

Space group (215) *P-43m*215
cP5

Fe_4C	<i>cP5</i>	(215) <i>P-43m</i> – ea
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Fe₄C [1]

Structural features: Close-packed Fe layers in c stacking, C in tetrahedral voids.

Pinsker Z.G., Kaverin S.V. (1956) [1]

 CFe_4 $a = 0.3878 \text{ nm}$, $V = 0.0583 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	4 <i>e</i>	.3 <i>m</i>	0.265	0.265	0.265		single atom C
C2	1 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron Fe ₄

Experimental: thin film, electron diffraction, $R = 0.280$ Remarks: A similar structure proposal for SnI_4 [2] is superseded; the correct space group, (205) *Pa-3*, was proposed in [3].

References: [1] Pinsker Z.G., Kaverin S.V. (1956), Sov. Phys. Crystallogr. (Engl. Transl.) 1, 48-53. [2] Ott H. (1926), Z. Kristallogr. 63, 222-230. [3] Dickinson R.G. (1923), J. Am. Chem. Soc. 45, 958-962.

215
cP6

$[\text{NH}_4]\text{Br}$	<i>cP6</i>	(215) <i>P-43m</i> – eba
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NH₄Br form IV [1]Structural features: NH_4 tetrahedra and Br atoms in a CsCl-type arrangement.

Levy H.A., Peterson S.W. (1953) [1]

 BrD_4N $a = 0.401 \text{ nm}$, $V = 0.0645 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	4 <i>e</i>	.3 <i>m</i>	0.148	0.148	0.148		single atom N
Br2	1 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron D ₄
N3	1 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron D ₄

Experimental: powder, diffractometer, neutrons, $T = 78 \text{ K}$ Remarks: Deuterized phase is stable at $T < 169 \text{ K}$. Correct symmetry is space group is (221) *Pm-3m* if the H positions are ignored.

References: [1] Levy H.A., Peterson S.W. (1953), J. Am. Chem. Soc. 75, 1536-1542.

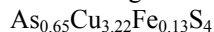
215
cP8

Cu_3AsS_4	<i>cP8</i>	(215) <i>P-43m</i> – eca
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Cu₃AsS₄ lazarevicite [1], lazarevicite

Structural features: Close-packed S layers in c stacking, Cu and As in tetrahedral voids. Substitution derivative of ZnS (sphalerite).

Schwendinger R.B., Mortensen J.L. (1960) [1]



$$a = 0.528 \text{ nm}, V = 0.1472 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	4e	.3m	0.25	0.25	0.25		tetrahedron AsCu ₃
Cu2	3c	-42.m	0	1/2	1/2		tetrahedron S ₄
M3	1a	-43m	0	0	0		tetrahedron S ₄

$$\text{M3} = 0.65\text{As} + 0.22\text{Cu} + 0.13\text{Fe}$$

Experimental: powder, film, X-rays

Remarks: Natural specimen from the Tilva Mika copper deposit at Bor, eastern Serbia. Composition Cu₃(As_{0.65}Cu_{0.20}Fe_{0.13})S₄ from electron microprobe analysis, trace amounts of V detected by spectroscopy. Idealized coordinates.

References: [1] Schwendinger R.B., Mortensen J.L. (1960), Geol. Soc. Am. Bull. 71, 1970.

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cP8

Cu ₃ VS ₄	cP8	(215) <i>P</i> -43m – eda
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Cu₃VS₄ [2], sylvanite, Strukturbericht notation H2₄; Cu₃TaSSe₃ [4]; "Cu₃SbS₄" (see remark)

Structural features: Distorted close-packed S layers in c stacking; V and Cu in tetrahedral voids. Single VS₄ tetrahedra share the six edges with surrounding CuS₄ tetrahedra. See Fig. II.23.

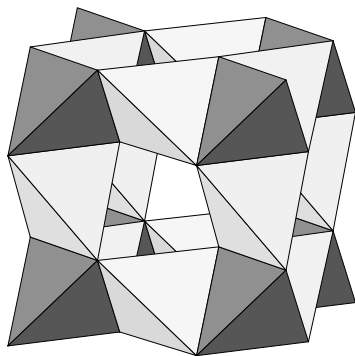


Fig. II.23. **Cu₃VS₄**

Arrangement of CuS₄ (light) and VS₄ (dark) tetrahedra.

Mujica C. et al. (1998) [1]



$$a = 0.5393 \text{ nm}, V = 0.1569 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	4e	.3m	0.2376	0.2376	0.2376		4-vertex polyhedron VCu ₃
Cu2	3d	-42.m	1/2	0	0		octahedron S ₄ V ₂
V3	1a	-43m	0	0	0		fourcapped trigonal prism S ₄ Cu ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.028, T = 293 K

Remarks: A structure proposal in space group (225) *Fm*-3*m* with an 8-fold unit cell [5] is superseded (see [6]); the same is valid for a similar structure proposal for Cu₃SbS₄ [7] (famatinite type). A structure proposal for tetrahedrite with the type described here [8] (Cu₃SbS₄) is also superseded (see [3]). The

description in space group (219) $F-43c$ with an 8-fold unit cell in [8] does not take into consideration all symmetry elements of the proposed model (see [9]).

References: [1] Mujica C., Carvajal G., Llanos J., Wittke O. (1998), Z. Kristallogr., New Cryst. Struct. 213, 12. [2] Pauling L., Hultgren R. (1933), Z. Kristallogr. 84, 204-212. [3] Makovicky E., Skinner B.J. (1979), Can. Mineral. 17, 619-634. [4] Müller A., Sievert W. (1974), Z. Anorg. Allg. Chem. 406, 80-91. [5] De Jong W.F. (1928), Z. Kristallogr. 68, 522-530. [6] Trojer F.J. (1966), Am. Mineral. 51, 890-894. [7] Alieva A.G., Pinsker Z.G. (1961), Sov. Phys. Crystallogr. (Engl. Transl.) 6, 161-164. [8] (1931), Strukturberichte 1, 335. [9] (1931), Strukturberichte 1, 335.

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cP9

$K_3[SO_4]F$	<i>cP9</i>	(215) $P-43m - ecba$
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K_3SO_4F **a** [1]

Structural features: SO_4 tetrahedra, F and K atoms in a $CaTiO_3$ -type arrangement.

Skakle J.M.S. et al. (1996) [1]

FK_3O_4S

$a = 0.5433 \text{ nm}$, $V = 0.1604 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4e	.3m	0.18	0.18	0.18		single atom S
K2	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_4F_2
F3	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		fourcapped trigonal prism K_6O_4
S4	1a	-43m	0	0	0		tetrahedron O_4

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, T = 873 K

Remarks: Phase stable at T > 858 K. A partly disordered model in space group (221) $Pm-3m$ with SO_4 units in two orientations could not be rejected.

References: [1] Skakle J.M.S., Fletcher J.G., West A.R. (1996), J. Chem. Soc., Dalton Trans. 1996, 2497-2501.

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cP10

$Zn[CN]_2$	<i>cP10</i>	(215) $P-43m - e^2ba$
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$Zn(CN)_2$ [2]

Structural features: ZnC_4 and ZnN_4 tetrahedra are interconnected via CN bonds (cyanide units) to form two interpenetrating frameworks. See Fig. II.24.

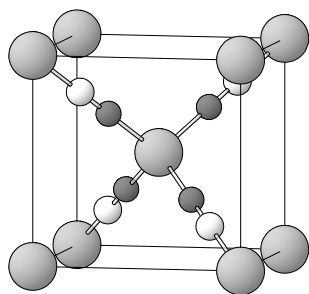
Hoskins B.F., Robson R. (1990) [1]

C_2N_2Zn

$a = 0.59002 \text{ nm}$, $V = 0.2054 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	4e	.3m	0.1882	0.1882	0.1882		single atom N
N2	4e	.3m	0.3007	0.3007	0.3007		single atom C
Zn3	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron N_4
Zn4	1a	-43m	0	0	0		tetrahedron C_4

Experimental: single crystal, diffractometer, X-rays, R = 0.028, T = 295 K

Fig. II.24. $\text{Zn}(\text{CN})_2$

Arrangement of Zn (large), C (light) and N (dark) atoms.

References: [1] Hoskins B.F., Robson R. (1990), J. Am. Chem. Soc. 112, 1546-1554. [2] Zhdanov G.S. (1941), Dokl. Akad. Nauk SSSR 31, 352-354.

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cP10

$\text{AgB}[\text{CN}]_4$	<i>cP10</i>	(215) $P\text{-}43m - e^2ba$
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Ag[B(CN)₄] [1]

Structural features: BC_4 and AgN_4 tetrahedra are interconnected via CN bonds (cyanide units) to form two interpenetrating frameworks.

Bernhardt E. et al. (2000) [1]

AgBC_4N_4

$a = 0.5732 \text{ nm}$, $V = 0.1883 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	4e	$.3m$	0.16	0.16	0.16		single atom N
N2	4e	$.3m$	0.2739	0.2739	0.2739		single atom C
Ag3	1b	$-43m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron N_4
B4	1a	$-43m$	0	0	0		tetrahedron C_4

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.008$, $T = 150 \text{ K}$

References: [1] Bernhardt E., Henkel G., Willner H. (2000), Z. Anorg. Allg. Chem. 626, 560-568.

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cP16

BiF_3	<i>cP16</i>	(215) $P\text{-}43m - e^2dcba$
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"BiF₃ α" [1]

Structural features: Close-packed Bi layers in c stacking, F occupies all octahedral and tetrahedral voids. BiF_8 and FF_8 cubes share all faces to form a 3D-framework. Substitution derivative of W (prototype for a b.c.c. atom arrangement), sequence along $\langle 111 \rangle$: $-\text{Bi-F-F-F}-$.

Hund F., Fricke R. (1949) [1]

BiF_3

$a = 0.5853 \text{ nm}$, $V = 0.2005 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Bi1	4e	$.3m$	0.237	0.237	0.237		rhombic dodecahedron F_{14}
F2	4e	$.3m$	0.75	0.75	0.75		rhombic dodecahedron F_8Bi_6
F3	3d	$-42.m$	$\frac{1}{2}$	0	0		rhombic dodecahedron Bi_4F_{10}

F4	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	rhombic dodecahedron $F_{10}Bi_4$
F5	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	bicapped hexagonal prism $F_{10}Bi_4$
F6	1a	-43m	0	0	0	rhombic dodecahedron Bi_4F_{10}

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, Debye-Scherrer film, X-rays

Remarks: Cubic BiF_3 is generally considered to adopt space group (225) $Fm-3m$ [2]. According to [3], pure BiF_3 is orthorhombic up to the melting point and the reported cubic compound contains oxygen ($\sim BiO_{0.5}F_2$).

References: [1] Hund F., Fricke R. (1949), Z. Anorg. Chem. 258, 198-204. [2] Hassel O., Nilssen S. (1929), Z. Anorg. Allg. Chem. 181, 172-176. [3] Greis O., Martinez Ripoll M. (1977), Z. Anorg. Allg. Chem. 436, 105-112.

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cP16

$Li_8Al_3Si_5$	cP16	(215) $P-43m - e^2dcba$
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$Li_8Al_3Si_5$ [1]

Structural features: Ordering variant of $\alpha-BiF_3$, substitution derivative of W (prototype for a b.c.c. atom arrangement). Single $SiSi_4$ tetrahedra.

Kevorkov D. et al. (2001) [1]

$Al_3Li_8Si_5$

$a = 0.61147$ nm, $V = 0.2286$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	4e	.3m	0.248	0.248	0.248		rhombic dodecahedron $Li_{10}Al_3Si$
Li2	4e	.3m	0.751	0.751	0.751		rhombic dodecahedron $Li_4Al_3Si_7$
Al3	3d	-42.m	$\frac{1}{2}$	0	0		rhombic dodecahedron Si_4Li_{10}
Li4	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron $Li_4Si_6Al_4$
Si5	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron $Li_{10}Si_4$
Li6	1a	-43m	0	0	0		rhombic dodecahedron $Si_4Li_4Al_6$

Experimental: powder, diffractometer, X-rays, $R_p = 0.070$

References: [1] Kevorkov D., Gröbner J., Schmid Fetzner R. (2001), J. Solid State Chem. 156, 500-505.

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cP17

$Rb[NO_3]$	cP17	(215) $P-43m - ieb$
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$RbNO_3$ form III [1]

Structural features: Rb atoms and NO_3 trigonal units (orientational disorder) in a W-type (b.c.c.) arrangement.

Shamsuzzoha M., Lucas B.W. (1987) [1]

NO_3Rb

$a = 0.44$ nm, $V = 0.0852$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.055	0.055	0.266	0.25	
N2	4e	.3m	0.055	0.055	0.055	0.25	

Rb3 1b -43m $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, neutrons, wR = 0.062, T = 461 K

Remarks: Phase stable at 437 < T < 492 K. Short interatomic distances for partly occupied site(s).

References: [1] Shamsuzzoha M., Lucas B.W. (1987), Acta Crystallogr. C 43, 385-388.

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cP21

Hf[BH ₄] ₄	cP21	(215) <i>P</i> -43m – ie ² a
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Hf(BH₄)₄ [1]

Structural features: Single BH₄ tetrahedra.

Broach R.W. et al. (1983) [1]

B₄H₁₆Hf

a = 0.5827 nm, *V* = 0.1978 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	12i	..m	0.258	0.258	0.019		single atom B
B2	4e	.3m	0.226	0.226	0.226		tetrahedron H ₄
H3	4e	.3m	0.34	0.34	0.34		single atom B
Hf4	1a	-43m	0	0	0		cuboctahedron H ₁₂

Experimental: single crystal, diffractometer, neutrons, R = 0.103, T = 110 K

References: [1] Broach R.W., Chuang I., Marks T.J., Williams J.M. (1983), Inorg. Chem. 22, 1081-1084.

215
cP24

TmNi ₂	cP24	(215) <i>P</i> -43m – ie ² ca
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TmNi₂ ht2 [1]

Structural features: Tm(Ni₁₂Tm₄) Friauf polyhedra (Ni₁₂ truncated tetrahedron + Tm₄ tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework, Tm forming a diamond-type sublattice. Distorted derivative of MgCu₂ (cubic Laves phase).

Deutz A.F. et al. (1989) [1]

Ni₂Tm

a = 0.7095 nm, *V* = 0.3572 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	12i	..m	0.122	0.122	0.612		icosahedron Ni ₆ Tm ₆
Tm2	4e	.3m	0.271	0.271	0.271		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Ni3	4e	.3m	0.622	0.622	0.622		icosahedron Ni ₆ Tm ₆
Tm4	3c	-42..m	0	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Tm5	1a	-43m	0	0	0		16-vertex Frank-Kasper Ni ₁₂ Tm ₄

Experimental: powder, diffractometer, X-rays, R_B = 0.079

Remarks: Phase stable at T > ~973 K. Space group (111) *P*-42m could not be excluded.

References: [1] Deutz A.F., Helmholtz R.B., Moleman A.C., De Mooij D.B., Buschow K.H.J. (1989), J. Less-Common Met. 153, 259-266.

215
cP26

$\text{Cs}_3\text{Mo}_4[\text{PO}_4]_3\text{O}_4$	<i>cP26</i>	(215) <i>P-43m</i> – ie^2dc
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Cs₃Mo₄P₃O₁₆ [1]

Structural features: Mo₄O₁₆ clusters consisting of four edge-linked MoO₆ octahedra (a Mo₄ tetrahedral cluster surrounded by an O₄ outer tetrahedron and an O₁₂ truncated tetrahedron) share vertices with PO₄ tetrahedra to form a 3D-framework.

Haushalter R.C. (1987) [1]

Cs₃Mo₄O₁₆P₃ $a = 0.7728 \text{ nm}$, $V = 0.4615 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	<i>..m</i>	0.1185	0.1185	0.3862		single atom P
Mo2	4e	<i>.3m</i>	0.118	0.118	0.118		octahedron O ₆
O3	4e	<i>.3m</i>	0.8576	0.8576	0.8576		non-coplanar triangle Mo ₃
P4	3d	<i>-42.m</i>	$\frac{1}{2}$	0	0		tetrahedron O ₄
Cs5	3c	<i>-42.m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		square prism (cube) O ₈

Transformation from published data: $-x, -y, -z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.034$

Remarks: Coordinates of the O sites not published, we derived approximate values from published Mo-O and Cs-O interatomic distances.

References: [1] Haushalter R.C. (1987), J. Chem. Soc., Chem. Commun. 1987, 1566-1568.

215
cP30

$\text{HK}_3\text{Ge}_7\text{O}_{16}[\text{H}_2\text{O}]_4$	<i>cP30</i>	(215) <i>P-43m</i> – ie^3dc
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K₃HGe₇O₁₆·4H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; K and H₂O in a system of interconnected channels. See Fig. II.25.

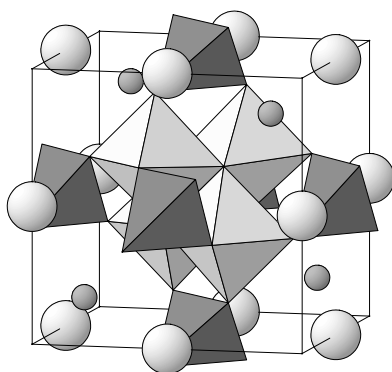
Bialek R., Gramlich V. (1992) [1]

Ge₇H₈K₃O₂₀ $a = 0.7709 \text{ nm}$, $V = 0.4581 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	<i>..m</i>	0.136	0.136	0.622		non-colinear Ge ₂
O2	4e	<i>.3m</i>	0.114	0.114	0.114		non-coplanar triangle Ge ₃
(OH ₂) ₃	4e	<i>.3m</i>	0.345	0.345	0.345		bicapped square prism O ₄ K ₃ (OH ₂) ₃
Ge4	4e	<i>.3m</i>	0.861	0.861	0.861		octahedron O ₆
Ge5	3d	<i>-42.m</i>	$\frac{1}{2}$	0	0		tetrahedron O ₄
K6	3c	<i>-42.m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		12-vertex polyhedron O ₈ (OH ₂) ₄

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.077$

Remarks: H not belonging to H₂O was not located. Average structure; the superstructure was refined in space group (197) *I23* with 8-fold cell volume. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

Fig. II.25. $\text{K}_3\text{HGe}_7\text{O}_{16}\cdot 4\text{H}_2\text{O}$

Arrangement of GeO_4 tetrahedra (dark), GeO_6 octahedra (light), K atoms (large) and H_2O molecules (O atoms small).

References: [1] Bialek R., Gramlich V. (1992), Z. Kristallogr. 198, 67-77.

215
cP30

$\text{HK}_3\text{Ti}_4[\text{SiO}_4]_3\text{O}_4[\text{H}_2\text{O}]_4$	cP30	(215) $P\text{-}43m - \text{ie}^3\text{dc}$
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$\text{K}_3\text{H}(\text{TiO})_4(\text{SiO}_4)_3\cdot 4\text{H}_2\text{O}$ [1], pharmacosiderite family

Structural features: Units of four edge-linked TiO_6 octahedra share vertices with SiO_4 tetrahedra to form a pharmacosiderite-type framework; K and H_2O in a system of interconnected channels.

Behrens E.A. et al. (1996) [1]

$\text{H}_9\text{K}_3\text{O}_{20}\text{Si}_3\text{Ti}_4$

$a = 0.77644 \text{ nm}$, $V = 0.4681 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	.m	0.1192	0.1192	0.6192		non-collinear SiTi
M2	4e	.3m	0.115	0.115	0.115		non-coplanar triangle Ti_3
(OH_2)3	4e	.3m	0.3335	0.3335	0.3335		single atom O
Ti4	4e	.3m	0.8547	0.8547	0.8547		octahedron O_6
Si5	3d	-42.m	$\frac{1}{2}$	0	0		tetrahedron O_4
K6	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		12-vertex polyhedron (OH_2) $_4\text{O}_8$

$\text{M2} = 0.75\text{O} + 0.25\text{OH}$

Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, X-rays, $R_p = 0.088$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Behrens E.A., Poojary D.M., Clearfield A. (1996), Chem. Mater. 8, 1236-1244.

215
cP30

$\text{KFe}_4[\text{AsO}_4]_3[\text{OH}]_4[\text{H}_2\text{O}]_7$	cP30	(215) $P\text{-}43m - \text{ie}^3\text{dc}$
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$\text{K}[\text{Fe}_4(\text{OH})_4(\text{AsO}_4)_3]\cdot 6\text{-}7\text{H}_2\text{O}$ [1], pharmacosiderite

Structural features: Units of four edge-linked $\text{Fe}(\text{O}_3[\text{OH}])_3$ octahedra share vertices with AsO_4 tetrahedra to form a pharmacosiderite-type framework; K and H_2O in a system of interconnected channels.

Zemann J. (1948) [1]

$\text{As}_3\text{Fe}_4\text{H}_{18}\text{O}_{23}$

$a = 0.791 \text{ nm}$, $V = 0.4949 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	<i>..m</i>	0.125	0.125	0.625		non-collinear AsFe
(OH)2	4e	<i>.3m</i>	0.125	0.125	0.125		non-coplanar triangle Fe ₃
(OH ₂)3	4e	<i>.3m</i>	0.3472	0.3472	0.3472		bicapped square prism (OH)(OH ₂) ₆ O ₃
Fe4	4e	<i>.3m</i>	0.8694	0.8694	0.8694		octahedron O ₃ (OH) ₃
As5	3d	<i>-42.m</i>	$\frac{1}{2}$	0	0		tetrahedron O ₄
(OH ₂)6	3c	<i>-42.m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		12-vertex polyhedron (OH ₂) ₄ O ₈

Transformation from published data: $-x, -y, -z$

Experimental: powder, film, X-rays

Remarks: Natural specimen from Cornwall. K not located. The structure was redetermined in [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Zemann J. (1948), *Tschermaks Mineral. Petrogr. Mitt.* 1, 1-13. [2] Buerger M.J., Dollase W.A., Garaycochea Wittke I. (1967), *Z. Kristallogr.* 125, 92-108.

215
cP31

$\text{Ti}_4[\text{SiO}_4]_3[\text{OH}]_4[\text{H}_2\text{O}]_8$	<i>cP31</i>	(215) <i>P-43m - ie³dca</i>
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H₄(TiO)₄(SiO₄)₃·8H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked Ti(O₃[OH]₃) octahedra share vertices with SiO₄ tetrahedra to form a pharmacosiderite-type framework; H₂O in a system of interconnected channels.

Behrens E.A. et al. (1996) [1]

H₂₀O₂₄Si₃Ti₄

$a = 0.78214 \text{ nm}$, $V = 0.4785 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	<i>..m</i>	0.3784	0.3784	0.8827		non-collinear SiTi
(OH ₂)2	4e	<i>.3m</i>	0.1949	0.1949	0.1949		collinear (OH)(OH ₂)
(OH)3	4e	<i>.3m</i>	0.3802	0.3802	0.3802		non-coplanar triangle Ti ₃
Ti4	4e	<i>.3m</i>	0.6511	0.6511	0.6511		octahedron O ₃ (OH) ₃
(OH ₂)5	3d	<i>-42.m</i>	$\frac{1}{2}$	0	0		12-vertex polyhedron (OH ₂) ₄ O ₈
Si6	3c	<i>-42.m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄
(OH ₂)7	1a	<i>-43m</i>	0	0	0		tetrahedron (OH ₂) ₄

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_p = 0.086$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Behrens E.A., Poojary D.M., Clearfield A. (1996), *Chem. Mater.* 8, 1236-1244.

215
cP33

$\text{Ca}_4\text{Mg}_4\text{Fe}_3\text{H}_{22}$	<i>cP33</i>	(215) <i>P-43m - hfe³d</i>
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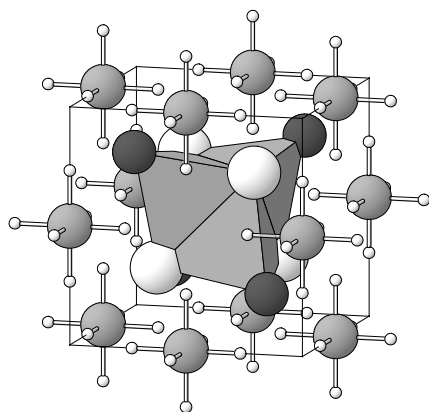
Ca₄Mg₄Fe₃H₂₂ [1]

Structural features: Single FeH₆ octahedra; additional H in Ca₃Mg tetrahedra. See Fig. II.26.

Huang B. et al. (1992) [1]

 $\text{Ca}_4\text{D}_{22}\text{Fe}_3\text{Mg}_4$ $a = 0.67016 \text{ nm}$, $V = 0.3010 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12h	2..	0.2362	$\frac{1}{2}$	0		single atom Fe
D2	6f	2.mm	0.267	0	0		single atom Fe
Mg3	4e	.3m	0.2153	0.2153	0.2153		10-vertex polyhedron D_{10}
D4	4e	.3m	0.3711	0.3711	0.3711		single atom Mg
Ca5	4e	.3m	0.709	0.709	0.709		9-vertex polyhedron D_9
Fe6	3d	-42.m	$\frac{1}{2}$	0	0		octahedron D_6

Experimental: powder, diffractometer, neutrons, $R_p = 0.054$, $T = 295 \text{ K}$ Fig. II.26. $\text{Ca}_4\text{Mg}_4\text{Fe}_3\text{H}_{22}$

Arrangement of $\text{H}(\text{Ca}_3\text{Mg})$ tetrahedra (Ca atoms light, Mg atoms dark) and FeH_6 octahedra (Fe atoms large, H atoms small).

References: [1] Huang B., Yvon K., Fischer P. (1992), J. Alloys Compd. 190, 65-68.

215
cP33

$\text{HFe}_4[\text{AsO}_4]_3[\text{OH}]_4[\text{H}_2\text{O}]_5$	<i>cP33</i>	(215) $P\text{-}43m - \text{ife}^3\text{c}$
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(K,H)Fe₄(AsO₄)₃(OH)₄·5H₂O [1], pharmacosiderite

Structural features: Units of four edge-linked $\text{Fe}(\text{O}_3[\text{OH}])_3$ octahedra share vertices with AsO_4 tetrahedra to form a pharmacosiderite-type framework; H_2O in a system of interconnected channels (partial disorder).

Buerger M.J. et al. (1967) [1]

 $\text{As}_3\text{Fe}_4\text{H}_{14}\text{O}_{21}$ $a = 0.798 \text{ nm}$, $V = 0.5082 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.3777	0.3777	0.8787		non-colinear AsFe
(OH ₂)2	6f	2.mm	0.18	0	0	0.5	trigonal prism $(\text{OH}_2)_6$
(OH ₂)3	4e	.3m	0.194	0.194	0.194	0.5	tetrahedron $(\text{OH}_2)_3(\text{OH})$
(OH)4	4e	.3m	0.3847	0.3847	0.3847		non-coplanar triangle Fe_3
Fe5	4e	.3m	0.6426	0.6426	0.6426		octahedron $\text{O}_3(\text{OH})_3$
As6	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O_4

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.066$

Remarks: Natural specimen from Cornwall. Only trace amounts of K detected. H not belonging to OH/H₂O was not located. Average structure. Supersedes a structure proposal with a different arrangement of H₂O in [2] (KFe₄(AsO₄)₃(OH)₄·5H₂O, K not located). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Buerger M.J., Dollase W.A., Garaycochea Wittke I. (1967), Z. Kristallogr. 125, 92-108. [2] Zemann J. (1948), Tschermaks Mineral. Petrogr. Mitt. 1, 1-13.

215
cP33



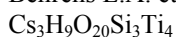
cP33

(215) *P*-43*m* – ige³d

Cs₃H(TiO)₄(SiO₄)₃·4H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked Ti(O,OH)₆ octahedra share vertices with SiO₄ tetrahedra to form a pharmacosiderite-type framework; Cs and H₂O in a system of interconnected channels (partial disorder).

Behrens E.A. et al. (1996) [1]



$$a = 0.78212 \text{ nm}, V = 0.4784 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.1208	0.1208	0.6177	0.5	non-collinear SiTi
Cs2	6g	2.mm	0.0587	¹ / ₂	¹ / ₂		
M3	4e	.3m	0.1275	0.1275	0.1275		non-coplanar triangle Ti ₃
(OH ₂)4	4e	.3m	0.3607	0.3607	0.3607		non-coplanar triangle Cs ₃
Ti5	4e	.3m	0.8563	0.8563	0.8563		octahedron O ₆
Si6	3d	-42.m	¹ / ₂	0	0		tetrahedron O ₄

$$\text{M3} = 0.75\text{O} + 0.25\text{OH}$$

Transformation from published data: -x,-y,-z

Experimental: powder, diffractometer, X-rays, R_p = 0.088

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Behrens E.A., Poojary D.M., Clearfield A. (1996), Chem. Mater. 8, 1236-1244.

215
cP34



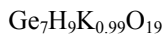
cP34

(215) *P*-43*m* – ie⁴dc

KH₃Ge₇O₁₆·3H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; K and H₃O in a system of interconnected channels (partial disorder).

Sturua G.I. et al. (1978) [1]



$$a = 0.7707 \text{ nm}, V = 0.4578 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.369	0.369	0.121	0.25	non-collinear Ge ₂
(OH ₃)2	4e	.3m	0.134	0.134	0.134		trigonal prism (OH ₃) ₃ O ₃
Ge3	4e	.3m	0.3633	0.3633	0.3633		octahedron O ₆
O4	4e	.3m	0.612	0.612	0.612		non-coplanar triangle Ge ₃

(OH ₃) ₅	4e	.3m	0.817	0.817	0.817	0.5	tetrahedron (OH ₃) ₃ O
K6	3d	-42.m	$\frac{1}{2}$	0	0	0.33	16-vertex Frank-Kasper (OH ₃) ₈ O ₈
Ge7	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄

Experimental: single crystal, diffractometer, X-rays, R = 0.068

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Sturua G.I., Belokoneva E.L., Simonov M.A., Belov N.V. (1978), Dokl. Akad. Nauk SSSR 242, 1078-1081.

215
cP34

[NH ₄] ₃ Mo ₄ P ₃ O ₁₆	cP34	(215) <i>P</i> -43m – ie ⁴ dc
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(NH₄)₃Mo₄P₃O₁₆ [1]

Structural features: Mo₄O₁₆ clusters consisting of four edge-linked MoO₆ octahedra (a Mo₄ tetrahedron surrounded by an O₄ tetrahedron and an O₁₂ truncated tetrahedron) share edges of the truncated tetrahedra with PO₄ tetrahedra to form a 3D-framework; NH₄ tetrahedra in voids (disorder).

King H.E. Jr. et al. (1991) [1]

H₁₂Mo₄N₃O₁₆P₃

a = 0.7736 nm, *V* = 0.4630 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	..m	0.384	0.384	0.11		single atom P
(NH ₄) ₂	4e	.3m	0.045	0.045	0.045	0.4	non-coplanar triangle (NH ₄) ₃
Mo3	4e	.3m	0.3826	0.3826	0.3828		octahedron O ₆
O4	4e	.3m	0.64	0.64	0.64		non-coplanar triangle Mo ₃
(NH ₄) ₅	4e	.3m	0.845	0.845	0.845	0.2	non-coplanar triangle (NH ₄) ₃
(NH ₄) ₆	3d	-42.m	$\frac{1}{2}$	0	0	0.2	12-vertex polyhedron (NH ₄) ₄ O ₈
P7	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄

Transformation from published data: -*x*, -*y*, -*z*

Experimental: single crystal, diffractometer, X-rays, R = 0.035, T = 303 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] King H.E. Jr., Mundi L.A., Strohmaier K.G., Haushalter R.C. (1991), J. Solid State Chem. 92, 154-158.

215
cP35

Na ₁₀ Be ₄ Si ₄ O ₁₇	cP35	(215) <i>P</i> -43m – ie ⁴ dca
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Na₁₀Be₄Si₄O₁₇ [1]

Structural features: Be₄Si₄O₁₇ units (four BeO₄ tetrahedra having a common vertex share the other vertices with four SiO₄ tetrahedra) in a Po-type (primitive cubic) arrangement.

Eriksson L. et al. (1990) [1]

Be₄Na₁₀O₁₇Si₄

a = 0.72811 nm, *V* = 0.3860 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.2612	0.2612	0.0009		non-colinear BeSi
Si2	4e	.3m	0.2201	0.2201	0.2201		tetrahedron O ₄
O3	4e	.3m	0.3464	0.3464	0.3464		single atom Si
Na4	4e	.3m	0.6589	0.6589	0.6589		7-vertex polyhedron O ₆ Be
Be5	4e	.3m	0.8688	0.8688	0.8688		tetrahedron O ₄
Na6	3d	-42.m	1/2	0	0		square prism (cube) O ₈
Na7	3c	-42.m	0	1/2	1/2		coplanar square O ₄
O8	1a	-43m	0	0	0		tetrahedron Be ₄

Experimental: single crystal, diffractometer, X-rays, wR = 0.031, T = 293 K

Remarks: Space group (195) *P*23 was tested and rejected.

References: [1] Eriksson L., Frostäng S., Grins J. (1990), Acta Crystallogr. B 46, 736-739.

215
cP36

HK ₃ Ge ₇ O ₁₆ [H ₂ O] ₄	cP36	(215) <i>P</i> -43m – ife ³ dc
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K₃HGe₇O₁₆·4H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; K and H₂O in a system of interconnected channels (partial disorder).

Nowotny H., Wittmann A. (1954) [1]

Ge₇H₉K₃O₂₀

a = 0.77 nm, *V* = 0.4565 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.39	0.39	0.86		non-colinear Ge ₂
K2	6f	2.mm	0.333	0	0	0.25	
(OH ₂)3	4e	.3m	0.185	0.185	0.185		tetrahedron K ₃ O
O4	4e	.3m	0.37	0.37	0.37		non-coplanar triangle Ge ₃
Ge5	4e	.3m	0.64	0.64	0.64		octahedron O ₆
K6	3d	-42.m	1/2	0	0	0.5	
Ge7	3c	-42.m	0	1/2	1/2		tetrahedron O ₄
H8	1b	-43m	1/2	1/2	1/2		

Transformation from published data: -x,-y,-z

Experimental: powder, film, X-rays

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nowotny H., Wittmann A. (1954), Monatsh. Chem. 85, 558-574.

215
cP38

Ni ₂ P ₂ O ₃ [CO] ₆	cP38	(215) <i>P</i> -43m – i ² fe ²
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P₄O₆[Ni(CO)₃]₄ [1]

Structural features: P₄O₆ units consisting of four vertex-linked :PO₃ ψ-tetrahedra (cage with four 6-membered rings) and non-planar Ni(CO)₃ trigonal units (linear Ni-C-O segments).

Pierron E.D. et al. (1966) [1]

 $\text{C}_6\text{Ni}_2\text{O}_9\text{P}_2$ $a = 0.8811 \text{ nm}$, $V = 0.6840 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	$\bar{3}m$	0.1898	0.1898	0.5793		single atom C
C2	12i	$\bar{3}m$	0.2161	0.2161	0.4553		single atom O
O3	6f	$2.mm$	0.2036	0	0		non-collinear P_2
P4	4e	$\bar{3}m$	0.1162	0.1162	0.1162		tetrahedron O_3Ni
Ni5	4e	$\bar{3}m$	0.2571	0.2571	0.2571		tetrahedron C_3P

Experimental: powder, diffractometer, X-rays, $R = 0.164$

References: [1] Pierron E.D., Wheatley P.J., Riess J.G. (1966), Acta Crystallogr. 21, 288-289.

215
cP38

$\text{K}_{10}\text{Mn}_4\text{Sn}_4\text{S}_{17}$	<i>cP38</i>	(215) $P\text{-}43m - \text{ig}e^4da$
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 $\text{K}_{10}\text{Mn}_4\text{Sn}_4\text{S}_{17}$ [1]Structural features: $\text{Mn}_4\text{Sn}_4\text{S}_{17}$ units (four MnS_4 tetrahedra having a common vertex share the other vertices with four SnS_4 tetrahedra) in a Po-type (primitive cubic) arrangement.

Palchik O. et al. (2003) [1]

 $\text{K}_{10}\text{Mn}_4\text{S}_{17}\text{Sn}_4$ $a = 1.0064 \text{ nm}$, $V = 1.0193 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12i	$\bar{3}m$	0.27676	0.27676	0.00117		non-collinear SnMn
K2	6g	$2.mm$	0.0562	$\frac{1}{2}$	$\frac{1}{2}$	0.5	
Mn3	4e	$\bar{3}m$	0.13607	0.13607	0.13607		tetrahedron S_4
K4	4e	$\bar{3}m$	0.33449	0.33449	0.33449		non-coplanar triangle S_3
S5	4e	$\bar{3}m$	0.63944	0.63944	0.63944		single atom Sn
Sn6	4e	$\bar{3}m$	0.77333	0.77333	0.77333		tetrahedron S_4
K7	3d	$\bar{4}2.m$	$\frac{1}{2}$	0	0		square prism (cube) S_8
S8	1a	$\bar{4}3m$	0	0	0		tetrahedron Mn_4

Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.021$, $T = 293 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s).

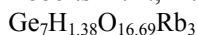
References: [1] Palchik O., Iyer R.G., Liao J.H., Kanatzidis M.G. (2003), Inorg. Chem. 42, 5052-5054.

215
cP39

$\text{HRb}_3\text{Ge}_7\text{O}_{16}[\text{H}_2\text{O}]_{0.69}$	<i>cP39</i>	(215) $P\text{-}43m - \text{if}^2e^3c$
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 $\text{Rb}_3\text{HGe}_7\text{O}_{16} \cdot 0.69\text{H}_2\text{O}$ [1], pharmacosiderite familyStructural features: Units of four edge-linked GeO_6 octahedra share vertices with GeO_4 tetrahedra to form a pharmacosiderite-type framework; Rb and H_2O in a system of interconnected channels (partial disorder).

Roberts M.A., Fitch A.N. (1996) [1]



$a = 0.76699 \text{ nm}$, $V = 0.4512 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	$\bar{3}m$	0.3671	0.3671	0.8761		non-collinear Ge ₂
Rb2	6f	2.mm	0.379	0	0	0.065	
Rb3	6f	2.mm	0.4758	0	0	0.435	
(OH ₂)4	4e	$\bar{3}m$	0.164	0.164	0.164	0.172	non-coplanar triangle Rb ₃
O5	4e	$\bar{3}m$	0.3846	0.3846	0.3846		non-coplanar triangle Ge ₃
Ge6	4e	$\bar{3}m$	0.6399	0.6399	0.6399		octahedron O ₆
Ge7	3c	$\bar{4}2.m$	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄

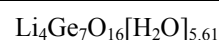
Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, X-rays, $R_B = 0.024$

Remarks: H not belonging to H₂O was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Roberts M.A., Fitch A.N. (1996), Z. Kristallogr. 211, 378-387.

215
cP41



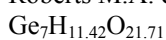
cP41

(215) $P\bar{4}3m - i^2ge^2d$

Li_{4-x}H_xGe₇O₁₆•5.61H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; Li and H₂O in a system of interconnected channels (partial disorder).

Roberts M.A. et al. (1995) [1]



$a = 0.77194 \text{ nm}$, $V = 0.4600 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	$\bar{3}m$	0.1308	0.1308	0.6284		non-collinear Ge ₂
(OH ₂)2	12i	$\bar{3}m$	0.3143	0.3143	0.371	0.237	
(OH ₂)3	6g	2.mm	0.0623	$\frac{1}{2}$	$\frac{1}{2}$	0.478	
O4	4e	$\bar{3}m$	0.1145	0.1145	0.1145		non-coplanar triangle Ge ₃
Ge5	4e	$\bar{3}m$	0.86503	0.86503	0.86503		octahedron O ₆
Ge6	3d	$\bar{4}2.m$	$\frac{1}{2}$	0	0		tetrahedron O ₄

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.033$

Remarks: Li and H not belonging to H₂O were not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Roberts M.A., Fitch A.N., Chadwick A.V. (1995), J. Phys. Chem. Solids 56, 1353-1358.

215
cP41



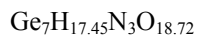
cP41

(215) $P\bar{4}3m - i^2ge^2d$

(NH₄)₃HGe₇O₁₆·2.72H₂O [1], pharmacosiderite family

Structural features: Units of four edge-linked GeO₆ octahedra share vertices with GeO₄ tetrahedra to form a pharmacosiderite-type framework; NH₄ and H₂O form a disordered network of hydrogen bonding in a system of interconnected channels.

Roberts M.A. et al. (1995) [1]



$a = 0.77107 \text{ nm}$, $V = 0.4584 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.1319	0.1319	0.6287		non-colinear Ge ₂
(OH ₂)2	12i	..m	0.3072	0.3072	0.37	0.227	
(NH ₄)3	6g	2.mm	0.0513	$\frac{1}{2}$	$\frac{1}{2}$	0.5	
O4	4e	.3m	0.1125	0.1125	0.1125		non-coplanar triangle Ge ₃
Ge5	4e	.3m	0.8625	0.8625	0.8625		octahedron O ₆
Ge6	3d	-42.m	$\frac{1}{2}$	0	0		tetrahedron O ₄

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.029$

Remarks: H not belonging to NH₄ or H₂O was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Roberts M.A., Fitch A.N., Chadwick A.V. (1995), J. Phys. Chem. Solids 56, 1353-1358.

215
cP44

K₁₀Co₄Sn₄S₁₇	cP44	(215) P-43m – ig²e⁴da
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K₁₀Co₄Sn₄S₁₇ [1]

Structural features: Co₄Sn₄S₁₇ units (four CoS₄ tetrahedra having a common vertex share the other vertices with four SnS₄ tetrahedra) in a Po-type (primitive cubic) arrangement.

Palchik O. et al. (2003) [1]



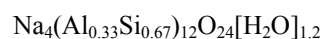
$a = 0.99332 \text{ nm}$, $V = 0.9801 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12i	..m	0.27202	0.27202	0.00739		non-colinear CoSn
K2	6g	2.mm	0.0249	$\frac{1}{2}$	$\frac{1}{2}$	0.187	
K3	6g	2.mm	0.0614	$\frac{1}{2}$	$\frac{1}{2}$	0.313	
Co4	4e	.3m	0.13351	0.13351	0.13351		tetrahedron S ₄
K5	4e	.3m	0.33176	0.33176	0.33176		non-coplanar triangle S ₃
S6	4e	.3m	0.64106	0.64106	0.64106		single atom Sn
Sn7	4e	.3m	0.7764	0.7764	0.7764		tetrahedron S ₄
K8	3d	-42.m	$\frac{1}{2}$	0	0		square prism (cube) S ₈
S9	1a	-43m	0	0	0		tetrahedron Co ₄

Experimental: single crystal, diffractometer, X-rays, $R = 0.009$, $T = 293 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Palchik O., Iyer R.G., Liao J.H., Kanatzidis M.G. (2003), Inorg. Chem. 42, 5052-5054.

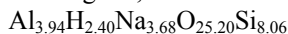
215
cP46

cP46

(215) $P\text{-}43m - i^2hfe$ **Na₄Al₄Si₈O₂₄·xH₂O** [1], zeolite SOD-H₂O

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); Na above the centers of 6-rings, H₂O above the centers of 4-rings.

Cartlidge S., Meier W.M. (1984) [1]



$$a = 0.893 \text{ nm}, V = 0.7121 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.157	0.157	0.471		non-colinear Si ₂
O2	12i	..m	0.3437	0.3437	0.966		non-colinear Si ₂
M3	12h	2..	0.255	1/2	0		tetrahedron O ₄
(OH ₂) ₄	6f	2.mm	0.333	0	0	0.2	non-colinear O ₂
Na5	4e	.3m	0.196	0.196	0.196	0.92	tricapped trigonal prism O ₆ (OH ₂) ₃

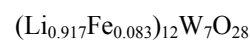
$$\text{M3} = 0.672\text{Si} + 0.328\text{Al}$$

Transformation from published data: -x,-y,-z; origin shift 1/2 1/2 1/2

Experimental: powder, Guinier-de Wolff, X-rays, R_B = 0.137, T = 723 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Cartlidge S., Meier W.M. (1984), Zeolites 4, 218-225.

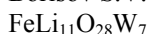
215
cP47

cP47

(215) $P\text{-}43m - i^3e^2c$ **Li₁₁Fe(WO₄)₇** [1]

Structural features: W₄O₁₆ units consisting of four edge-linked WO₆ octahedra (W₄ tetrahedral cluster), and single WO₄ tetrahedra are interconnected via (Li,Fe)O₆ octahedra to form a 3D-framework.

Borisov S.V. et al. (1969) [1]



$$a = 0.825 \text{ nm}, V = 0.5615 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.115	0.115	0.617		tetrahedron Li ₃ W
M2	12i	..m	0.125	0.125	0.374		octahedron O ₆
O3	12i	..m	0.376	0.376	0.142		non-coplanar triangle WLi ₂
O4	4e	.3m	0.117	0.117	0.117		octahedron Li ₃ W ₃
W5	4e	.3m	0.856	0.856	0.856		octahedron O ₆
W6	3c	-42.m	0	1/2	1/2		tetrahedron O ₄

$$\text{M2} = 0.917\text{Li} + 0.083\text{Fe}$$

Transformation from published data: origin shift 1/2 1/2 1/2

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.130

References: [1] Borisov S.V., Klevtsova R.F., Belov N.V. (1969), Sov. Phys. Crystallogr. (Engl. Transl.) 13, 852-855.

215
cP48

$\text{Cd}_{19}(\text{Cd}_{0.2}\text{Ni}_{0.8})_5$	<i>cP48</i>	(215) <i>P-43m</i> – i^2gfe^3
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NiCd₅ [1]

Structural features: 26-atom γ brass- (a Cd_4 inner tetrahedron surrounded by a Cd_4 outer tetrahedron, a Cd_6 octahedron and a Cd_{12} cuboctahedron) and 22-atom Ti_2Ni -type (a $(\text{Ni},\text{Cd})_6$ octahedron surrounded by a $(\text{Ni},\text{Cd})_4$ tetrahedron and a Cd_{12} cuboctahedron) nested polyhedra units in a CsCl-type arrangement.

Ljung H., Westman S. (1970) [1]

 $\text{Cd}_{20}\text{Ni}_4$ $a = 0.97878 \text{ nm}$, $V = 0.9377 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cd1	12 <i>i</i>	.. <i>m</i>	0.2052	0.2052	0.5526		icosahedron Ni_3Cd_9
Cd2	12 <i>i</i>	.. <i>m</i>	0.3096	0.3096	0.0403		15-vertex Frank-Kasper $\text{Ni}_3\text{Cd}_{12}$
M3	6 <i>g</i>	2.. <i>mm</i>	0.2492	$\frac{1}{2}$	$\frac{1}{2}$		14-vertex polyhedron Ni_6Cd_8
Cd4	6 <i>f</i>	2.. <i>mm</i>	0.3631	0	0		pseudo Frank-Kasper Cd_{13}
Cd5	4 <i>e</i>	.. <i>3m</i>	0.1066	0.1066	0.1066		pseudo Frank-Kasper Cd_{12}Ni
M6	4 <i>e</i>	.. <i>3m</i>	0.3169	0.3169	0.3169		bicapped square prism Ni_3Cd_7
Cd7	4 <i>e</i>	.. <i>3m</i>	0.8361	0.8361	0.8361		icosahedron Cd_{12}

M3 = 0.8Ni + 0.2Cd; M6 = 0.8Ni + 0.2Cd

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.080$

Remarks: Phase referred to as γ -(CdNi). Preliminary data in [2] and [3]. In [1] the Wyckoff positions 6*f* and 6*g* are interchanged.

References: [1] Ljung H., Westman S. (1970), Acta Chem. Scand. 24, 611-617. [2] Ekman W. (1931), Z. Phys. Chem., Abt. B 12, 57-78. [3] Lihl F., Buhl E. (1955), Z. Metallkd. 46, 787-791.

215
cP49

$\text{Zn}_{36}\text{Ni}_8\text{Ga}_5$	<i>cP49</i>	(215) <i>P-43m</i> – i^2gfe^3a
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Ni₈Zn₃₆Ga₅ [1]

Structural features: 26-atom γ brass- (a Ga_4 inner tetrahedron surrounded by a Ni_4 outer tetrahedron, a Zn_6 octahedron and a Zn_{12} cuboctahedron) and 23-atom Ti_2Ni -type (a Ga central atom surrounded by a Zn_6 octahedron, a Ni_4 tetrahedron and a Zn_{12} cuboctahedron) nested polyhedra units in a CsCl-type arrangement.

Sarah N. et al. (1981) [1]

 $\text{Ga}_5\text{Ni}_8\text{Zn}_{36}$ $a = 0.88483 \text{ nm}$, $V = 0.6928 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	12 <i>i</i>	.. <i>m</i>	0.1863	0.1863	0.4562		15-vertex Frank-Kasper $\text{Ni}_2\text{Zn}_{12}\text{Ga}$
Zn2	12 <i>i</i>	.. <i>m</i>	0.2959	0.2959	0.9483		12-vertex polyhedron $\text{Ni}_2\text{Zn}_{10}$
Zn3	6 <i>g</i>	2.. <i>mm</i>	0.1417	$\frac{1}{2}$	$\frac{1}{2}$		pseudo Frank-Kasper $\text{Zn}_9\text{Ga}_2\text{Ni}_2$
Zn4	6 <i>f</i>	2.. <i>mm</i>	0.323	0	0		icosahedron $\text{Ni}_2\text{Zn}_9\text{Ga}$
Ni5	4 <i>e</i>	.. <i>3m</i>	0.1746	0.1746	0.1746		pseudo Frank-Kasper Zn_9Ga_2
Ga6	4 <i>e</i>	.. <i>3m</i>	0.3934	0.3934	0.3934		pseudo Frank-Kasper $\text{Ni}_4\text{Zn}_6\text{Ga}_3$
Ni7	4 <i>e</i>	.. <i>3m</i>	0.671	0.671	0.671		icosahedron Zn_9Ga_3

Ga8 1a -43m 0 0 0 fourcapped trigonal prism Ni₄Zn₆

Transformation from published data: -x,-y,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.056

References: [1] Sarah N., Rajasekharan T., Schubert K. (1981), Z. Metallkd. 72, 732-735.

215
cP49

Na₈(Al_{0.5}Si_{0.5})₁₂[SO₄]O₂₄ cP49 (215) *P*-43m – i²he³a

Na₈Al₆Si₆O₂₄SO₄ [2], nosean, zeolite SOD-SO₄

Structural features: (Al,Si)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), every second of which is centered by a SO₄ tetrahedron; Na above the centers of 6-rings.

Schulz H. (1970) [1]

Al₆Na₈O₂₈SSi₆

a = 0.905 nm, *V* = 0.7412 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	..m	0.149	0.149	0.458		non-collinear Al ₂
O2	12i	..m	0.351	0.351	0.958		non-collinear Al ₂
M3	12h	2..	0.25	¹ / ₂	0		tetrahedron O ₄
O4	4e	.3m	0.1	0.1	0.1		collinear SNa
Na5	4e	.3m	0.203	0.203	0.203		single atom O
Na6	4e	.3m	0.797	0.797	0.797		non-coplanar triangle O ₃
S7	1a	-43m	0	0	0		tetrahedron O ₄

M3 = 0.5Al + 0.5Si

Experimental: single crystal, Weissenberg and precession photographs, X-rays, R = 0.074

Remarks: Natural specimen from Laacher See. Composition Na_{5.7}Ca_{0.23}K_{0.17}[Al₆Si₆O₂₄](SO₄)_{1.05}Cl_{0.1} from electron microprobe analysis (elements within square brackets not analyzed). Short interatomic distances: d(Na5-O4) = 0.162 nm. In table 7 of [1] the *z*-coordinate of the (Si,Al) site is misprinted as ¹/₂ instead of 0 (agreement with Wyckoff position 12h).

References: [1] Schulz H. (1970), Z. Kristallogr. 131, 114-138. [2] Barth T.F.W. (1932), Z. Kristallogr. 83, 405-414.

215
cP49

CsBe₄Al₄B₁₂O₂₈ cP49 (215) *P*-43m – i²he³a

CsBe₄Al₄B₁₂O₂₈ [1], rhodizite

Structural features: Al₄Be₄O₂₈ units (four edge-linked AlO₆ octahedra sharing vertices with BeO₄ tetrahedra) share vertices with BO₄ tetrahedra to form a 3D-framework; Cs in large voids.

Buerger M.J., Taxer K. (1966) [1]

Al₄B₁₂Be₄CsO₂₈

a = 0.7319 nm, *V* = 0.3921 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	..m	0.1339	0.1339	0.3981		non-coplanar triangle B ₂ Be
O2	12i	..m	0.3635	0.3635	0.8983		non-coplanar triangle B ₂ Al

B3	12h	2..	0.245	$\frac{1}{2}$	0	tetrahedron O ₄
Be4	4e	.3m	0.245	0.245	0.245	tetrahedron O ₄
O5	4e	.3m	0.3805	0.3805	0.3805	tetrahedron BeAl ₃
Al6	4e	.3m	0.6425	0.6425	0.6425	octahedron O ₆
Cs7	1a	-43m	0	0	0	tetrahedron Be ₄

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, wR = 0.071

Remarks: Natural specimen from Manjaka, Madagascar. Supersedes a structure proposal for rhodizite in the same space group in [2].

References: [1] Buerger M.J., Taxer K. (1966), Science (Washington D.C.) 152, 500-502. [2] Strunz H. (1943), Naturwissenschaften 31, 68.

215
cP49

$(\text{K}_{0.5}\text{Na}_{0.5})_2\text{Li}_4\text{Be}_3\text{Al}_4\text{B}_{10}\text{O}_{27}$	cP49	(215) $P\text{-}43m - i^3e^2dba$
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KNaLi₄Be₃Al₄B₁₀O₂₇ [1], rhodizite

Structural features: AlO₆ octahedra and (B,Be)O₄ tetrahedra share vertices to form a 3D-framework.

Strunz H. (1943) [1]

$\text{Al}_4\text{B}_{10}\text{Be}_2\text{KLi}_4\text{NaO}_{27}$

$a = 0.73 \text{ nm}$, $V = 0.3890 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12i	..m	0.125	0.125	0.375		trigonal bipyramid O ₄ Li
O2	12i	..m	0.25	0.25	0.0		non-colinear B ₂
O3	12i	..m	0.25	0.25	0.5		non-coplanar triangle BAlLi
Li4	4e	.3m	0.25	0.25	0.25		9-vertex polyhedron B ₃ O ₆
Al5	4e	.3m	0.75	0.75	0.75		octahedron O ₆
O6	3d	-42.m	$\frac{1}{2}$	0	0		tetrahedron B ₄
M7	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		cuboctahedron O ₁₂
M8	1a	-43m	0	0	0		cuboctahedron O ₁₂

M1 = 0.833B + 0.167Be; M7 = 0.5K + 0.5Na; M8 = 0.5K + 0.5Na

Remarks: Part of Be not located. Short interatomic distances: d(M1-Li4) = 0.158 nm. The structure of rhodizite was later redetermined in the same space group [2].

References: [1] Strunz H. (1943), Naturwissenschaften 31, 68. [2] Buerger M.J., Taxer K. (1966), Science (Washington D.C.) 152, 500-502.

215
cP52

Cu_9Al_4	cP52	(215) $P\text{-}43m - i^2gfe^4$
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Cu₉Al₄ [2], γ -brass, Strukturbericht notation D8₃; Cu₉Ga₄ γ_1 [3]; Mn₃In [4]

Structural features: Two kinds of 26-atom γ brass-type nested polyhedra unit (an Al₄/Cu₄ inner tetrahedron surrounded by a Cu₄/Cu₄ outer tetrahedron, a Cu₆/Cu₆ octahedron and a Cu₁₂/Al₁₂ cuboctahedron) in a CsCl-type arrangement.

Arnberg L., Westman S. (1978) [1]

Al_4Cu_9

$a = 0.8707 \text{ nm}$, $V = 0.6601 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	12i	..m	0.1847	0.1847	0.5322		pentacapped trigonal prism Cu ₆ Al ₅
Al2	12i	..m	0.3113	0.3113	0.0332		pentacapped trigonal prism Cu ₁₁
Cu3	6g	2.mm	0.1447	1/2	1/2		pseudo Frank-Kasper Al ₆ Cu ₇
Cu4	6f	2.mm	0.3549	0	0		pseudo Frank-Kasper Cu ₉ Al ₄
Cu5	4e	.3m	0.1066	0.1066	0.1066		icosahedron Cu ₉ Al ₃
Cu6	4e	.3m	0.3296	0.3296	0.3296		icosahedron Cu ₆ Al ₆
Al7	4e	.3m	0.6157	0.6157	0.6157		pseudo Frank-Kasper Cu ₁₀ Al ₃
Cu8	4e	.3m	0.8253	0.8253	0.8253		pseudo Frank-Kasper Al ₄ Cu ₉

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.024

Remarks: For Mn₃In mixed occupation is reported for the tetrahedron sites of one unit, all other sites being occupied exclusively by Mn. In [1] the positions of former A:OH and B:OH are misprinted as 6g 0 0 z instead of 6f 0 0 z for A:OH and 6g $\frac{1}{2} \frac{1}{2} z$ for B:OH (see [5]). In [3] the position of former B:OH is misprinted as 6f 0 0 z instead of 6g $\frac{1}{2} \frac{1}{2} z$ (see [6]).

References: [1] Arnberg L., Westman S. (1978), Acta Crystallogr. A 34, 399-404. [2] (1931), Strukturberichte 1, 498. [3] Stokhuyzen R., Brandon J.K., Chieh P.C., Pearson W.B. (1974), Acta Crystallogr. B 30, 2910-2911. [4] Brandon J.K., Kim H.S., Pearson W.B. (1979), Acta Crystallogr. B 35, 1937-1944. [5] (1980), Structure Reports 44A, 5. [6] (1976), Structure Reports 40A, 54.

215
cP52

Ti ₈ In ₅	cP52	(215) <i>P</i> -43 <i>m</i> – i ² gfe ⁴
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Ti₈In₅ [1]

Structural features: Two kinds of 26-atom γ brass-type nested polyhedra unit (a Ti₄/In₄ inner tetrahedron surrounded by a Ti₄/In₄ outer tetrahedron, a Ti₆/Ti₆ octahedron and a In₁₂/Ti₁₂ cuboctahedron) in a CsCl-type arrangement. Ordering variant of Cu₉Al₄.

Gulay L.D., Schuster J.C. (2003) [1]

In₅Ti₈

$a = 0.99578$ nm, $V = 0.9874$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	12i	..m	0.1838	0.1838	0.5204		pentacapped trigonal prism Ti ₁₀ In
Ti2	12i	..m	0.31	0.31	0.042		pentacapped trigonal prism Ti ₅ In ₆
Ti3	6g	2.mm	0.122	1/2	1/2		pseudo Frank-Kasper Ti ₉ In ₄
Ti4	6f	2.mm	0.347	0	0		pseudo Frank-Kasper In ₈ Ti ₅
In5	4e	.3m	0.1162	0.1162	0.1162		icosahedron Ti ₆ In ₆
Ti6	4e	.3m	0.337	0.337	0.337		icosahedron In ₃ Ti ₉
Ti7	4e	.3m	0.625	0.625	0.625		pseudo Frank-Kasper In ₄ Ti ₉
In8	4e	.3m	0.8293	0.8293	0.8293		pseudo Frank-Kasper Ti ₇ In ₆

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, R_B = 0.038

References: [1] Gulay L.D., Schuster J.C. (2003), J. Alloys Compd. 360, 137-142.

215
cP52

$\text{Cd}_{10.75}\text{Pd}_2$	<i>cP52</i>	(215) <i>P-43m</i> – i^2gfe^4
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Pd₈Cd₄₃ [1], γ -brass

Structural features: 26-atom γ brass-type nested polyhedra units (a Cd₄ inner tetrahedron surrounded by a Pd₄ outer tetrahedron, a Cd₆ octahedron and Cd₁₂ cuboctahedron) in a W-type (b.c.c.) arrangement; disordered vacancies in the inner tetrahedron of every second unit.

Arnberg L. (1980) [1]

 $\text{Cd}_{10.75}\text{Pd}_2$ $a = 0.99415 \text{ nm}$, $V = 0.9826 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cd1	12 <i>i</i>	.. <i>m</i>	0.1924	0.1924	0.5448		15-vertex Frank-Kasper Pd ₂ Cd ₁₃
Cd2	12 <i>i</i>	.. <i>m</i>	0.3038	0.3038	0.0474		15-vertex Frank-Kasper Pd ₂ Cd ₁₃
Cd3	6 <i>g</i>	2.. <i>mm</i>	0.1444	$\frac{1}{2}$	$\frac{1}{2}$		pseudo Frank-Kasper Cd ₁₁ Pd ₂
Cd4	6 <i>f</i>	2.. <i>mm</i>	0.3493	0	0		pseudo Frank-Kasper Cd ₁₁ Pd ₂
Cd5	4 <i>e</i>	.. <i>3m</i>	0.1048	0.1048	0.1048	0.75	icosahedron Cd ₉ Pd ₃
Pd6	4 <i>e</i>	.. <i>3m</i>	0.3292	0.3292	0.3292		icosahedron Cd ₁₂
Cd7	4 <i>e</i>	.. <i>3m</i>	0.6073	0.6073	0.6073		pseudo Frank-Kasper Cd ₉ Pd ₄
Pd8	4 <i>e</i>	.. <i>3m</i>	0.8266	0.8266	0.8266		pseudo Frank-Kasper Cd ₁₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.132$

Remarks: Preliminary data in [2]. In table 2 of [1] the Wyckoff positions of former A OH and B OH are interchanged.

References: [1] Arnberg L. (1980), Acta Crystallogr. B 36, 527-532. [2] Nowotny H., Stempf A., Bittner H. (1951), Monatsh. Chem. 82, 949-958.

215
cP52

$\text{Sc}_{4.75}\text{OsBr}_7$	<i>cP52</i>	(215) <i>P-43m</i> – i^3e^4
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Sc₁₉Os₄Br₂₈ [1]

Structural features: Os₄Sc₁₆ clusters (an Os₄ tetrahedron surrounded by a Sc₁₂ truncated tetrahedron and a Sc₄ tetrahedron) and Sc₃ trigonal units (partial occupation of the vertices of a Sc₄ tetrahedron) in a CsCl-type arrangement, interconnected via Br atoms (Os₄Sc₁₆Br₂₀ and (Sc₃□)Br₈ clusters).

Steinwand S.J. et al. (1997) [1]

 $\text{Br}_7\text{OsSc}_{4.72}$ $a = 1.10032 \text{ nm}$, $V = 1.3322 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sc1	12 <i>i</i>	.. <i>m</i>	0.1169	0.1169	0.3286		octahedron OsBr ₅
Br2	12 <i>i</i>	.. <i>m</i>	0.1274	0.1274	0.6027		tetrahedron Sc ₄
Br3	12 <i>i</i>	.. <i>m</i>	0.3651	0.3651	0.1259		non-coplanar triangle Sc ₃
Os4	4 <i>e</i>	.. <i>3m</i>	0.0973	0.0973	0.0973		tricapped trigonal prism Sc ₆ Os ₃
Sc5	4 <i>e</i>	.. <i>3m</i>	0.384	0.384	0.384	0.72	octahedron Br ₆
Br6	4 <i>e</i>	.. <i>3m</i>	0.6265	0.6265	0.6265		non-coplanar triangle Sc ₃
Sc7	4 <i>e</i>	.. <i>3m</i>	0.8614	0.8614	0.8614		octahedron Os ₃ Br ₃

Experimental: single crystal, diffractometer, X-rays, $wR = 0.034$

References: [1] Steinwand S.J., Corbett J.D., Martin J.D. (1997), Inorg. Chem. 36, 6413-6422.

215
cP52

$(\text{Cu}_{0.1}\text{Zn}_{0.4}\text{Ni}_{0.5})_{10.4}\text{Sn}_{8.7}$	<i>cP52</i>	(215) <i>P-43m</i> – i^3ge^2ba
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Sn_{8.7}(Ni_{0.5}Zn_{0.4}Cu_{0.1})_{10.4} [1]

Structural features: Defect derivative of W (prototype for a b.c.c. atom arrangement) with 14 of 54 positions per unit cell vacant (ignoring additional disordered vacancies).

Larsson A.K. et al. (1994) [1]

$\text{Cu}_{0.99}\text{Ni}_{4.95}\text{Sn}_{8.75}\text{Zn}_{3.96}$

$a = 0.8854 \text{ nm}$, $V = 0.6941 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	12i	..m	0.1296	0.1296	0.5066	0.44	
M2	12i	..m	0.1807	0.1807	0.4969	0.52	
M3	12i	..m	0.3477	0.3477	0.0061	0.86	
Sn4	6g	2.mm	0.2108	$\frac{1}{2}$	$\frac{1}{2}$	0.97	tricapped trigonal prism Ni ₉
M5	4e	.3m	0.1737	0.1737	0.1737		
Sn6	4e	.3m	0.827	0.827	0.827		
M7	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.87	octahedron Sn ₆
M8	1a	-43m	0	0	0	0.75	square prism (cube) Sn ₈

M2 = 0.5Ni + 0.4Zn + 0.1Cu; M3 = 0.5Ni + 0.4Zn + 0.1Cu; M5 = 0.60Sn + 0.20Ni + 0.16Zn + 0.04Cu; M7 = 0.5Ni + 0.4Zn + 0.1Cu; M8 = 0.5Ni + 0.4Zn + 0.1Cu

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.054, T = 293 K

Remarks: Ni/Cu/Zn ratio from electron microprobe analysis. Short interatomic distances for partly occupied site(s).

References: [1] Larsson A.K., Lidin S., Jacob M. (1994), Acta Crystallogr. C 50, 9-12.

215
cP53

$\text{Li}_{14}\text{W}_7\text{O}_{28}[\text{H}_2\text{O}]_4$	<i>cP53</i>	(215) <i>P-43m</i> – i^2fe^4dcb
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7Li₂WO₄·4H₂O [1]

Structural features: LiW₄O₁₆ units (a central Li atom surrounded by four edge-linked WO₆ octahedra) and single WO₄ tetrahedra are interconnected via Li(O₃[OH₂]) tetrahedra to form a 3D-framework.

Hüllen A. (1966) [1]

$\text{H}_8\text{Li}_{14}\text{O}_{32}\text{W}_7$

$a = 0.832 \text{ nm}$, $V = 0.5759 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.125	0.125	0.625		non-collinear WLi
O2	12i	..m	0.368	0.368	0.132		non-coplanar triangle Li ₂ W
Li3	6f	2.mm	0.23	0	0		tetrahedron (OH ₂) ₂ O ₂
(OH ₂)4	4e	.3m	0.13	0.13	0.13		tetrahedron Li ₄
Li5	4e	.3m	0.25	0.25	0.25		trigonal bipyramid WO ₃ (OH ₂)
W6	4e	.3m	0.356	0.356	0.356		8-vertex polyhedron Li ₂ O ₆
O7	4e	.3m	0.62	0.62	0.62		4-vertex polyhedron LiW ₃
W8	3d	-42.m	$\frac{1}{2}$	0	0		octahedron O ₄ Li ₂

Li9	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	tetrahedron O ₄
Li10	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	square prism (cube) O ₄ W ₄

Experimental: single crystal, diffractometer, X-rays, R = 0.144

Remarks: Short interatomic distances: d(W6-Li3) = 0.153 nm. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hüllen A. (1966), Ber. Bunsen-Ges. 70, 598-606.

215
cP53

Fe ₂₁ O ₃₁ [OH]	cP53	(215) <i>P</i> -43m – i ³ e ³ dba
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Fe₂O₃ γ deficient [1]

Structural features: Close-packed O layers in c stacking; Fe in tetrahedral and octahedral voids. Defect derivative of γ-Fe₂O₃ with four octahedral Fe replaced by a central Fe in tetrahedral coordination.

Sinha K.P., Sinha A.P.B. (1957) [1]

Fe₂₁HO₃₂

a = 0.835 nm, *V* = 0.5822 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	..m	0.125	0.125	0.625		non-coplanar triangle Fe ₃
O2	12i	..m	0.375	0.375	0.125		tetrahedron Fe ₄
Fe3	12i	..m	0.375	0.375	0.875		octahedron O ₆
O4	4e	.3m	0.125	0.125	0.125		colinear Fe ₂
Fe5	4e	.3m	0.25	0.25	0.25		tetrahedron O ₄
O6	4e	.3m	0.625	0.625	0.625		tetrahedron Fe ₄
Fe7	3d	-42.m	$\frac{1}{2}$	0	0		tetrahedron O ₄
Fe8	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄
Fe9	1a	-43m	0	0	0		tetrahedron O ₄
H10	4e	.3m	0.875	0.875	0.875	0.25	

Transformation from published data: -*x*, -*y*, -*z*; origin shift $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$

Experimental: powder, film, X-rays

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Ambiguous data: OH units are considered in the text, but the published H site is closer to Fe than to O.

References: [1] Sinha K.P., Sinha A.P.B. (1957), Z. Anorg. Allg. Chem. 293, 228-232.

215
cP54

Cd ₅ Pt	cP54	(215) <i>P</i> -43m – i ² gf ² e ³
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Pt₈Cd₄₀ [1]

Structural features: 26-atom γ brass- (a Cd₄ inner tetrahedron surrounded by a Pt₄ outer tetrahedron, a Cd₆ octahedron and a Cd₁₂ cuboctahedron) and 22-atom Ti₂Ni-type (a Cd₆ octahedron (split site) surrounded by a Pt₄ tetrahedron and a Cd₁₂ cuboctahedron) nested polyhedra units in a CsCl-type arrangement.

Arnberg L. (1980) [1]

Cd₅Pt

a = 0.992 nm, *V* = 0.9762 nm³, *Z* = 8

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	12i	..m	0.182	0.182	0.464		
Cd2	12i	..m	0.296	0.296	0.949		
Cd3	6g	2.mm	0.144	1/2	1/2		pseudo Frank-Kasper Cd ₁₁ Pt ₂
Cd4	6f	2.mm	0.260	0	0	0.4	
Cd5	6f	2.mm	0.337	0	0	0.6	
Pt6	4e	.3m	0.1832	0.1832	0.1832		
Cd7	4e	.3m	0.390	0.390	0.390		pseudo Frank-Kasper Pt ₄ Cd ₉
Pt8	4e	.3m	0.6688	0.6688	0.6688		icosahedron Cd ₁₂

Transformation from published data: -x,-y,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.107

Remarks: Phase referred to as γ -(CdPt), homogeneity range Cd_{100-x}Pt_x, 14.5 < x < 17.5. Short interatomic distances for partly occupied site(s). In table 4 of [1] the Wyckoff positions 6f and 6g are interchanged.

References: [1] Arnberg L. (1980), Acta Crystallogr. B 36, 527-532.

215
cP54

Na ₈ (Al _{0.5} Si _{0.5}) ₁₂ [SO ₄]O ₂₄ -a	cP54	(215) <i>P</i> -43m – i ² he ⁴ ba
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Na₈Al₆Si₆O₂₄SO₄ [1], nosean, zeolite SOD-SO₄

Structural features: (Al,Si)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), part of which are centered by SO₄ tetrahedra (disorder); Na near the centers of and above 6-rings.

Saalfeld A. (1959) [1]

Al₆Na₈O₂₈SSi₆

a = 0.905 nm, *V* = 0.7412 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.144	0.144	0.527		non-colinear Al ₂
O2	12i	..m	0.355	0.355	0.028		non-colinear Al ₂
M3	12h	2..	0.25	1/2	0		tetrahedron O ₄
O4	4e	.3m	0.117	0.117	0.117	0.5	single atom S
Na5	4e	.3m	0.265	0.265	0.265		4-vertex polyhedron O ₄
O6	4e	.3m	0.627	0.627	0.627	0.5	single atom S
Na7	4e	.3m	0.825	0.825	0.825		7-vertex polyhedron O ₆ S
S8	1b	-43m	1/2	1/2	1/2	0.5	tetrahedron O ₄
S9	1a	-43m	0	0	0	0.5	tetrahedron O ₄

M3 = 0.5Al + 0.5Si

Transformation from published data: -x,-y,-z

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Natural specimen from Laacher See. In [1] the coordinates of the Na sites are given as 0.150-0.200 and 0.720-0.750, respectively; we took average values.

References: [1] Saalfeld A. (1959), Neues Jahrb. Mineral., Monatsh. 1959, 38-46.

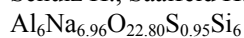
215
cP54

Na ₈ (Al _{0.5} Si _{0.5}) ₁₂ [SO ₄]O ₂₄ -b	cP54	(215) <i>P</i> -43m – i ² he ⁴ ba
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Na₈Al₆Si₆O₂₄SO₄ [1], nosean, zeolite SOD-SO₄

Structural features: (Al,Si)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra), part of which are centered by SO₄ tetrahedra; Na distributed over several sites along <111> (disorder).

Schulz H., Saalfeld H. (1966) [1]



$$a = 0.905 \text{ nm}, V = 0.7412 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.133	0.133	0.529	0.95	non-colinear Al ₂
O2	12i	..m	0.342	0.342	0.04	0.95	non-colinear Al ₂
M3	12h	2..	0.252	1/2	0		tetrahedron O ₄
Na4	4e	.3m	0.228	0.228	0.228	0.52	
Na5	4e	.3m	0.309	0.309	0.309	0.31	
Na6	4e	.3m	0.686	0.686	0.686	0.53	
Na7	4e	.3m	0.78	0.78	0.78	0.38	
S8	1b	-43m	1/2	1/2	1/2	0.48	square prism (cube) Na ₈
S9	1a	-43m	0	0	0	0.47	square prism (cube) Na ₈

$$\text{M3} = 0.5\text{Al} + 0.5\text{Si}$$

Transformation from published data: -x,-y,-z; origin shift 1/2 1/2 1/2

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.150

Remarks: Natural specimen from Laacher See. O of sulfate groups not located; refinements including more partly occupied sites did not give a better agreement. Short interatomic distances for partly occupied site(s). In table 1 of [1] the Wyckoff position of former S(2) is misprinted as 1a instead of 1b.

References: [1] Schulz H., Saalfeld H. (1966), Tschermarks Mineral. Petrogr. Mitt. 10, 225-232.

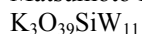
215
cP56

$\text{K}_8\text{W}_{11}[\text{SiO}_4]\text{O}_{35}[\text{H}_2\text{O}]_{13}$	cP56	(215) <i>P</i> -43m – i ⁴ eda
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K₈SiW₁₁O₃₉·13H₂O α [1]

Structural features: SiW₁₁O₃₉ Keggin units (twelve edge- and vertex-linked (W,□)O₆ octahedra sharing vertices with a central SiO₄ tetrahedron, every twelfth octahedron being vacant in statistical disorder) in a Po-type (primitive cubic) arrangement.

Matsumoto K.Y., Sasaki Y. (1976) [1]



$$a = 1.0654 \text{ nm}, V = 1.2093 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	..m	0.112	0.112	0.7092		non-colinear W ₂
O2	12i	..m	0.1412	0.1412	0.3328		non-colinear W ₂
W3	12i	..m	0.2349	0.2349	0.9962	0.917	octahedron O ₆
O4	12i	..m	0.3438	0.3438	0.9715	0.917	single atom W
O5	4e	.3m	0.0877	0.0877	0.0877		single atom Si
K6	3d	-42.m	1/2	0	0		square prism (cube) O ₈
Si7	1a	-43m	0	0	0		tetrahedron O ₄

Transformation from published data: -x,-y,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.069

Remarks: H₂O and part of K not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Matsumoto K.Y., Sasaki Y. (1976), Bull. Chem. Soc. Jpn. 49, 156-158.

215
cP58

Cu ₄ In ₉ Se ₁₆	cP58	(215) $P\text{-}43m - i^2hfe^4$
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Cu₄In₉Se₁₆ [1]

Structural features: Close-packed Se layers in c stacking, Cu and In in tetrahedral voids.

Djega Mariadassou C. et al. (1980) [1]

Cu₄In₉Se₁₆

$a = 1.1533 \text{ nm}$, $V = 1.5340 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	12i	..m	0.138	0.138	0.6169		tetrahedron CuIn ₃
Se2	12i	..m	0.3803	0.3803	0.1486		non-coplanar triangle CuIn ₂
In3	12h	2..	0.2647	$\frac{1}{2}$	0		tetrahedron Se ₄
In4	6f	2.mm	0.2561	0	0		tetrahedron Se ₄
Se5	4e	.3m	0.1273	0.1273	0.1273		tetrahedron CuIn ₃
Cu6	4e	.3m	0.2494	0.2494	0.2494		tetrahedron Se ₄
Se7	4e	.3m	0.6336	0.6336	0.6336		single atom Cu
Cu8	4e	.3m	0.7505	0.7505	0.7505		tetrahedron Se ₄

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.100

Remarks: Idealized coordinates are reported in [2] (Cu-rich β -phase). Composition doubtful according to [3], Cu₇In₁₉Se₃₂ would be in agreement with valence electron rules.

References: [1] Djega Mariadassou C., Rimsky A., Lesueur R., Albany J.H. (1980), Jpn. J. Appl. Phys. Suppl. 19-3, 89-93. [2] Hönle W., Kühn G., Boehnke U.C. (1989), J. Mater. Sci. 24, 2483-2487. [3] Parthé E., Gelato L., Chabot B., Penzo M., Cenzual K., Gladyshevskii R. (1993/1994), Gmelin Handbook of Inorganic and Organometallic Chemistry, 8th Ed., TYPX – Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Vol. 4, p. 1541.

215
cP60

BaAu ₂ F ₁₂	cP60	(215) $P\text{-}43m - i^4e^2da$
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Ba(AuF₆)₂ [1]

Structural features: Single AuF₆ octahedra.

Popov A.I. et al. (1990) [1]

Au₂BaF₁₂

$a = 0.9901 \text{ nm}$, $V = 0.9706 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12i	..m	0.123	0.123	0.311		single atom Au
F2	12i	..m	0.126	0.126	0.686		single atom Au
F3	12i	..m	0.374	0.374	0.186		single atom Au
F4	12i	..m	0.377	0.377	0.811		single atom Au
Au5	4e	.3m	0.249	0.249	0.249		octahedron F ₆

Au6	4e	.3m	0.748	0.748	0.748	octahedron F ₆
Ba7	3d	-42.m	$\frac{1}{2}$	0	0	square prism (cube) F ₈
Ba8	1a	-43m	0	0	0	24-vertex polyhedron F ₂₄

Transformation from published data: -x,-y,-z

Experimental: powder, diffractometer, X-rays, R_p = 0.084

References: [1] Popov A.I., Val'kovskii M.D., Kiselev Y.M., Chumaevskii N.A., Sokolov V.B., Spirin S.N. (1990), Russ. J. Inorg. Chem. 35, 1122-1127.

215
cP63

Cu ₁₄ In _{16.7} Se ₃₂	cP63	(215) <i>P</i> -43m – i ⁴ e ² dca
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Cu₁₄In_{16.7}Se₃₂ [1]

Structural features: Close-packed Se layers in c stacking, Cu and In in tetrahedral voids (partial disorder).

Hönle W. et al. (1989) [1]

Cu_{12.32}In_{18.04}Se₃₂

a = 1.1534 nm, *V* = 1.5344 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	12i	.m	0.1219	0.1219	0.6293		tetrahedron Cu ₃ In
In2	12i	.m	0.25	0.25	0.4989		tetrahedron Se ₄
M3	12i	.m	0.2502	0.2502	0.0		tetrahedron Se ₄
Se4	12i	.m	0.3793	0.3793	0.1144		tetrahedron Cu ₂ In ₂
Se5	4e	.3m	0.1278	0.1278	0.1278		tetrahedron Cu ₃ In
Se6	4e	.3m	0.6138	0.6138	0.6138		non-coplanar triangle In ₃
M7	3d	-42.m	$\frac{1}{2}$	0	0		tetrahedron Se ₄
Cu8	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.816	tetrahedron Se ₄
In9	1a	-43m	0	0	0	0.912	tetrahedron Se ₄

M3 = 0.68Cu + 0.32In; M7 = 0.57Cu + 0.43In

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.046

Remarks: In the abstract of [1] the cell parameter is misprinted as 1.1534 nm instead of 1.1543 nm (given in table II; checked on interatomic distances).

References: [1] Hönle W., Kühn G., Boehnke U.C. (1989), J. Mater. Sci. 24, 2483-2487.

215
cP64

Cu ₂₅ (V _{0.57} Sn _{0.43}) ₃ (Sb _{0.08} As _{0.92}) ₄ S ₃₂	cP64	(215) <i>P</i> -43m – i ⁴ e ² dcb
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Cu₂₅(V_{0.57}Sn_{0.43})₃(As_{0.92}Sb_{0.08})₄S₃₂ [1], colusite

Structural features: Close-packed S layers in c stacking; Cu, (V,Sn) and (As,Sb) in tetrahedral voids.

Dangel P.N., Wuensch B.J. (1970) [1]

As_{3.68}Cu₂₅S₃₂Sb_{0.32}Sn_{1.29}V_{1.71}

a = 1.0629 nm, *V* = 1.2008 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	12i	.m	0.125	0.125	0.625		tetrahedron Cu ₃ V
Cu2	12i	.m	0.25	0.25	0.0		tetrahedron S ₄

Cu3	12i	$\bar{3}m$	0.25	0.25	0.5	tetrahedron S ₄
S4	12i	$\bar{3}m$	0.375	0.375	0.125	tetrahedron Cu ₃ As
S5	4e	$\bar{3}m$	0.125	0.125	0.125	tetrahedron Cu ₄
S6	4e	$\bar{3}m$	0.625	0.625	0.625	tetrahedron AsCu ₃
M7	3d	$\bar{4}2.m$	$\frac{1}{2}$	0	0	tetrahedron S ₄
M8	3c	$\bar{4}2.m$	0	$\frac{1}{2}$	$\frac{1}{2}$	tetrahedron S ₄
M9	1b	$\bar{4}3m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	tetrahedron S ₄
Cu10	1a	$\bar{4}3m$	0	0	0	tetrahedron S ₄

M7 = 0.57V + 0.43Sn; M8 = 0.92As + 0.08Sb; M9 = 0.92As + 0.08Sb

Experimental: single crystal, Weissenberg and precession photographs, X-rays

Remarks: Natural specimen of unknown origin. Composition Cu_{25.04}(V_{0.57}Sn_{0.43})_{3.25}(Sb_{0.08}As_{0.92})_{4.00}S_{31.68} from electron microprobe analysis, small amounts of Fe detected. Idealized coordinates. Ambiguous data: ordered arrangement of 25 Cu, 3 (V,Sn) and 4 (As,Sb) is stated, but several possibilities exist; we arbitrarily assigned one of them. The structure was later redetermined in space group (218) *P*-43*n* [2].

References: [1] Dangel P.N., Wuensch B.J. (1970), Am. Mineral. 55, 1787-1791. [2] Spry P.G., Merlino S., Wang S., Zhang X., Buseck P.R. (1994), Am. Mineral. 79, 750-762.

215
*cP*68

Gd ₅ MnI ₇	<i>cP</i> 68	(215) <i>P</i> -43 <i>m</i> – i ⁴ e ⁵
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Gd₅I₇Mn [1]

Structural features: Mn₄Gd₁₆I₂₀ units (a Mn₄ tetrahedron surrounded by a Gd₁₂ truncated tetrahedron, a large Gd₄ tetrahedron and an I₂₀ polyhedron) and Gd₄I₄ clusters (a Gd₄ tetrahedron surrounded by an I₄ tetrahedron) share atoms to form a 3D-framework.

Ebihara M. et al. (1994) [1]

Gd₅I₇Mn

a = 1.21765 nm, *V* = 1.8054 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Gd1	12i	$\bar{3}m$	0.11504	0.11504	0.32288		
I2	12i	$\bar{3}m$	0.133	0.133	0.59775		4-vertex polyhedron Gd ₄
I3	12i	$\bar{3}m$	0.3705	0.3705	0.1268	0.75	
I4	12i	$\bar{3}m$	0.3724	0.3724	0.1057	0.25	
Mn5	4e	$\bar{3}m$	0.0821	0.0821	0.0821		tricapped trigonal prism Mn ₃ Gd ₆
Gd6	4e	$\bar{3}m$	0.3521	0.3521	0.3521	0.241	
Gd7	4e	$\bar{3}m$	0.3883	0.3883	0.3883	0.759	
I8	4e	$\bar{3}m$	0.634	0.634	0.634		
Gd9	4e	$\bar{3}m$	0.85765	0.85765	0.85765		octahedron Mn ₃ I ₃

Experimental: single crystal, diffractometer, X-rays, wR = 0.034

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Ebihara M., Martin J.D., Corbett J.D. (1994), Inorg. Chem. 33, 2079-2084.

215
*cP*72

YMn ₂ H _{1.26}	<i>cP</i> 72	(215) <i>P</i> -43 <i>m</i> – i ⁵ e ² ca
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YMn₂H_{1.15} It [1]

Structural features: Filled-up derivative of MgCu_2 (cubic Laves phase) with H in tetrahedral (Y_2Mn_2) voids.

Latroche M. et al. (2000) [1]

$\text{D}_{1.26}\text{Mn}_2\text{Y}$

$a = 0.7855 \text{ nm}$, $V = 0.4847 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12i	$\dots m$	0.0344	0.0344	0.7429	0.184	
Mn2	12i	$\dots m$	0.1358	0.1358	0.3837		non-collinear D_2
D3	12i	$\dots m$	0.1808	0.1808	0.0039	0.076	non-coplanar triangle D_3
D4	12i	$\dots m$	0.3064	0.3064	0.0258	0.416	non-coplanar triangle DMn_2
D5	12i	$\dots m$	0.4575	0.4575	0.7315	0.164	
Mn6	4e	$\dots m$	0.3659	0.3659	0.3659		
Y7	4e	$\dots m$	0.7496	0.7496	0.7496		
Y8	3c	$\dots m$	0	$\frac{1}{2}$	$\frac{1}{2}$		
Y9	1a	$\dots m$	0	0	0		

Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, neutrons, $R_B = 0.076$, $T = 10 \text{ K}$

Remarks: Phase stable at $T < 217 \text{ K}$.

References: [1] Latroche M., Paul Boncour V., Percheron Guégan A., Bourée Vigneron F., André G. (2000), J. Solid State Chem. 154, 398-404.

215
cP74

$\text{K}_7\text{V}(\text{V}_{0.33}\text{W}_{0.67})_{12}\text{O}_{40}[\text{H}_2\text{O}]_{12}$	<i>cP74</i>	(215) $P\text{-}43m - i^5\text{geda}$
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$\text{K}_7[\text{V}(\text{V}_4\text{W}_8)\text{O}_{40}] \cdot 12\text{H}_2\text{O}$ [1]; $\text{K}_3\text{H}_6[\text{P}(\text{W}_9\text{O}_{34})\text{O}_{34}] \cdot 18\text{H}_2\text{O}$ [2]

Structural features: $\text{V}(\text{W},\text{V})_{12}\text{O}_{40}$ Keggin units (twelve edge- and vertex-linked $(\text{W},\text{V})\text{O}_6$ octahedra sharing vertices with a central VO_4 tetrahedron) in a Po-type (primitive cubic) arrangement; K and H_2O between the units (partial disorder for the former).

Nishikawa K. et al. (1975) [1]

$\text{H}_{24}\text{K}_7\text{O}_{52}\text{V}_5\text{W}_8$

$a = 1.062 \text{ nm}$, $V = 1.1978 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	$\dots m$	0.1101	0.1101	0.7194		non-collinear W_2
O2	12i	$\dots m$	0.1428	0.1428	0.3211		non-collinear W_2
M3	12i	$\dots m$	0.2351	0.2351	0.003		octahedron O_6
$(\text{OH}_2)_4$	12i	$\dots m$	0.3113	0.3113	0.4766		7-vertex polyhedron $(\text{OH}_2)_4\text{K}_2\text{O}$
O5	12i	$\dots m$	0.3476	0.3476	0.9818		single atom W
K6	6g	$2.m.m$	0.1423	$\frac{1}{2}$	$\frac{1}{2}$	0.667	tricapped trigonal prism $\text{O}_4(\text{OH}_2)_4\text{K}$
O7	4e	$\dots m$	0.0948	0.0948	0.0948		single atom V
K8	3d	$\dots m$	$\frac{1}{2}$	0	0		square prism (cube) O_8
V9	1a	$\dots m$	0	0	0		tetrahedron O_4

$\text{M3} = 0.667\text{W} + 0.333\text{V}$

Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.057$

Remarks: Space groups (207) $F432$ and (221) $Pm-3m$ were tested and rejected. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nishikawa K., Kobayashi A., Sasaki Y. (1975), Bull. Chem. Soc. Jpn. 48, 3152-3155. [2] Fuchs J., Palm R. (1984), Z. Naturforsch. B 39, 757-762.

215
cP75

$K_6V(V_{0.17}Mo_{0.83})_{12}O_{40}[H_2O]_{13}$	<i>cP75</i>	(215) $P-43m - i^5gedba$
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$K_6[V(V_2Mo_{10})O_{40}] \cdot 13H_2O$ [1]

Structural features: $V(Mo,V)_{12}O_{40}$ Keggin units (twelve edge- and vertex-linked $(Mo,V)O_6$ octahedra sharing vertices with a central VO_4 tetrahedron) in a Po-type (primitive cubic) arrangement; K and H_2O between the units (partial disorder for the former).

Björnberg A., Hedman B. (1980) [1]

$H_{26}K_6Mo_{10}O_{53}V_3$

$a = 1.06124 \text{ nm}$, $V = 1.1952 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	$\dots m$	0.1072	0.1072	0.7214		non-collinear Mo_2
O2	12i	$\dots m$	0.1396	0.1396	0.3201		non-collinear Mo_2
M3	12i	$\dots m$	0.23264	0.23264	0.99981		octahedron O_6
$(OH_2)_4$	12i	$\dots m$	0.2771	0.2771	0.5057		non-coplanar triangle K_2O
O5	12i	$\dots m$	0.3401	0.3401	0.0093		single atom Mo
K6	6g	$2.mmm$	0.1339	$\frac{1}{2}$	$\frac{1}{2}$	0.5	tricapped trigonal prism $O_4(OH_2)_4K$
O7	4e	$.3m$	0.0895	0.0895	0.0895		single atom V
K8	3d	$-42.m$	$\frac{1}{2}$	0	0		square prism (cube) O_8
$(OH_2)_9$	1b	$-43m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		18-vertex polyhedron $(OH_2)_{12}K_6$
V10	1a	$-43m$	0	0	0		tetrahedron O_4

$M3 = 0.833Mo + 0.167V$

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.061$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Björnberg A., Hedman B. (1980), Acta Crystallogr. B 36, 1018-1022.

215
cP76

$Au_6(Au_{0.5}In_{0.5})_6In$	<i>cP76</i>	(215) $P-43m - j^2gfe^4$
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In_4Au_9 [1], γ -brass

Structural features: Two kinds of 26-atom γ brass-type nested polyhedra unit (an In_4/Au_4 inner tetrahedron surrounded by a Au_4/Au_4 outer tetrahedron, an Au_6/Au_6 octahedron and an $(Au,In)_{12}/(In,Au)_{12}$ cuboctahedron) in a CsCl-type arrangement; splitting of the atom sites forming cuboctahedra.

Brandon J.K. et al. (1977) [1]

Au_9In_4

$a = 0.9829 \text{ nm}$, $V = 0.9496 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24j	1	0.0361	0.3000	0.3259	0.5	
M2	24j	1	0.1681	0.1969	0.5307	0.5	
Au3	6g	2.mm	0.1425	$\frac{1}{2}$	$\frac{1}{2}$		
Au4	6f	2.mm	0.3566	0	0		
Au5	4e	.3m	0.1080	0.1080	0.1080		
Au6	4e	.3m	0.3341	0.3341	0.3341		
In7	4e	.3m	0.6212	0.6212	0.6212		
Au8	4e	.3m	0.8241	0.8241	0.8241		

M1 = 0.75In + 0.25Au; M2 = 0.75Au + 0.25In

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.082

Remarks: Short interatomic distances for partly occupied site(s). In [2] the cuboctahedron sites are reported to be occupied exclusively by Au and In, respectively, and no site splitting was observed (Cu₉Al₄ type).

References: [1] Brandon J.K., Brizard R.Y., Pearson W.B., Tozer D.J.N. (1977), Acta Crystallogr. B 33, 527-537. [2] Puselj M., Schubert K. (1975), J. Less-Common Met. 41, 33-44.

215
cP76

UO _{2.25}	cP76	(215) <i>P</i> -43 <i>m</i> – j ³ e ² dcba
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U₄O₉ β [1]

Structural features: Close-packed U layers in c stacking; O mainly in tetrahedral voids (high degree of disorder).

Lauriat J.P. et al. (1989) [1]

O_{9.38}U₄

$a = 0.544$ nm, $V = 0.1610$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24j	1	0.126	0.267	0.367	0.055	
O2	12i	..m	0.129	0.129	0.249	0.082	
O3	12i	..m	0.295	0.295	0.166	0.01	
O4	12i	..m	0.379	0.379	0.245	0.034	
O5	4e	.3m	0.123	0.123	0.123	0.025	
U6	4e	.3m	0.7492	0.7492	0.7492		
O7	3d	-42.m	$\frac{1}{2}$	0	0	0.52	
O8	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.99	
O9	1b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.94	
O10	1a	-43m	0	0	0	0.98	tetrahedron O ₄

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, neutrons, R = 0.049, T = 393 K

Remarks: Phase stable at T > 393 K. Average structure. An alternative refinement in space group (216) *F*-43*m* gave R = 0.036. The superstructure was refined in space group (220) *I*-43*d* with 8-fold cell volume. Short interatomic distances for partly occupied site(s).

References: [1] Lauriat J.P., Chevrier G., Boucherle J.X. (1989), J. Solid State Chem. 80, 80-93.

215
cP78

CsRe ₂ I ₂ Cl ₅ [H ₂ O]							cP78	(215) <i>P</i> -43 <i>m</i> – i ⁶ eba
Cs_{1.5}[Re₃I₃Cl_{7.5}(H₂O)_{1.5}] [1]								
Structural features: Re ₃ I ₃ (Cl,OH ₂) ₉ clusters (a Re ₃ triangle surrounded by a coplanar I ₃ triangle, a Cl ₆ trigonal prism and a large (Cl,OH ₂) ₃ triangle, distinct positions for Cl and O).								
Jung B., Meyer G. (1992) [1]								
Cl _{5.04} CsH _{1.92} I ₂ O _{0.96} Re ₂								
<i>a</i> = 1.24106 nm, <i>V</i> = 1.9115 nm ³ , <i>Z</i> = 6								
site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment	
Cl1	12i	..m	0.09	0.09	0.2734		single atom Re	
Cl2	12i	..m	0.1259	0.1259	0.5263	0.52		
(OH ₂)3	12i	..m	0.139	0.139	0.502	0.48		
Re4	12i	..m	0.20939	0.20939	0.34988			
Cl5	12i	..m	0.2985	0.2985	0.4872		single atom Re	
I6	12i	..m	0.3594	0.3594	0.0498		non-collinear Re ₂	
Cs7	4e	.3m	0.7701	0.7701	0.7701			
Cs8	1b	-43 <i>m</i>	¹ / ₂	¹ / ₂	¹ / ₂		cuboctahedron Cl ₁₂	
Cs9	1a	-43 <i>m</i>	0	0	0		12-vertex polyhedron Cl ₁₂	

Transformation from published data: -*x*, -*y*, -*z*

Experimental: single crystal, diffractometer, X-rays, wR = 0.037

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the Wyckoff position of the 12-fold sites is misprinted as 12*m* instead of 12*i*.

References: [1] Jung B., Meyer G. (1992), Z. Anorg. Allg. Chem. 610, 15-19.

215
cP80

HK ₈ W ₁₁ BO ₃₉ [H ₂ O] ₁₃							cP80	(215) <i>P</i> -43 <i>m</i> – i ⁵ g ² eda
K₈H[BW₁₁O₃₉]·13H₂O [1]								
Structural features: BW ₁₁ O ₃₉ Keggin units (twelve edge- and vertex-linked (W,□)O ₆ octahedra sharing vertices with a central BO ₄ tetrahedron, every twelfth octahedron being vacant in statistical disorder) in a Po-type (primitive cubic) arrangement; K and H ₂ O between the units (partial disorder for the former).								
Guoyi F. et al. (1989) [1]								
BH ₂₄ K ₈ O ₅₂ W ₁₁								
<i>a</i> = 1.071 nm, <i>V</i> = 1.2285 nm ³ , <i>Z</i> = 1								
site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment	
O1	12i	..m	0.1025	0.1025	0.2757		non-coplanar triangle W ₂ O	
O2	12i	..m	0.1402	0.1402	0.6859		non-collinear W ₂	
W3	12i	..m	0.2313	0.2313	0.9986	0.917	octahedron O ₆	
(OH ₂)4	12i	..m	0.2779	0.2779	0.4976		non-collinear K ₂	
O5	12i	..m	0.3432	0.3432	0.012		single atom W	
K6	6g	2. <i>mm</i>	0.1257	¹ / ₂	¹ / ₂	0.667		
K7	6g	2. <i>mm</i>	0.2939	¹ / ₂	¹ / ₂	0.167		
O8	4e	.3 <i>m</i>	0.0817	0.0817	0.0817		single atom B	
K9	3d	-42. <i>m</i>	¹ / ₂	0	0		square prism (cube) O ₈	

B10 1a -43m 0 0 0 tetrahedron O₄

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.045

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Guoyi F., Enbo W., Jingfu L., Yonghua L., Songchun J., Endong S. (1989), Yingyong Huaxue 6, 16-20.

215
cP207

Fe₁₁O₁₂

cP207

(215) *P*-43m - j²i²h²g²f²e⁵dca

Fe_{0.902}O [1], wüstite

Structural features: Close-packed O layers in c stacking, Fe mainly in octahedral, in part in tetrahedral voids. Derivative of NaCl with clusters with 13 Fe vacancies and 4 tetrahedral Fe.

Koch F., Cohen J.B. (1969) [1]

Fe₁₁O₁₂

a = 1.284 nm, *V* = 2.1169 nm³, *Z* = 9

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	24j	1	0.000	0.167	0.333		octahedron O ₆
O2	24j	1	0.162	0.332	0.500		square pyramid Fe ₅
O3	12i	..m	0.162	0.162	0.340		octahedron Fe ₆
O4	12i	..m	0.162	0.162	0.660		octahedron Fe ₆
O5	12i	..m	0.167	0.167	0.000		octahedron Fe ₆
Fe6	12i	..m	0.1705	0.1705	0.500		octahedron O ₆
O7	12i	..m	0.333	0.333	0.000		octahedron Fe ₆
Fe8	12i	..m	0.342	0.342	0.176		octahedron O ₆
Fe9	12i	..m	0.342	0.342	0.824		octahedron O ₆
O10	12h	2..	0.167	$\frac{1}{2}$	0		octahedron Fe ₆
Fe11	12h	2..	0.333	$\frac{1}{2}$	0		octahedron O ₆
Fe12	6g	2.mm	0.171	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
O13	6g	2.mm	0.328	$\frac{1}{2}$	$\frac{1}{2}$		coplanar triangle Fe ₃
Fe14	6f	2.mm	0.167	0	0		octahedron O ₆
O15	6f	2.mm	0.333	0	0		octahedron Fe ₆
Fe16	4e	.3m	0.170	0.170	0.170		octahedron O ₆
O17	4e	.3m	0.326	0.326	0.326		tetrahedron Fe ₄
Fe18	4e	.3m	0.410	0.410	0.410		tetrahedron O ₄
O19	4e	.3m	0.674	0.674	0.674		non-coplanar triangle Fe ₃
Fe20	4e	.3m	0.830	0.830	0.830		octahedron O ₆
Fe21	3d	-42.m	$\frac{1}{2}$	0	0		octahedron O ₆
O22	3c	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Fe ₆
O23	1a	-43m	0	0	0		octahedron Fe ₆

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.095

Remarks: The amount of Fe vacancies and tetrahedral Fe could not be determined with accuracy. We derived an approximate cell parameter from the interatomic distances to the tetrahedral Fe site. In [1] the Wyckoff position of the third published O site is misprinted as 24*k* instead of 24*j*.

References: [1] Koch F., Cohen J.B. (1969), Acta Crystallogr. B 25, 275-287.