The crystal structure of the new mineral wilhelmkleinite – ZnFe$_2^{3+}$(OH)$_2$(AsO$_4$)$_2$

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Abstract. The new mineral wilhelmkleinite has ideal chemical composition ZnFe$_2^{3+}$(OH)$_2$(AsO$_4$)$_2$ and crystallizes monoclinic, space group $P2_1/n$, $Z = 2$ with lattice parameters $a = 6.631(1)$ Å, $b = 7.611(1)$ Å, $c = 7.377(1)$ Å and $\beta = 91.80(1)°$. The structure was solved using direct methods. Refinement led to a final $R(F)$ value of 0.014 for 1092 symmetrically independant reflections $\geq 3\sigma(I)$.

The structure is characterized by chains of edge-linked [Fe(OH)$_2$O$_4$]$^{7-}$ octahedra which are connected via common (OH)$^-$ groups. The chains have composition [Fe(OH)O$_4$]$^{6-}$ and run parallel to [010]. Different chains are bridged by [AsO$_4$]$^{3-}$ tetrahedra in the directions of [100] and [001] and thus a three dimensional framework is formed. The Zn^{2+} ions are incorporated in cavities and are surrounded by six oxygen atoms in the form of a distorted octahedron.

Alternatively, one [ZnO$_4$(OH)$_2$] octahedron shares opposite faces with two [FeO$_4$(OH)$_2$] octahedra, to form a face sharing trimer trans-M$_3\Phi_{12}$ ($\Phi = O^{2-}, OH^-$) of composition [ZnFe$_2(OH)_4O_8$]. Different trimers are connected via the arsenate tetrahedra. The structure can be mapped onto a {3^6} net.

Distances and angles in wilhelmkleinite are in good agreement with values observed in comparable compounds. The face sharing of the octahedra leads to a pronounced shortening of the common edges.

Wilhelmkleinite is closely related to the orthorhombic modification of CuFe$_2$(OH)$_2$(AsO$_4$)$_2$. The framework of [FeO$_6$]$^{9-}$ octahedra and [AsO$_4$]$^{3-}$ tetrahedra are nearly identical in the two compounds. However, the Zn^{2+} (or Cu^{2+} ions respectively) are incorporated into different vacancies and this leads to a doubling of two of the axes of CuFe$_2$(OH)$_2$(AsO$_4$)$_2$ with respect to wilhelmkleinite.

Introduction

The new mineral wilhelmkleinite with ideal formula ZnFe$_2^{3+}$(AsO$_4$)$_2$(OH)$_2$ was found in the Tsumeb mine, Na-

mibia, accompanied by crystals of Al-rich scorodite, adamite and gerdtremmelite. For further information see [1]. The mineral was approved by the I. M. A. Commision on New Minerals and Mineral Names in 1998.

The chemical composition suggested close relationships to other hydroxyl arsenate-hydrate minerals like tsumcorite [2], mapimite [3], ojuélaïte [4] as well as to the hydroxyl phosphate minerals hentschelite [5] and lazulite [6] (see Table 1). Yet surprisingly neither the powder patterns nor the lattice parameters of these compounds showed similarities to wilhelmkleinite. On the other hand the synthetic compound CuFe$_2$(OH)$_2$(AsO$_4$)$_2$ – of which an orthorhombic and a triclinic modification are known [7, 8] – seemed to be related. In particular, the powder pattern of the orthorhombic modification appeared similar to that of wilhelmkleinite.

We considered it prudent to carry out a complete structural analysis to gain more insight about the relationship of wilhelmkleinite with the above mentioned minerals and compounds.

Experimental details and structure refinement

Details concerning the crystal data, measurement of intensities and structure refinement are given in Table 2. The structure solution by direct methods yielded the positions of the Zn, Fe, As and oxygen atoms. After refinement of the coordinates and the displacement parameters, a difference Fourier synthesis showed the position of the hydrogen atom. The positional and atomic displacement parameters of the hydrogen atom were not refined. Final atomic coordinates and equivalent atomic displacement parameters are given in Table 3[I].

Table 1. Lattice parameters and chemical composition of related compounds.

Wilhelmkleinite $ZnFe_2^{3+}(AsO_4)_2(OH)_2$	$a - 6.631(1)$ Å	$b = 7.611(1)$ Å $\beta = 91.80(2)°$	$c = 7.377(1)$ Å	$V = 372.12(9)$ Å^3	$P2_1/n$	this work
Mapimite $Zn_2Fe_3^{3-}(AsO_4)_3(OH)_4 \cdot 10\ H_2O$	$a = 11.415(5)$ Å	$b = 11.259(5)$Å $\beta = 107.74(4)°$	$c = 8.661(3)$ Å	$V = 1060$ Å^3	Cm	[3]
Ojuélaïte $ZnFe_2^{3+}(AsO_4)_2(OH)_2 \cdot 4\ H_2O$	$a = 10.247(6)$ Å	$b = 9.665(5)$ Å $\beta = 94.22°$	$c = 5.569(4)$ Å	$V = 549.7$ Å^3	$P2_1/c$	[4]
Tsumcorite $Pb(Zn, Fe^{3+}, Fe^{2+})_2(AsO_4)_2(OH)_2(H_2O)_2$	$a = 9.124(3)$ Å	$b = 6.329(2)$ Å $\beta - 115.17(2)°$	$c = 7.577(2)$ Å	$V = 395.5(4)$ Å^3	$C2/m$	[2]
Hentschelite $CuFe_2^{3+}(PO_4)_2(OH)_2$	$a = 6.984(3)$ Å	$b = 7.786(3)$ Å $\beta = 117.68(2)°$	$c - 7.266(3)$ Å	$V = 349.9(5)$ Å^3	$P2_1/n$	[5]
Lazulite $(Mg, Fe)Al_2(PO_4)_2(OH)_2$	$a = 7.144(1)$ Å	$b = 7.278(1)$ Å $\beta = 120.50(1)°$	$c = 7.228(1)$ Å	$V = 323.8$ Å^3	$P2_1/c$	[6]
Beraunite $Fe^{2+}Fe_5^{3-}(PO_4)_4(OH)_5(H_2O)_4 \cdot 2\ H_2O$	$a = 20.953(5)$ Å	$b = 5.171(1)$ Å $\beta = 93.34(2)°$	$c = 19.266(4)$ Å	$V = 2083.9$ Å^3	$C2/c$	[9]
orthorhombic $CuFe_2^{3+}(AsO_4)_2(OH)_2$	$a = 7.717(3)$ Å	$b = 13.225(5)$ Å	$c = 14.549(5)$ Å	$V = 1484.8$ Å^3	$Pbca$	[7]
triclinic $CuFe_2^{3+}(AsO_4)_2(OH)_2$	$a = 5.094(2)$ Å $\alpha = 102.52(2)°$	$b = 5.273(2)$ Å $\beta = 104.45(2)°$	$c = 7.572(3)$ Å $\gamma = 102.07(2)°$	$V - 184.7$ Å^3	$P\bar{1}$	[8]

Table 2. Experimental conditions and structure refinement.

Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	6.631(1)
b [Å]	7.611(1)
c [Å]	7.377(1)
β [°]	91.80(2)
Lattice parameters from	25 reflections
in θ range	$8.7° \leq \theta \leq 15.3°$
V [Å^3]	372.12(9)
μ [mm^{-1}]	8.34
Diffractometer	CAD-4
Wavelength [Å]	0.71073
Scan	$\omega - 2\theta$
Scan angle	$0.7 + 0.15 \sin\theta$
θ range	$3° < \theta < 25°$
$hkl_{min} \quad hkl_{max}$	9. $\overline{11}$. $\overline{11}$ — 0. 11. 11
2 standard reflections	every 120 min
Absorption correction	experimental
with program	MOLEN [14]
$T_{min} \cdot T_{max}$	76.7, 99.9
Measured reflections	2844
Observed reflections $\geq 3\sigma$	2359
Independent reflections	1092
$R(F^2)_{int}$	0.024
Structure solution	Sir92 [15]
Structure refinement	Shelxl93 [16]
$R(F)$	0.014
$wR(F^2)$	0.039
Number of variable parameters	71
Extinction correction	Shelxl93 [16]
Extinction coefficient	0.0237(9)
Difference density maximum	0.516
Difference density minimum	−0.590
Weighting scheme	$w = 1/[\sigma^2(F_{obs})^2 + (0.017 \cdot P)^2]$
with	$P = (Max\ (F_{obs}^2) + 2F_{calc}^2)/3$

Table 3. Positional and equivalent atomic displacement parameters [Å]^2 for the atoms with e.s.d.'s in parentheses.

Atom	x	y	z	U_{eq}
Zn	0	0	$^1/_2$	0.01115(7)
Fe	0.22856(3)	0.36444(3)	0.26271(3)	0.00717(7)
As	0.24265(2)	0.623976(19)	0.633213(19)	0.00579(6)
O1	0.2220(2)	0.44359(16)	0.50673(16)	0.0123(2)
O2	0.06002(18)	0.63490(16)	0.78564(16)	0.0097(2)
O3	0.46181(17)	0.61580(16)	0.75421(15)	0.0104(2)
O4	0.23482(18)	0.80790(16)	0.50638(15)	0.0097(2)
O5	0.24552(18)	0.11675(15)	0.35613(15)	0.0087(2)
H	0.336	0.118	0.422	0.050

with an Fe-O-Fe angle of $135.4(2)°$ (see Fig. 1). The resulting composition of the chain is $[Fe^{3+}(OH)(O_A)_4]^{6-}$. Different chains are bridged by $[AsO_4]^3$ tetrahedra in the directions of [100] and [001] and a three dimensional network is formed (see Fig. 1).

Description of the structure

The structure of wilhelmkleinite is characterized by chains of edge linked octahedra of composition $[Fe^{3+}(OH)_2(O_A)_4]^{7-}$ (with O_A designating oxygen atoms which form part of the $[AsO_4]^{3-}$ tetrahedra). The octahedra are corner connected via common (OH)$^-$ groups and form chains parallel to [010]
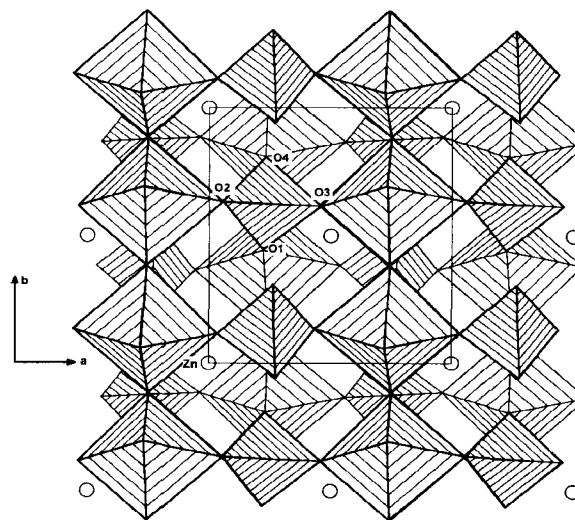

Fig. 1. $a - b$-Projection of the crystal structure of wilhelmkleinite; octahedra and tetrahedra around Fe and As are shown; Zn^{2+} ions are shown as circles; H atoms are not shown for reasons of clearness. Drawn with STRUPLO84 [19].

Fig. 2. $a - c$-Projection of the crystal structure of wilhelmkleinite: octahedra and tetrahedra around Zn. Fe and As are shown; Zn^{2+} ions are shown as circles; H atoms are not shown for reasons of clearness. Drawn with STRUPLO84 [19].
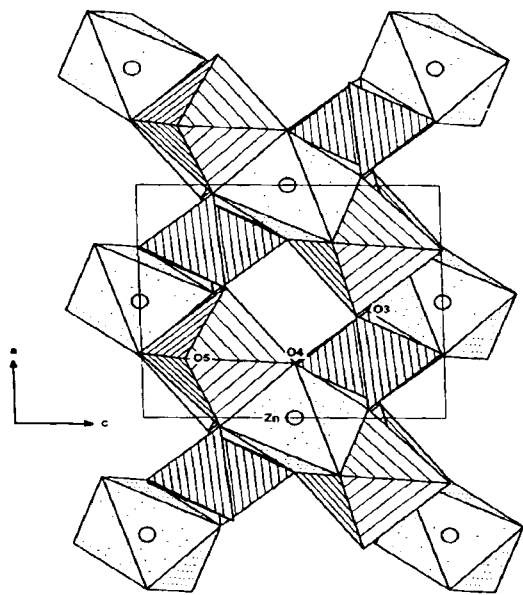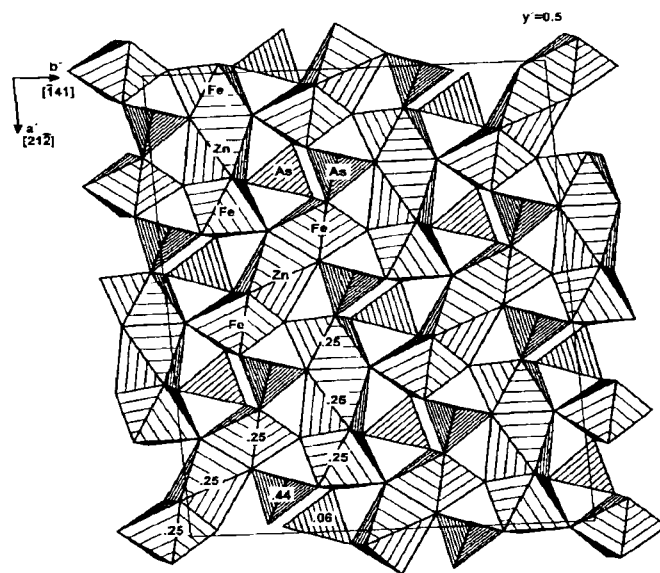

Fig. 3. Partial $a' - b'$-projection of wilhelmkleinite $(-0.1 \leq y' \leq 0.6;$ $-0.11 \leq z' \leq 0.61)$. Matrix for transformation with respect to lattice parameters given in Table 2 is $[21\bar{2} \mid \bar{1}41 \mid 101]$. Octahedra around Zn and Fe and tetrahedra around As are shown. H atoms are not drawn for reasons of clearness. Drawn with STRUPLO84 [19].

In the projection along [010] (see Fig. 2) the structure can be described as consisting of slices arranged at heights $z = \pm \frac{1}{4}$. For the Fe, As and part of the oxygen atoms the pseudotranslation vector $a/2 + b/4$ can be used to describe the displacement of neighbouring slices. Between adjacent slices cavities are formed in which the Zn^{2+} ions at height $z = 0$ and $z = \frac{1}{2}$ are incorporated. Only every second cavity is occupied. These Zn^{2+} ions are coordinated by six oxygen atoms in the form of a distorted octahedron of composition $[Zn(OH)_2(O_A)_4]^{8-}$.

In addition, a hydrogen atom is located at a distance of 0.76 Å from O5 and 2.25 Å from O2. A hydrogen bond is formed in which O5 is the donor atom and O2 the receptor (distance O5–O2: 2.891(2) Å; angle O5–H–O2: 145.6(2)°).

However, the most conspicuous building units in wilhelmkleinite are triple octahedra, each one containing a $[ZnO_4(OH)_2]^{8-}$ octahedron which shares opposite faces with two $[FeO_4(OH)_2]^{7-}$ octahedra. In this way a trimer $trans$-$[M_3\Phi_{12}]^{12-}$ ($\Phi = O^{2-}, OH^-$) of composition $[ZnFe_2(OH)_4O_8]^{12-}$ is formed.

These trimers can be best observed after carrying out a transformation of wilhelmkleinite according to $a' = 2a + 1b - 2c = 21.535$ Å; $b' = -a + 4b + c = 32.067$ Å; $c' = a + c = 9.763$ Å; $\alpha' = 88.05°$; $\beta' = 95.42°$; $\gamma' = 87.37°$ (Matrix $A' = [21\bar{2}/\bar{1}41/101]$, $|A'| = 18$). The resulting cell is centered at eighteen points: $(0, 0, 0)$, $(^7/_9,$ $^1/_{18}, ^1/_2)$, $(^5/_9, ^1/_9, 0)$, $(^1/_3, ^1/_6, ^1/_2)$, $(^1/_9, ^2/_9, 0)$, $(^8/_9,$ $^5/_{18}, ^1/_2)$, $(^2/_3, ^1/_3, 0)$, $(^4/_9, ^7/_{18}, ^1/_2)$, $(^2/_9, ^4/_9, 0)$, $(0, ^1/_2,$ $^1/_2)$, $(^7/_9, ^5/_9, 0)$, $(^5/_9, ^{11}/_{18}, ^1/_2)$, $(^1/_3, ^2/_3, 0)$, $(^1/_9, ^{13}/_{18},$ $^1/_2)$, $(^8/_9, ^7/_9, 0)$, $(^2/_3, ^5/_6, ^1/_2)$, $(^4/_9, ^8/_9, 0)$ and $(^2/_9, ^{17}/_{18},$ $^1/_2)$.

Fig. 3 is a partial projection $(-0.1 \leq y \leq 0.6;$ $-0.11 \leq z \leq 0.61)$ along the new c' axis. Here the trimers of octahedra are arranged within the plane with the centering cations at heights $z = \frac{1}{4}$. Different trimers are con-

nected via the $[AsO_4]^3$ tetrahedra with the centering atoms at heights $z = 0.06$ and $z = 0.44$. Fig. 4 is a schematic representation seen along the new a' axis. Here
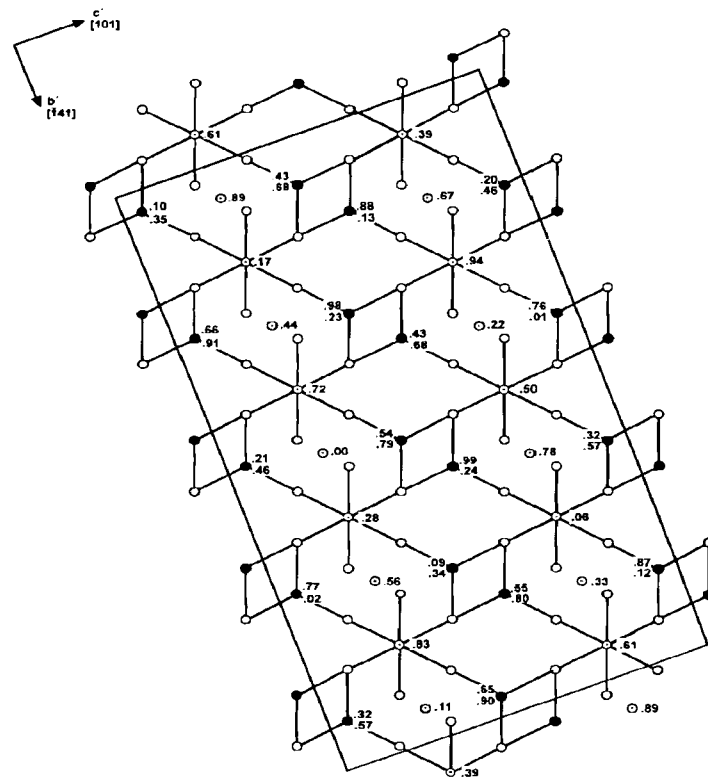

Fig. 4. Schematic representation of the structure of wilhelmkleinite as a mapping onto a $\{3^6\}$ net. Matrix for transformation with respect to lattice parameters given in Table 2 is $[21\bar{2} \mid \bar{1}41 \mid 101]$. Zn and Fe trimeric ions are shown as circles with a dot, oxygen is represented by open circles and As as filled circles, bonds are represented as solid lines. Heights of Zn and As are given as fractional coordinates.

Table 4. Distances and angles for the $[AsO_4]^{3-}$ tetrahedra with e.s.d.'s in parentheses.

		[A]			[A]				[°]
As	O1	1.663(1)	O2	O3	2.686(2)	O2	As	O3	105.99(6)
	O2	1.680(1)	O1	O3	2.720(2)	O1	As	O3	108.76(6)
	O3	1.683(1)	O2	O4	2.733(2)	O2	As	O4	108.69(6)
	O4	1.684(1)	O3	O4	2.752(2)	O3	As	O4	109.67(6)
		1.678	O1	O2	2.765(2)	O1	As	O2	111.58(6)
			O1	O4	2.774(2)	O1	As	O4	111.96(6)
					2.738				109.44

Table 5. Distances and angles in the FeO_6 octahedra with e.s.d.'s in parentheses; $\Phi = O^{2-}$, OH^-; bond lengths, edge lengths and angles involving atoms common to ZnO_6 and FeO_6 are marked with an asterisk.

Φ		[A]	Φ	Φ	[A]
Fe	−O1	1.900(1)	O4^{vi}−Fe−O5^{viii}		77.09(6)*
	−O2^{vi}	1.936(1)	O4^{vi}−Fe−O3^{vii}		78.98(6)*
	−O5	2.009(1)	O3^{vii}−Fe−O5^{viii}		79.37(6)*
	−O4^{vi}	2.053(1)*	O1 −Fe−O5		88.59(6)
	−O3^{vii}	2.066(1)*	O2^{iv}−Fe−O4^{vi}		88.21(6)
	−O5^{viii}	2.120(1)*	O1 −Fe−O2^{iv}		96.99(6)
		2.014	O2^{iv}−Fe−O5^{viii}		90.81(6)
O4^{vi}−O5^{viii}		2.601(1)*	O1 −Fe−O3^{vii}		94.96(6)
O4^{vi}−O3^{vii}		2.620(1)*	O2^{iv}−Fe−O5		96.31(6)
O3^{vii}−O5^{viii}		2.674(1)*	O5 −Fe−O3^{vii}		92.52(6)
O1 −O5		2.731(1)	O1 −Fe−O5^{viii}		96.25(6)
O2^{iv}−O4^{vi}		2.777(1)	O5 −Fe−O4^{vi}		97.35(6)
O1 −O2^{iv}		2.872(1)			89.79
O2^{iv}−O5^{viii}		2.891(1)			
O1 −O3^{vii}		2.925(1)			
O2^{iv}−O5		2.939(1)			
O5 −O3^{vii}		2.945(1)			
O1 −O5^{viii}		2.997(1)			
O5 −O4^{vi}		3.051(1)			
		2.835			

Symmetry operators for generating equivalent atoms
(i) $−x + \tfrac{1}{2}$, $y − \tfrac{1}{2}$, $−z + \tfrac{3}{2}$; (ii) $x − \tfrac{1}{2}$, $−y + \tfrac{1}{2}$, $z − \tfrac{1}{2}$;
(iii) x, $y − 1$, z; (iv) $−x$, $−y + 1$, $−z + 1$; (v) $−x$, $−y$, $−z + 1$;
(vi) $−x + \tfrac{1}{2}$, $y − \tfrac{1}{2}$, $−z + \tfrac{1}{2}$; (vii) $−x + 1$, $−y + 1$, $−z + 1$;
(viii) $−x + \tfrac{1}{2}$, $y + \tfrac{1}{2}$, $−z + \tfrac{1}{2}$

bonds between cations and anions are drawn and the centering of the cell can be easily observed. It is remarkable that in this view the structure can be mapped onto a regular $\{3^6\}$ net.

Results and discussion

Within the tetrahedra, the As—O distances range from 1.663(1) Å to 1.684(1) Å, the O—O edges from 2.686(2) Å to 2.774(2) Å (see Table 4) and the angles from 105.99(6)–111.96(6)°. The bond length distortion parameter[2] of the [AsO$_4$] groups is 0.42% and is of similar magnitude as the corresponding parameters in e.g. orthorhombic $CuFe_2(OH)_2(AsO_4)_2$ (0.37% and 0.64%; [7]). The bond angle variances are on the other hand smaller in wilhelmkleinite than in $CuFe_2(OH)_2(AsO_4)_2$ (wilhelmkleinite: 4.46%; $CuFe_2(OH)_2(AsO_4)_2$: 6.05% and 6.90%).

The Fe^{3+}—O distances (Table 5) are comparable with distances in other compounds (Table 6) and are a clear indication that no Zn-ions are incorporated within the octahedra since this would immediately lead to an increase of the bond lengths.

The average Zn—O distance in wilhelmkleinite is 2.107 Å. The largest Zn—O distance in the ZnO_6-octahedra is to the $(OH)^-$ ions (2.162 Å) while the distances to the four oxygen atoms which are further connected to the arsenate group are 2.035 Å and 2.135 Å (Table 7). The distances in the ZnO_6-octahedra are in good agreement with distances observed in other compounds for such coordination polyhedron. In mapimite [3] for example the average distances for the Zn—O octahedra are 2.075 Å and 2.117 Å with single distances ranging from 1.968(8) Å to 2.237(6) Å.

The *trans*-$M_3\Phi_{12}$ trimers as building units were also observed in orthorhombic $CuFe_2(OH)_2(AsO_4)_2$ and are found in many other structures (e.g. hentschelite [5], beraunite [9], lazulite and isostructural minerals [6, 10]; see also [11]). In all these compounds the shared faces lead to

Table 6. Fe—O bond lengths in [Å] in wilhelmkleinite and comparable compounds.

	Min.	Max.	Mean	Lit.
Wilhelmkleinite	1.900(1)	2.120(1)	2.014	this work
Mapimite	1.928(7)	2.128(7)	2.013	[3]
	1.943(4)	2.107(5)	2.012	[3]
Hentschelite	1.926(2)	2.158(2)	2.010	[5]
Beraunite	1.931(4)	2.133(4)	2.011	[9]
	1.938(4)	2.134(4)	2.023	[9]
$CuFe_2(OH)_2(AsO_4)_2$ (orthorh.)	1.924(3)	2.180(3)	2.018	[7]
$CuFe_2(OH)_2(AsO_4)_2$ (tricl.)	1.916(2)	2.152(2)	2.016	[8]
Mawbyite $(PbFe_2(OH)_2(AsO_4)_2)$	1.993(9)	2.114(10)	2.045	[17]
Tsumcorite (Fe, Zn at one position)	2.019(6)	2.131(6)	2.065	[2]

Table 7. Distances and angles in the ZnO_6 octahedra with e.s.d.'s in parentheses; $\Phi = O^{2-}$, OH^-; Φ — Φ edges common with FeO_6 octahedra and angles involving atoms common to ZnO_6 and FeO_6 are marked with an asterisk.

Φ	[A]	Φ	Φ	[A]			[°]
Zn−O3	2.025(1)	O4−O5		2.601(2)*	O4−Zn−O5		74.50(6)*
−O4	2.135(1)	O3−O4		2.620(2)*	O3−Zn−O4		78.02(6)*
−O5	2.162(1)	O3−O5		2.674(2)*	O3−Zn−O5		79.30(6)*
	2.407	O3−O5		3.225(2)	O3−Zn−O5		100.70(6)
		O3−O4		3.233(2)	O3−Zn−O4		101.98(6)
		O4−O5		3.421(2)	O4−Zn−O5		105.50(6)
				2.962			90.0

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[2] The bond length distortion parameter of a [TO$_4$] group is defined as

$$BLD = \frac{100}{4} \sum_{i=1}^{4} \left[\frac{|(T-X)_i - (T-X)_{average}|}{(T-X)_{average}} \right] \% \; ;$$

the angular distortion is defined as

$$AD = \sum_{i=1}^{4} \frac{a_j}{4} \times 100\%; \text{ with } a_j = \sum_{i=1}^{3} \frac{|\alpha_i - \alpha_{ideal}|}{\alpha_{ideal}} \times 100\% \; [18].$$

	Wilhelmkleinite $ZnFe_2(OH)_2(AsO_4)_2$	Orthorhombic $CuFe_2(OH)_4(AsO_4)_2$	Hentschelite $CuFe_2(OH)_2(PO_4)_2$
Common edges	2.601(2)–2.674(2)	2.577(5)–2.638(5)	2.596(2)–2.676(2)
Other edges (Fe)	2.731(1)–3.051(1)	2.702(5)–3.095(5)	2.769(2)–3.034(2)
Other edges (Cu/Zn)	3.225(2)–3.421(2)	3.010(5)–3.587(5)	2.976(2)–3.547(2)

Table 8. $\Phi - \Phi$ lengths in [Å] in octahedra of wilhelmkleinite and comparable compounds; $\Phi = O^{2-}$, OH^-.

Table 9. Bond-valence sums in [v.u.] calculated using parameters by Brese and O'Keeffe [12]; $\sum c_i'$: sum of the bond valences reaching the anion; $\sum c_i'$: sum of the bond valences reaching the anion after introduction of the hydrogen bond contribution [13].

	$\sum c_i$		$\sum c_i$	$\sum c_i'$
Zn	2.04	O1	2.01	
Fe	3.08	O2	1.89	2.01
As	5.10	O3	2.11	
		O4	2.02	
		O5	1.18	1.05

a significant shortening of the corresponding common edges of the octahedra with respect to the unshared ones (see Table 8 for examples).

Results of bond valence calculations which were corrected for the hydrogen bond distribution [12, 13] are given in Table 9. They lead to nearly ideal values for the
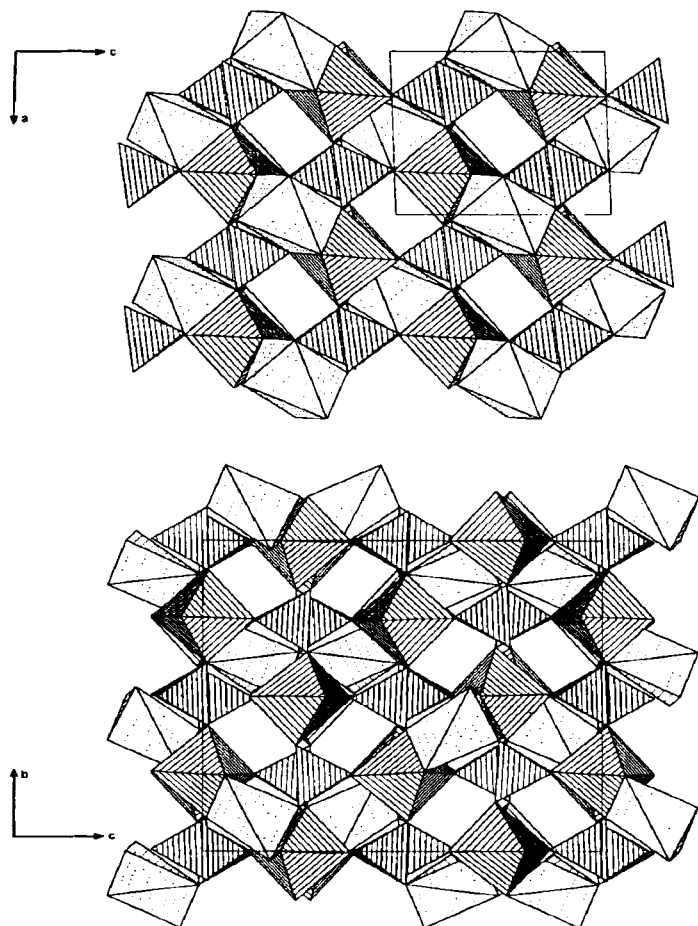
bond-valence sums of the cations and differentiate clearly between the O^{2-} ions and the oxygen atom O5 which forms part of the hydroxyl group.

The structure is very closely related to the orthorhombic modification of $CuFe_2(OH)_2(AsO_4)_2$ (Table 1, [7]). The cell of wilhelmkleinite corresponds to a theoretical cell of orthorhombic $CuFe_2(OH)_2(AsO_4)_2$ which results when one does not take into account the Cu and H atoms. The relation of lattice parameters between the two compounds is $a_{WIL} \simeq b_{OCF}/2$; $b_{WIL} \simeq a_{OCF}$; $c_{WIL} \simeq c_{OCF}/2$. The differences between wilhelmkleinite and orthorhombic $CuFe_2(OH)_2(AsO_4)_2$ are best seen when looking at Fig. 5. The framework of $[Fe(OH)_2(O_A)_4]^{7-}$ octahedra and arsenate tetrahedra is nearly identical in the two structures. Yet the Zn^{2+} (or Cu^{2+} ions respectively) are incorporated into different vacancies and this leads to a doubling of two of the axes of $CuFe_2(OH)_2(AsO_4)_2$ with respect to wilhelmkleinite.

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Fig. 5. $a - c$-Projection of the crystal structure of wilhelmkleinite and b–c projection of the structure of orthorhombic $CuFe_2(OH)_2(AsO_4)_2$. Octahedra and tetrahedra around Zn (Cu). Fe and As are shown. Drawn with STRUPLO84 [19].

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