds the Cu–O distances (the average Cu–O distance and the Cu–Cl distance for four $\text{Cu}\phi_5$ pentahedra are 1.96 and 2.76 Å, respectively).

In both structures the AsO_4 tetrahedra are linked to each cluster of four $\text{Cu}(1)\phi_5$ pentahedra (four tetrahedra below and four tetrahedra above). Each tetrahedron shares two vertices with two $\text{Cu}\phi_5$ pentahedra of one cluster and one vertex with a $\text{Cu}\phi_5$ pentahedron from the adjacent cluster. The fourth vertex of each AsO_4 tetrahedron (O(3)) in mahnertite is linked to the $\text{Cu}(2)\phi_5$ pentahedron, which does not belong to clusters. Like the $\text{Cu}(1)\phi_5$ pentahedra considered above, the latter copper polyhedron is also a pentahedron and represents a distorted tetragonal pyramid. However, the Cu(2) atom is co-ordinated (along with four oxygen atoms) either by Cl atoms or by the water molecule statistically distributed in Cl(2) sites and oriented toward the interlayer space. All the oxygen atoms in this tetragonal

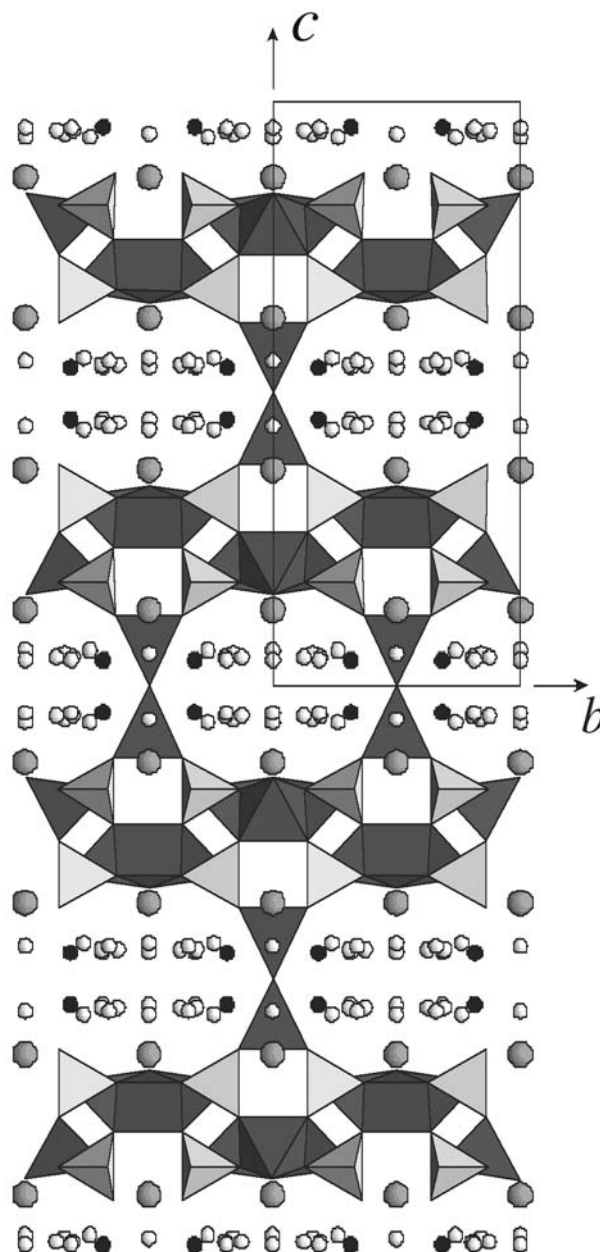


Fig. 2. The crystal structure of mahnertite: a general view along [100].

pyramid are located in its base and simultaneously serve as vertices of the AsO_4 tetrahedra.

Mirror planes m parallel to (001) pass through the apical Cl(2) atoms (partially substituted by H_2O molecules) of these pyramids providing linkage between the polyhedral sheets adjacent along [001] (Fig. 2). As a result a heterogeneous framework is formed. In common with zdenekite, there could be stacking faults of the sheets which are the main elements of the framework. This is consistent with the observed diffuse scattering parallel to the c -axis. All the Bragg reflections in reciprocal lattice lie on rods of weak diffuse intensity projecting along the c -axis. The Bragg peaks themselves are also slightly extended in this direction too. However, this is much less

marked than in the case of zdenekite, where the Bragg peaks extend in such a way that their tails run into each other, forming a continuous rod of intensity. Thus, both structures can contain different stacking variations of the identical adjacent sheets.

The large interlayer voids of the framework accommodate $(\text{Na,Ca})\text{O}_4\text{W}(1)_2$ slightly distorted trigonal prisms formed by 4 O(1) atoms and 2 water molecules, Cu(3) atoms and W(2-4) water molecules. Cu(3) is located in the compressed pseudotrigonal pyramid with one additional 5th vertex which accommodate $\text{Cl}(2) = (\text{Cl},\text{H}_2\text{O})$. The equatorial plane of this polyhedron is formed by H_2O molecules.

The strongest reflection 002 in the powder diffraction pattern (Table 5) confirms the orientation of polyhedral sheets in mahnertite. As a conclusion it can be emphasized that both mahnertite and zdenekite contain a new type of mixed polyhedral sheets which are characterized by a different mode of stacking. Another alternation of the similar modules and consequently another polytype may be found in chemically related mineral species.

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