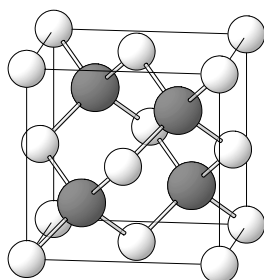


Space group (216) $F\bar{4}3m$ 216
 $cF8$

ZnS	$cF8$	(216) $F\bar{4}3m - ca$
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ZnS 3C [2], sphalerite, zinc blende, Strukturbericht notation B3

Structural features: Close-packed S layers in c stacking, Zn in tetrahedral voids (stacking sequence AaBbCc). ZnS_4 tetrahedra share vertices to form a 3D-framework. Substitution derivative of diamond. See Fig. II.13.

Fig. II.13. **ZnS 3C**

Arrangement of Zn (dark) and S (light) atoms.

Jamieson J.C., Demarest H.H. Jr. (1980) [1]

SZn

 $a = 0.54102 \text{ nm}$, $V = 0.1584 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	4c	$\bar{4}3m$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron Zn_4
Zn2	4a	$\bar{4}3m$	0	0	0		tetrahedron S_4

Experimental: powder, film, X-rays

Remarks: The two atom sites are crystallographically equivalent (may be interchanged).

References: [1] Jamieson J.C., Demarest H.H. Jr. (1980), J. Phys. Chem. Solids 41, 963-964. [2] (1931), Strukturberichte 1, 76.

216
 $cF12$

$Cu_{1.9}S$	$cF12$	(216) $F\bar{4}3m - cba$
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 $Cu_{1.9}S$ [1]; Cu_5FeS_4 [2], bornite; $CuI \gamma$ [3]

Structural features: Close-packed S layers in c stacking; Cu in octahedral and tetrahedral voids.

Kazinets M.M. (1970) [1]

 $Cu_{1.90}S$ $a = 0.5564 \text{ nm}$, $V = 0.1723 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	4c	$\bar{4}3m$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		square prism (cube) Cu_4S_4
Cu2	4b	$\bar{4}3m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.9	fourcapped trigonal prism Cu_4S_6
S3	4a	$\bar{4}3m$	0	0	0		fourcapped trigonal prism Cu_{10}

Experimental: polycrystalline sample, electron diffraction, $R = 0.192$

References: [1] Kazinets M.M. (1970), Sov. Phys. Crystallogr. (Engl. Transl.) 14, 599-600. [2] Tunell G., Adams C.E. (1949), Am. Mineral. 34, 824-829. [3] Kurdyumova R.N., Semiletov S.A. (1962), Sov. Phys. Crystallogr. (Engl. Transl.) 7, 292-295.

216
cF12

MgAgAs	cF12	(216) $F-43m - cba$
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MgAgAs [2], Strukturbericht notation $C1_b$; LiAlSi β [1]; YPtSb [4]; CuMnSb [5]
Structural features: Close-packed As layers in c stacking, Mg and Ag in tetrahedral voids. Alternatively: Mg and Ag form a NaCl-type framework, As in cubic voids. Al and Si form a tetrahedral 3D-framework in β -LiAlSi. See Fig. II.14.

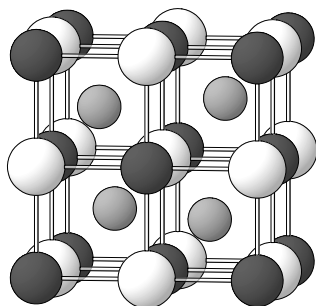


Fig. II.14. **MgAgAs**

Arrangement of Mg (light), Ag (dark) and As (medium) atoms.

Nowotny H., Holub F. (1960) [1]

AgAsMg

$a = 0.621 \text{ nm}$, $V = 0.2395 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	4c	$-43m$	$1/4$	$1/4$	$1/4$		square prism (cube) Mg_4Ag_4
Mg2	4b	$-43m$	$1/2$	$1/2$	$1/2$		fourcapped trigonal prism As_4Ag_6
Ag3	4a	$-43m$	0	0	0		fourcapped trigonal prism As_4Mg_6

Transformation from published data: origin shift $3/4 \ 3/4 \ 3/4$

Experimental: powder, film, X-rays

Remarks: Strukturbericht notation $C1_b$ is not in agreement with the stoichiometry. In [2] the cell parameter is expressed in kX instead of Å as indicated (see [3]). In most isotypic compounds the cubic site is occupied by the most electronegative element, however, exceptions occur.

References: [1] Nowotny H., Holub F. (1960), Monatsh. Chem. 91, 877-887. [2] Nowotny H., Sibert W. (1941), Z. Metallkd. 33, 391-394. [3] (1956), Structure Reports 8, 28. [4] Wenski G., Mewis A. (1986), Z. Kristallogr. 176, 125-134. [5] Forster R.H., Johnston G.B., Wheeler D.A. (1968), J. Phys. Chem. Solids 29, 855-861.

216
cF12

$\text{Hg}_{0.6}(\text{Te}_{0.2}\text{I}_{0.8})$	cF12	(216) $F-43m - cba$
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Hg₃TeI₄ [1]; CuI γ [2]

Structural features: Close-packed (I,Te) layers in c stacking; Hg in tetrahedral voids (partial order).

Wiedemeier H. et al. (1997) [1]

$\text{Hg}_{0.62}\text{I}_{0.80}\text{Te}_{0.20}$

$a = 0.6244 \text{ nm}$, $V = 0.2434 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		square prism (cube) Hg ₈
Hg2	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.119	fourcapped trigonal prism I ₄ Hg ₆
Hg3	4a	-43m	0	0	0	0.5	fourcapped trigonal prism I ₄ Hg ₆

M1 = 0.80I + 0.20Te

Experimental: powder, diffractometer, X-rays, $R_B = 0.059$

Remarks: Correct symmetry is space group (225) $Fm\bar{3}m$ if sites Hg2 and Hg3 have the same occupancy. The authors suggest local ordering exists with red HgI₂-type regions interconnected by SiS₂-type fragments.

References: [1] Wiedemeier H., Hutchins M.A., Grin Y., Feldmann C., Von Schnering H.G. (1997), Z. Anorg. Allg. Chem. 623, 1843-1846. [2] Kurdyumova R.N., Semiletov S.A. (1962), Sov. Phys. Crystallogr. (Engl. Transl.) 7, 292-295.

216
cF16

Li ₂ AgSb	cF16	(216) $F\bar{4}3m$ – dcba
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Li₂AgSb [1]; Li₂AuSn [1]; Li₂CaGe [4]; Li₂MgSn [1]; Li₂RhAl [2]; TiCuHg₂ [3]

Structural features: Close-packed Sb layers in c stacking; part of Li in octahedral, Ag and remaining Li in tetrahedral voids. AgSb₄ tetrahedra share vertices to form a 3D-framework. Substitution derivative of W (prototype for a b.c.c. atom arrangement), sequence along <111>: -Li-Li-Ag-Sb-.

Pauly H. et al. (1968) [1]

AgLi₂Sb

$a = 0.6583$ nm, $V = 0.2853$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		rhombic dodecahedron Li ₁₀ Sb ₄
Li2	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Li ₄ Sb ₄ Ag ₆
Li3	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron Ag ₄ Li ₄ Sb ₆
Sb4	4a	-43m	0	0	0		rhombic dodecahedron Ag ₄ Li ₁₀

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

Remarks: A partly disordered distribution of Li and Ca is reported for Li₂CaGe in [4]. In table 3 of [2] the chemical formula is misprinted as LiRhAl instead of Li₂RhAl.

References: [1] Pauly H., Weiss A., Witte H. (1968), Z. Metallkd. 59, 47-58. [2] Czybulka A., Petersen A., Schuster H.U. (1990), J. Less-Common Met. 161, 303-312. [3] Puselj M., Ban Z. (1969), Croat. Chem. Acta 41, 79-83. [4] Pavlyuk V.V., Dmytriv G.C., Bodak O.I. (1993), Inorg. Mater. 29, 833-834.

216
cF16

LiMgPdSn	cF16	(216) $F\bar{4}3m$ – dcba
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LiMgPdSn [1]

Structural features: Close-packed Sn layers in c stacking; Mg in octahedral, Li and Pd in tetrahedral voids. PdSn₄ tetrahedra share vertices to form a 3D-framework. Substitution derivative of W (prototype for a b.c.c. atom arrangement), sequence along <111>: -Sn-Pd-Mg-Li-. See Fig. II.15.

Eberz U. et al. (1980) [1]

LiMgPdSn

$a = 0.642 \text{ nm}$, $V = 0.2646 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	4 <i>d</i>	-43 <i>m</i>	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		rhombic dodecahedron $\text{Mg}_4\text{Sn}_4\text{Pd}_6$
Pd2	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron $\text{Mg}_4\text{Sn}_4\text{Li}_6$
Mg3	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron $\text{Li}_4\text{Pd}_4\text{Sn}_6$
Sn4	4 <i>a</i>	-43 <i>m</i>	0	0	0		rhombic dodecahedron $\text{Li}_4\text{Pd}_4\text{Mg}_6$

Experimental: single crystal, diffractometer, X-rays, $R = 0.044$

Remarks: The atom sites are crystallographically equivalent (may be interchanged, maintaining the relative shifts along $\langle 111 \rangle$ for the different elements). In table II of [1] the Wyckoff position of the Li site is misprinted as 4*b* instead of 4*d*.

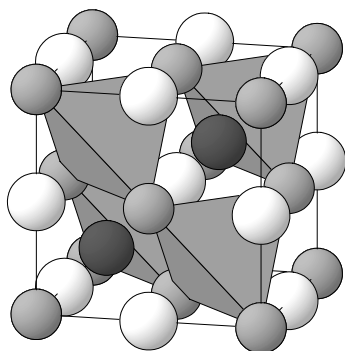


Fig. II.15. **LiMgPdSn**

Arrangement of PdSn_4 tetrahedra (Sn atoms medium), Li (dark) and Mg (light) atoms.

References: [1] Eberz U., Seelentag W., Schuster H.U. (1980), Z. Naturforsch. B 35, 1341-1343.

216
cF20

CuI	<i>cF20</i>	(216) <i>F-43m - ea</i>
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CuI γ [2], marssite

Structural features: Close-packed I layers in c stacking; Cu in tetrahedral voids (displaced along $\langle 111 \rangle$).

Keen D.A., Hull S. (1995) [1]

CuI

$a = 0.60847 \text{ nm}$, $V = 0.2253 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	16 <i>e</i>	.3 <i>m</i>	0.276	0.276	0.276	0.250	
I2	4 <i>a</i>	-43 <i>m</i>	0	0	0		

Experimental: powder, diffractometer, neutrons, time-of-flight, $T = 573 \text{ K}$

Remarks: Phase stable at $T < 643 \text{ K}$; above $\sim 600 \text{ K}$ partial occupation of the remaining tetrahedral positions was observed (Pearson symbol *cF36*). Short interatomic distances for partly occupied site(s). In [1] the occupancy of former Cu2 is misprinted as $1-n(\text{Cu1})$ instead of $\frac{1}{4}-n(\text{Cu1})$.

References: [1] Keen D.A., Hull S. (1995), J. Phys.: Condens. Matter 7, 5793-5804. [2] Bührer W., Hälg W. (1977), Electrochim. Acta 22, 701-704.

216
cF24

K[ClO₄]	<i>cF24</i>	(216) <i>F-43m</i> – eba
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KClO₄ ht [1], Strukturbericht notation H0₅Structural features: K atoms and ClO₄ tetrahedra in a NaCl-type arrangement.

Herrmann K., Ilge W. (1930) [1]

KlKO₄*a* = 0.747 nm, *V* = 0.4168 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	16 <i>e</i>	.3 <i>m</i>	0.125	0.125	0.125		single atom Cl
K2	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		18-vertex polyhedron O ₁₂ Cl ₆
Cl3	4 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron O ₄

Experimental: powder, Debye-Scherrer film, X-rays, *T* = 613 KRemarks: Phase stable at *T* > 573 K.

References: [1] Herrmann K., Ilge W. (1930), Z. Kristallogr. 75, 41-66.

216
cF24

CuI	<i>cF24</i>	(216) <i>F-43m</i> – eca
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CuI α [1]

Structural features: Close-packed I layers in c stacking; Cu in tetrahedral and trigonal voids (disorder).

Miyake S. et al. (1952) [1]

CuI

a = 0.619 nm, *V* = 0.2372 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	16 <i>e</i>	.3 <i>m</i>	0.34	0.34	0.34	0.2	
Cu2	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.2	
I3	4 <i>a</i>	-43 <i>m</i>	0	0	0		

Experimental: powder, Debye film, X-rays, *T* = 703 KRemarks: Phase stable at *T* > 680 K. Partial occupation of a single off-centered tetrahedral site is observed below ~600 K. Short interatomic distances for partly occupied site(s). Correct symmetry is space group (225) *Fm-3m* if sites Cu1 and Cu2 have the same occupancy.

References: [1] Miyake S., Hoshino S., Takenaka T. (1952), J. Phys. Soc. Jpn. 7, 19-24.

216
cF24

Be₅Au	<i>cF24</i>	(216) <i>F-43m</i> – eca
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AuBe₅ [1], Strukturbericht notation C15_b; PdBe₅ [1]; UNi₅ [2]Structural features: Substitution derivative of MgCu₂. AuBe₁₂ and BeBe₁₂ truncated tetrahedra share hexagonal faces to form a 3D-framework. Alternatively: empty Be₄ tetrahedra share vertices to form a 3D-framework; Au and additional Be in truncated tetrahedral voids. Tetrahedrally close-packed structure (Frank-Kasper phase).

Misch L. (1935) [1]

 AuBe_5 $a = 0.6097 \text{ nm}$, $V = 0.2267 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Be1	16e	.3m	0.625	0.625	0.625		icosahedron Be_9Au_3
Be2	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper $\text{Be}_{12}\text{Au}_4$
Au3	4a	-43m	0	0	0		16-vertex Frank-Kasper Be_{16}

Experimental: powder, film, X-rays

Remarks: Idealized coordinates. The Strukturbericht notation is not in agreement with the stoichiometry.

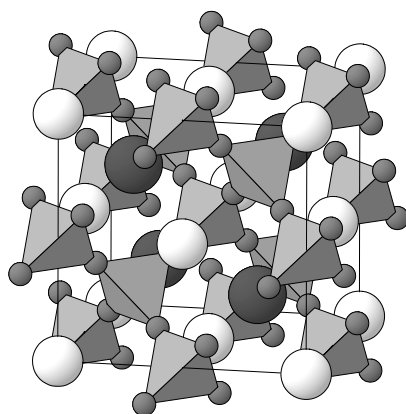
References: [1] Misch L. (1935), Metallwirtsch. Metallwiss. Metalltech. 14, 897-899. [2] Baenziger N.C., Rundle R.E., Snow A.I., Wilson A.S. (1950), Acta Crystallogr. 3, 34-40.

216
 $cF24$

MgCu_4Sn	$cF24$	$(216) F-43m - eca$
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MgCu₄Sn [2]; CaCu_4In [4]; MgCu_4In [6]; YbCu_4In [3]; MgYNi_4 [5]

Structural features: Substitution derivative of MgCu_2 . $\text{Mg}(\text{Sn}_4\text{Cu}_{12})$ and $\text{Sn}(\text{Mg}_4\text{Cu}_{12})$ Friauf polyhedra (Cu_{12} truncated tetrahedron + Sn_4/Mg_4 tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. Alternatively: Cu_4 tetrahedra share vertices to form a 3D-framework; Mg and Sn in truncated tetrahedral voids. Tetrahedrally close-packed structure (Frank-Kasper phase). See Fig. II.16.

Fig. II.16. **MgCu₄Sn**

Arrangement of Cu_4 tetrahedra (Cu atoms medium), Mg (dark) and Sn (light) atoms.

Osamura K., Murakami Y. (1978) [1]

 Cu_4MgSn $a = 0.7042 \text{ nm}$, $V = 0.3492 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	16e	.3m	0.625	0.625	0.625		icosahedron $\text{Cu}_6\text{Mg}_3\text{Sn}_3$
Mg2	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper $\text{Cu}_{12}\text{Sn}_4$
Sn3	4a	-43m	0	0	0		16-vertex Frank-Kasper $\text{Cu}_{12}\text{Mg}_4$

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates. In [1] the x -coordinate of the Cu site is misprinted as $\frac{3}{8}$ instead of $\frac{5}{8}$.

References: [1] Osamura K., Murakami Y. (1978), J. Less-Common Met. 60, 311-313. [2] Gladyshevskii E.I., Kripyakevich P.I., Teslyuk M.Y. (1952), Dokl. Akad. Nauk SSSR 85, 81-84. [3] Kojima K., Nakai Y., Suzuki T., Asano H., Izumi F., Fujita T., Hihara T. (1990), J. Phys. Soc. Jpn. 59, 792-795. [4] Cordier G., Röhr C. (1991), Z. Kristallogr. 197, 314-315. [5] Aono K., Orimo S., Fujii H. (2000), J. Alloys Compd. 309, L1-L4. [6] Teslyuk M.Y., Kripyakevich P.I. (1961), Dopov. Akad. Nauk Ukr. RSR 1961, 1039-1041.

216
cF24

Zn[SO ₄]	cF24	(216) <i>F</i> -43 <i>m</i> – eca
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ZnSO₄ β [1]

Structural features: Zn atoms and SO₄ tetrahedra in a ZnS-type (sphalerite) arrangement.

Spiess M., Gruehn R. (1979) [1]

O₄SZn

a = 0.718 nm, *V* = 0.3701 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	16 <i>e</i>	.3 <i>m</i>	0.12	0.12	0.12		colinear SZn
Zn2	4 <i>c</i>	-43 <i>m</i>	¹ / ₄	¹ / ₄	¹ / ₄		tetrahedron O ₄
S3	4 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron O ₄

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

Experimental: powder, Guinier-Simon film, X-rays, R_B = 0.060, T = 973 K

Remarks: Phase stable at T > ~968 K.

References: [1] Spiess M., Gruehn R. (1979), Z. Anorg. Allg. Chem. 456, 222-240.

216
cF28

Cu _{1.43} Te	cF28	(216) <i>F</i> -43 <i>m</i> – edba
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Cu_{3-x}Te₂ f.c.c. [1]

Structural features: Close-packed Te layers in c stacking; Cu in tetrahedral (in part displaced towards a face) and octahedral voids.

Stevens A.L.N., Wiegers G.A. (1971) [1]

Cu_{1.50}Te

a = 0.6032 nm, *V* = 0.2195 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	16 <i>e</i>	.3 <i>m</i>	0.21	0.21	0.21	0.075	
Cu2	4 <i>d</i>	-43 <i>m</i>	³ / ₄	³ / ₄	³ / ₄		
Te3	4 <i>b</i>	-43 <i>m</i>	¹ / ₂	¹ / ₂	¹ / ₂		
Cu4	4 <i>a</i>	-43 <i>m</i>	0	0	0	0.2	

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

Experimental: powder, Guinier film, X-rays, T = 633 K

Remarks: Phase stable at T > 633 K. Short interatomic distances for partly occupied site(s).

References: [1] Stevens A.L.N., Wiegers G.A. (1971), Recl. Trav Chim. Pays-Bas 90, 352-359.

216
cF32

(Ag _{0.5} Hg _{0.25})I	cF32	(216) <i>F</i> -43 <i>m</i> – e ²
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Ag₂HgI₄ α [1]

Structural features: Distorted close-packed I layers in c stacking (split site); (Ag,Hg) in trigonal voids (partial disorder).

Kasper J.S., Browall K.W. (1975) [1]

Ag_{0.50}Hg_{0.25}I

a = 0.635 nm, *V* = 0.2560 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	16 <i>e</i>	.3 <i>m</i>	0.0207	0.0207	0.0207	0.25	
M2	16 <i>e</i>	.3 <i>m</i>	0.725	0.725	0.725	0.188	

M2 = 0.67Ag + 0.33Hg

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.037, *T* = 339 K

Remarks: Phase stable at *T* > 323 K. Short interatomic distances for partly occupied site(s).

References: [1] Kasper J.S., Browall K.W. (1975), J. Solid State Chem. 13, 49-56.

216
cF32

Na _{1.67} AlSiO _{4.33}	cF32	(216) <i>F</i> -43 <i>m</i> – edcba
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(Na₂O)_{0.33}NaAlSiO₄ [1]

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a cristobalite-type 3D-framework; (Na₂O) in voids.

Klingenberg R., Felsche J. (1986) [1]

AlNa_{1.67}O_{4.33}Si

a = 0.73209 nm, *V* = 0.3924 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	16 <i>e</i>	.3 <i>m</i>	0.125	0.125	0.125		colinear AlSi
M2	4 <i>d</i>	-43 <i>m</i>	³ / ₄	³ / ₄	³ / ₄		pseudo Frank-Kasper O ₁₂ Na ₄ Si ₄
Al3	4 <i>c</i>	-43 <i>m</i>	¹ / ₄	¹ / ₄	¹ / ₄		tetrahedron O ₄
M4	4 <i>b</i>	-43 <i>m</i>	¹ / ₂	¹ / ₂	¹ / ₂		pseudo Frank-Kasper O ₁₂ Al ₄ Na ₄
Si5	4 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron O ₄

M2 = 0.833Na + 0.167O; M4 = 0.833Na + 0.167O

Experimental: powder, Guinier film, X-rays

Remarks: Homogeneity range (Na₂O)_xNaAlSiO₄, 0.01 < *x* < 0.33. In the abstract of [1] the cell parameter is misprinted as 0.73029 nm instead of 0.73209 nm (given in table 1); in fig. 4 of the same reference the Wyckoff positions of the interstitial sites (4*b* and 4*c*) are interchanged.

References: [1] Klingenberg R., Felsche J. (1986), J. Solid State Chem. 61, 40-46.

216
cF36

CuI	cF36	(216) <i>F</i> -43 <i>m</i> – e ² <i>a</i>
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CuI γ [1], marshite

Structural features: Close-packed I layers in c stacking; Cu in tetrahedral voids (displaced towards a face, disorder).

Keen D.A., Hull S. (1995) [1]

CuI

$a = 0.60991 \text{ nm}$, $V = 0.2269 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	16e	.3m	0.281	0.281	0.281	0.245	
Cu2	16e	.3m	0.719	0.719	0.719	0.005	
I3	4a	-43m	0	0	0		

Experimental: powder, diffractometer, neutrons, time-of-flight, $T = 628 \text{ K}$

Remarks: Phase stable at $T < \sim 643 \text{ K}$; partial occupation of a second tetrahedral site was observed above 600 K. Short interatomic distances for partly occupied site(s). Correct symmetry is space group (225) $Fm\bar{3}m$ if sites Cu1 and Cu2 have the same occupancy. We assume that in table 1 of [1] the occupation factor $n(\text{Cu}2)$ is misprinted as $1-n(\text{Cu}1)$ instead of $1/4-n(\text{Cu}1)$ (agreement with the nominal composition).

References: [1] Keen D.A., Hull S. (1995), J. Phys.: Condens. Matter 7, 5793-5804.

216
cF40

$\text{K}_9[\text{C}_{70}]$	cF40	(216) $F\bar{4}3m - e^2da$
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K₉C₇₀ [1]

Structural features: C₇₀ fullerene units (fused 6- and 5-membered rings) in a Cu-type (c.c.p.) arrangement; K in "octahedral" (two concentric K₄ tetrahedra) and "tetrahedral" voids.

Kobayashi M. et al. (1993) [1]

C₇₀K₉

$a = 1.569 \text{ nm}$, $V = 3.8625 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	16e	.3m	0.1461	0.1461	0.1461		7-vertex polyhedron K ₇
K2	16e	.3m	0.4061	0.4061	0.4061		trigonal prism K ₆
(C ₇₀)3	4d	-43m	$3/4$	$3/4$	$3/4$		28-vertex polyhedron K ₂₈
K4	4a	-43m	0	0	0		tetrahedron K ₄

Transformation from published data: $-x, -y, -z$; origin shift $1/4 \ 1/4 \ 1/4$

Experimental: powder, diffractometer, X-rays, $R_B = 0.168$

Remarks: The atom coordinates correspond to the positions of K atoms and the centers of C₇₀ units.

References: [1] Kobayashi M., Akahama Y., Kawamura H., Shinohara H., Sato H., Saito Y. (1993), Phys. Rev. B: Condens. Matter 48, 16877-16880.

216
cF40

$\text{Ba}(\text{Ba}_{0.33}\text{Y}_{0.67})\text{Cu}(\text{Cu}_{0.33}\text{W}_{0.67})\text{O}_{5.67}$	cF40	(216) $F\bar{4}3m - fdcba$
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Ba₂Cu₂WYO_{8.5-8} [1], perovskite AA'BB'O₆

Structural features: (W,Cu)O₆ and CuO₆ octahedra share vertices to form a 3D-framework; Ba and (Y,Ba) in cuboctahedral voids. Substitution derivative of CaTiO₃ of ideal composition [AA'] [BB']O₆.

Kitahama K. et al. (1991) [1]

Ba_{1.33}Cu_{1.33}O_{5.66}W_{0.67}Y_{0.67}

$a = 0.8345 \text{ nm}$, $V = 0.5811 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24 <i>f</i>	2. <i>mm</i>	0.25	0	0	0.944	colinear CuW
Ba2	4 <i>d</i>	-43 <i>m</i>	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		cuboctahedron O ₁₂
M3	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		cuboctahedron O ₁₂
M4	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Cu5	4 <i>a</i>	-43 <i>m</i>	0	0	0		octahedron O ₆

M3 = 0.667Y + 0.333Ba ; M4 = 0.667W + 0.333Cu

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, diffractometer, X-rays, R = 0.094

References: [1] Kitahama K., Hori Y., Kawai T., Kawai S. (1991), Jpn. J. Appl. Phys., Part 2, 30, L809-L812.

216
cF44

Cu ₂ Se	<i>cF44</i>	(216) <i>F-43m</i> – e ² dca
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Cu₂Se α [1]

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

Rahlf's P. (1936) [1]

Cu₂Se

$a = 0.584 \text{ nm}$, $V = 0.1992 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	16 <i>e</i>	.3 <i>m</i>	0.08333	0.08333	0.08333	0.025	
Cu2	16 <i>e</i>	.3 <i>m</i>	0.41667	0.41667	0.41667	0.1	
Se3	4 <i>d</i>	-43 <i>m</i>	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		
Cu4	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.5	
Cu5	4 <i>a</i>	-43 <i>m</i>	0	0	0		

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, film, X-rays, T = 443 K

Remarks: Phase stable at T > 383 K. Short interatomic distances for partly occupied site(s).

References: [1] Rahlfs P. (1936), Z. Phys. Chem., Abt. B 31, 157-194.

216
cF48

PrI ₂	<i>cF48</i>	(216) <i>F-43m</i> – e ³
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PrI₂ form V [1]

Structural features: Close-packed I layers in c stacking; Pr in octahedral voids. Units of four edge-linked PrI₆ octahedra (a central Pr₄ tetrahedral cluster) share additional edges to form a 3D-framework.

Warkentin E., Bärnighausen H. (1979) [1]

I₂Pr

$a = 1.236 \text{ nm}$, $V = 1.8882 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	16e	.3m	0.11142	0.11142	0.11142		non-coplanar triangle Pr ₃
Pr2	16e	.3m	0.36083	0.36083	0.36083		tricapped trigonal prism I ₆ Pr ₃
I3	16e	.3m	0.62596	0.62596	0.62596		non-coplanar triangle Pr ₃

Experimental: single crystal, diffractometer, X-rays, R = 0.041

Remarks: Space group (227) *Fd-3m* was tested and rejected (R = 0.196).

References: [1] Warkentin E., Bärnighausen H. (1979), Z. Anorg. Allg. Chem. 459, 187-200.

216
cF48

MoSBr	cF48	(216) <i>F-43m</i> – e ³
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MoSBr [1]; ReTeS [2]

Structural features: Distorted close-packed SBr layers in c stacking; Mo in octahedral (S₃Br₃) voids. Mo₄S₄ clusters (a Mo₄ inner tetrahedron and a S₄ outer tetrahedron). Ordering variant of PrI₂. See Fig. II.17.

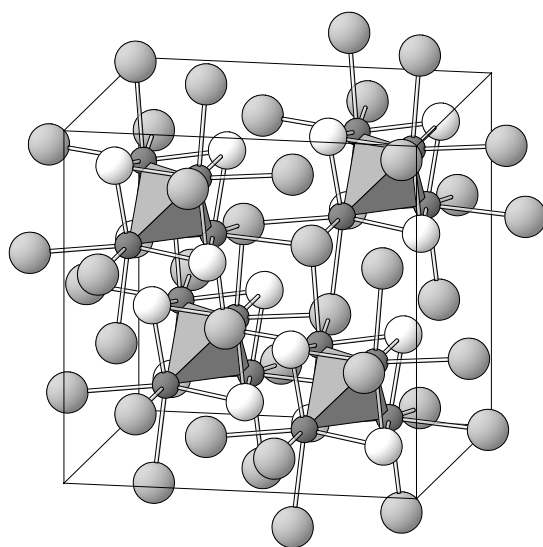


Fig. II.17. **MoSBr**

Arrangement of Mo₄ tetrahedra (Mo atoms dark), S (light) and Br (medium) atoms.

Perrin C. et al. (1975) [1]

BrMoS

$a = 0.9945 \text{ nm}$, $V = 0.9836 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	16e	.3m	0.1184	0.1184	0.1184		non-coplanar triangle Mo ₃
Mo2	16e	.3m	0.3494	0.3494	0.3494		tricapped trigonal prism S ₃ Br ₃ Mo ₃
Br3	16e	.3m	0.6227	0.6227	0.6227		non-coplanar triangle Mo ₃

Transformation from published data: -x,-y,-z; origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

References: [1] Perrin C., Chevrel R., Sergent M. (1975), C. R. Seances Acad. Sci., Ser. C 281, 23-25. [2] Fedorov V.E., Mironov Y.V., Fedin V.P., Mironov Y.I. (1994), J. Struct. Chem. (Engl. Transl.) 35, 146-147.

216
cF48

Be_4TeO_7	$cF48$	$(216) F-43m - \text{feca}$
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Be₄TeO₇ [1]

Structural features: TeO_6 octahedra and BeO_4 tetrahedra share vertices to form a 3D-framework. Alternatively: TeO_6 octahedra and OBe_4 tetrahedra in a ZnS-type (sphalerite) arrangement.

Trömel M. et al. (1977) [1]

 $\text{Be}_4\text{O}_7\text{Te}$ $a = 0.7577 \text{ nm}$, $V = 0.4350 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	2. mm	0.2532	0	0		coplanar triangle Be_2Te
Be2	16e	.3m	0.373	0.373	0.373		tetrahedron O_4
O3	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron Be_4
Te4	4a	-43m	0	0	0		octahedron O_6

Transformation from published data: $-x, -y, -z$ Experimental: powder, diffractometer, neutrons, $R_B = 0.042$

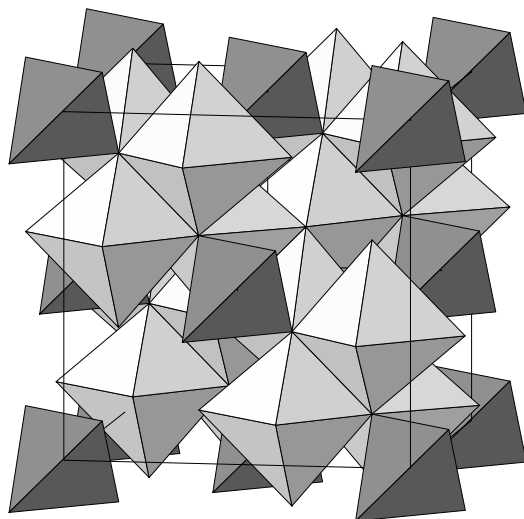
References: [1] Trömel M., Maetz J., Müllner M. (1977), Acta Crystallogr. B 33, 3959-3961.

216
cF52

Mo_4GaS_8	$cF52$	$(216) F-43m - e^3a$
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GaMo₄S₈ rt [2]; $(\text{Cu}_{0.85}\text{Fe}_{0.15})(\text{Re}_{2.85}\text{Mo}_{1.15})\text{S}_8$ [3]; $\text{Li}_{1.3}\text{V}_{1.2}\text{Cl}_4$ rt [4]

Structural features: Close-packed S layers in c stacking; Mo in octahedral, Ga in tetrahedral voids. MoS_6 octahedra share edges to form a 3D-framework with Mo_4 tetrahedral clusters. Vacancy derivative of MgAl_2O_4 (spinel). See Fig. II.18.

Fig. II.18. **Mo₄GaS₈**

Arrangement of GaS_4 tetrahedra (dark) and MoS_6 octahedra (light).

Francois M. et al. (1991) [1]

 GaMo_4S_8 $a = 0.97356 \text{ nm}$, $V = 0.9228 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	16e	.3m	0.1345	0.1345	0.1345		tetrahedron GaMo ₃
Mo2	16e	.3m	0.3978	0.3978	0.3978		tricapped trigonal prism S ₆ Mo ₃
S3	16e	.3m	0.6343	0.6343	0.6343		non-coplanar triangle Mo ₃
Ga4	4a	-43m	0	0	0		tetrahedron S ₄

Experimental: powder, diffractometer, X-rays, $R_B = 0.040$, $T = 300$ K

Remarks: Phase stable at $T > 45$ K.

References: [1] Francois M., Lengauer W., Yvon K., Yaich Aerrache H.B., Gougeon P., Potel M., Sergent M. (1991), Z. Kristallogr. 196, 111-120. [2] Perrin C., Chevrel R., Sergent M. (1975), C. R. Seances Acad. Sci., Ser. C 280, 949-951. [3] Kohlmann M., Schulz H. (1993), Z. Kristallogr. 204, 287-288. [4] Partik M., Lutz H.D. (1997), Mater. Res. Bull. 32, 1073-1078.

216
cF52

$\text{Re}_4\text{As}_5(\text{As}_{0.25}\text{S}_{0.75})_4$	cF52	(216) $F\bar{4}3m - e^3a$
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Re₄As₆S₃ [1]

Structural features: Close-packed (As,S) layers in c stacking; Re in octahedral, additional As in tetrahedral voids (AsAs₄ tetrahedra). Units of four edge-linked Re(As,S)₆ octahedra (Re₄ tetrahedral cluster) are interconnected to form a 3D-framework. Ordering variant of Mo₄GaS₈.

Besnard C. et al. (2003) [1]

$\text{As}_{6.04}\text{Re}_4\text{S}_{2.96}$

$a = 0.98608$ nm, $V = 0.9588$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	16e	.3m	0.1425	0.1425	0.1425		tetrahedron AsRe ₃
Re2	16e	.3m	0.40047	0.40047	0.40047		tricapped trigonal prism S ₃ As ₃ Re ₃
M3	16e	.3m	0.6386	0.6386	0.6386		non-coplanar triangle Re ₃
As4	4a	-43m	0	0	0		tetrahedron As ₄

$M3 = 0.74S + 0.26As$

Experimental: powder, diffractometer, X-rays, $R_B = 0.007$

References: [1] Besnard C., Svensson C., Stahl K., Siegrist T. (2003), J. Solid State Chem. 172, 446-450.

216
cF52

$\text{CsMg}[\text{AsO}_4][\text{H}_2\text{O}]_6$	cF52	(216) $F\bar{4}3m - fecba$
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CsMgAsO₄·6H₂O [1]

Structural features: Mg(OH₂)₆ octahedra and AsO₄ tetrahedra in a ZnS-type (sphalerite) arrangement.

Ferrari A. et al. (1955) [1]

$\text{AsCsH}_{12}\text{MgO}_{10}$

$a = 1.0178$ nm, $V = 1.0544$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24f	2.mm	0.3	0	0		single atom Mg
O2	16e	.3m	0.156	0.156	0.156		single atom As
As3	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O ₄

Mg4	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	octahedron (OH ₂) ₆
Cs5	4a	-43m	0	0	0	fourcapped trigonal prism O ₄ (OH ₂) ₆

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

Experimental: single crystal, Weissenberg photographs, X-rays

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

References: [1] Ferrari A., Cavalca L., Nardelli M. (1955), Gazz. Chim. Ital. 85, 169-174.

216
cF52

Cu ₂ Al ₄ O ₇	cF52	(216) F-43m – fedca
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Cu₂Al₄O₇ [1]

Structural features: AlO₄ tetrahedra share vertices to form a 3D-framework; Cu in octahedral and cuboctahedral voids.

Meyer H., Müller Buschbaum H. (1981) [1]

Al₄Cu₂O₇

$a = 0.809$ nm, $V = 0.5295$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24f	2.mm	0.243	0	0		coplanar triangle Al ₂ Cu
Al2	16e	.3m	0.3842	0.3842	0.3842		tetrahedron O ₄
Cu3	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		cuboctahedron O ₁₂
O4	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron Al ₄
Cu5	4a	-43m	0	0	0		octahedron O ₆

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

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

Remarks: In the abstract of [1] the cell parameter is misprinted as 0.9080 nm instead of 0.8090 nm (given on page 52; checked on interatomic distances).

References: [1] Meyer H., Müller Buschbaum H. (1981), Monatsh. Chem. 112, 51-57.

216
cF56

Co _{2.95} O ₄	cF56	(216) F-43m – e ³ da
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Co_{3-x}O₄ thin film [1]

Structural features: Close-packed O layers in c stacking, Co in octahedral and tetrahedral voids. Vacancy derivative of Fe₃O₄ (magnetite) with partly ordered vacancies on the tetrahedral sites.

Kotousova I.S., Polyakov S.M. (1972) [1]

Co_{2.97}O₄

$a = 0.8065$ nm, $V = 0.5246$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	16e	.3m	0.140	0.140	0.140		tetrahedron Co ₄
(Co ³⁺)2	16e	.3m	0.375	0.375	0.375		octahedron O ₆
O3	16e	.3m	0.610	0.610	0.610		tetrahedron Co ₄
M4	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.95	tetrahedron O ₄

(Co²⁺)₅ 4a -43m 0 0 0 tetrahedron O₄

$$M4 = 0.89\text{Co}^{2+} + 0.11\text{Co}^{3+}$$

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: thin film, electron diffraction, R = 0.136

Remarks: Approximate composition. Correct symmetry is space group (227) *Fd-3m* if sites Co4 and Co5 have the same occupancy.

References: [1] Kotousova I.S., Polyakov S.M. (1972), Sov. Phys. Crystallogr. (Engl. Transl.) 17, 572-574.

216
cF56

Mo₄Al_{1.1}S₈ cF56 (216) *F-43m* – e³da

Mo₂Al_xS₄ [1], spinel family; Mo₂Ga_xS₄ [1]

Structural features: Close-packed S layers in c stacking; Mo in octahedral, Al in tetrahedral voids. Vacancy derivative of MgAl₂O₄ with partly ordered vacancies on the tetrahedral sites.

Vandenberg J.M., Brasen D. (1975) [1]

Al_{1.10}Mo₄S₈

$$a = 0.9726 \text{ nm}, V = 0.9200 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	16e	.3m	0.113	0.113	0.113		tetrahedron AlMo ₃
Mo2	16e	.3m	0.355	0.355	0.355		tricapped trigonal prism S ₆ Mo ₃
S3	16e	.3m	0.618	0.618	0.618		tetrahedron AlMo ₃
Al4	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		tetrahedron S ₄
Al5	4a	-43m	0	0	0	0.1	tetrahedron S ₄

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, diffractometer, X-rays, R = 0.134

Remarks: Correct symmetry is space group (227) *Fd-3m* if sites Al4 and Al5 have the same occupancy.

References: [1] Vandenberg J.M., Brasen D. (1975), J. Solid State Chem. 14, 203-208.

216
cF56

LiCr_{3.2}Fe_{1.8}O₈ cF56 (216) *F-43m* – e³da

Li_{0.32}Fe_{0.68}(Li_{0.18}Fe_{0.22}Cr_{1.6})O₄ [1], spinel family

Structural features: Close-packed O layers in c stacking; Fe and (Li,Fe) in tetrahedral, (Cr,etc.) in octahedral voids. Single FeO₄ and (Li,Fe)O₄ tetrahedra and edge-linked CrO₆ octahedra share vertices to form a spinel-type 3D-framework. Substitution derivative of MgAl₂O₄ (spinel) of ideal composition [AA']B₄O₈.

Dargel L. et al. (1972) [1]

Cr_{3.20}Fe_{1.80}LiO₈

$$a = 0.8278 \text{ nm}, V = 0.5673 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	16e	.3m	0.135	0.135	0.135		tetrahedron LiCr ₃
M2	16e	.3m	0.376	0.376	0.376		octahedron O ₆
O3	16e	.3m	0.614	0.614	0.614		tetrahedron FeCr ₃

Fe4	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	tetrahedron O ₄
M5	4a	-43m	0	0	0	tetrahedron O ₄

M2 = 0.80Cr + 0.11Fe + 0.09Li; M5 = 0.64Li + 0.36Fe

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.023$

Remarks: General formula $\text{Fe}_x\text{Li}_{1-x}(\text{Li}_{x-0.5}\text{Fe}_{2.5-x}\text{Cr})\text{O}_4$. On page 691 of [1] the Wyckoff positions of former (Li,Fe,Cr), O1 and O2 are misprinted as 16a and 16c instead of 16e.

References: [1] Dargel L., Kubel W., Olkiewicz K. (1972), Acta Phys. Pol., A 41, 689-700.

216
cF60

$\text{Cu}_2\text{Fe}[\text{CN}]_6$	cF60	(216) $F-43m - \bar{1}^2cba$
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$\text{Cu}_2[\text{Fe}(\text{CN})_6]$ [1]

Structural features: $\text{Fe}(\text{CN})_6$ octahedral units (FeC_6 octahedron, linear Fe-C-N segments) in a Cu-type (c.c.p.) arrangement; Cu in "octahedral" and "tetrahedral" voids.

Rigamonti R. (1937) [1]

$\text{C}_6\text{Cu}_2\text{FeN}_6$

$a = 0.998 \text{ nm}$, $V = 0.9940 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24f	2.mm	0.1875	0	0		single atom N
N2	24f	2.mm	0.3125	0	0		single atom C
Cu3	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		truncated cube (dice) $\text{C}_{12}\text{N}_{12}$
Cu4	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N_6
Fe5	4a	-43m	0	0	0		octahedron C_6

Experimental: powder, film, X-rays

Remarks: C and N could not be distinguished in [1]; we assigned probable atom distribution based on more recent refinements. Unusual interatomic distances are reported in [2]: $d(\text{Fe5-C1}) = 0.1105 \text{ nm}$, $d(\text{C1-N2}) = 0.1922 \text{ nm}$.

References: [1] Rigamonti R. (1937), Gazz. Chim. Ital. 67, 137-146. [2] Juszczak S., Johansson C., Hanson M., Ratuszna A., Malecki G. (1994), J. Magn. Magn. Mater. 138, 281-286.

216
cF60

$\text{CsLi}[\text{WO}_4]$	cF60	(216) $F-43m - hcba$
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CsLiWO_4 [1]

Structural features: WO_4 tetrahedra (split O site) in a Cu-type (c.c.p.) arrangement; Cs in octahedral, Li in tetrahedral voids.

Okada K., Osaka J. (1980) [1]

CsLiO_4W

$a = 0.835 \text{ nm}$, $V = 0.5822 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	.m	0.11	0.11	0.147	0.333	
Li2	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Cs3	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		

W4	$4a$	$-43m$	0	0	0
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Experimental: single crystal, diffractometer, X-rays, R = 0.050, T = 298 K

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

References: [1] Okada K., Ossaka J. (1980), *Acta Crystallogr. B* 36, 657-659.

216
cF60
$$\text{Cs}_2\text{Al}[\text{OH}]_3\text{F}_2[\text{H}_2\text{O}] \quad cF60 \quad (216) F\text{-}43m - \text{hcba}$$

Cs₂Al(OH)₃F₂·H₂O [1]

Structural features: $\text{Al}(\text{OH}, \text{F}, \text{OH}_2)_6$ octahedral units and Cs atoms in a CaF_2 -type arrangement.

Petrosyants S.P. et al. (1996) [1]

$$\text{AlCs}_2\text{F}_2\text{H}_5\text{O}_4$$
$$a = 0.8915 \text{ nm}, V = 0.7085 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	$48h$	$\bar{..}m$	0.24	0.24	0.0608	0.5	
Al2	$4c$	$-43m$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Cs3	$4b$	$-43m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Cs4	$4a$	$-43m$	0	0	0		

$$M1 = 0.5OH + 0.333F + 0.167OH_2$$

Transformation from published data: -x,-y,-z; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.036

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] Petrosyants S.P., Ilyukhin A.B., Malyarik M.A. (1996), Russ. J. Inorg. Chem. 41, 1521-1524.

216
cF64
$$\text{Cu}_2\text{Fe}[\text{CN}]_6[\text{H}_2\text{O}]_{0.5} \quad cF64 \quad (216) F-43m - f^2dcba$$

$\text{Cu}_2[\text{Fe}(\text{CN})_6] \cdot 0.5\text{H}_2\text{O}$ [1], Prussian blue family

Structural features: Fe(CN)₆ octahedral units (central FeC₆ octahedron, linear Fe-C-N segments) in a Cu-type (c.c.p.) arrangement; part of Cu in "octahedral", H₂O and remaining Cu in "tetrahedral" voids.

Ratuszna A. et al. (1995) [1]

$$\text{C}_6\text{Cu}_{1.70}\text{FeH}_{1.10}\text{N}_6\text{O}_{0.55}$$
$$a = 1.0022 \text{ nm}, V = 1.0066 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	$24f$	$2.mm$	0.1798	0	0		single atom N
N2	$24f$	$2.mm$	0.2944	0	0		single atom C
(OH ₂)3	$4d$	$-43m$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.55	truncated cube (dice) N ₁₂ C ₁₂
Cu4	$4c$	$-43m$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.7	truncated cube (dice) N ₁₂ C ₁₂
Cu5	$4b$	$-43m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N ₆
Fe6	$4a$	$-43m$	0	0	0		octahedron C ₆

Experimental: powder, diffractometer, X-rays, $wR_p = 0.026$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table IV of [1] the chemical formula is misprinted as $\text{Cu}_2[\text{Fe}(\text{CN})_6] \cdot \text{H}_2\text{O}$ instead of $\text{Cu}_2[\text{Fe}(\text{CN})_6] \cdot \frac{1}{2}\text{H}_2\text{O}$ (better agreement with refined composition, analogy with other compounds reported in the same paper).

References: [1] Ratuszna A., Juszczak S., Matecki G. (1995), Powder Diffraction, 10, 300-305.

216
cF64

$\text{CsCrMn}[\text{CN}]_6[\text{H}_2\text{O}]$	cF64	(216) $F-43m - f^2dcba$
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CsMn[Cr(CN)₆]·H₂O [1], Prussian blue family

Structural features: CrC_6 and MnN_6 octahedra in a NaCl-type arrangement are interconnected via C-N bonds (cyanide units) to form a 3D-framework; Cs in "cubic" voids (partial disorder). Ordering variant of $\text{Cu}_2[\text{Fe}(\text{CN})_6] \cdot 0.5\text{H}_2\text{O}$.

Ziegler B. et al. (1999) [1]

$\text{C}_6\text{CrCsMnN}_6$

$a = 1.0843 \text{ nm}$, $V = 1.2748 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24f	2.mm	0.1906	0	0		single atom N
N2	24f	2.mm	0.2956	0	0		single atom C
Cs3	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.18	truncated cube (dice) $\text{N}_{12}\text{C}_{12}$
Cs4	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.82	truncated cube (dice) $\text{N}_{12}\text{C}_{12}$
Mn5	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N_6
Cr6	4a	-43m	0	0	0		octahedron C_6

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.043$, $T = 295 \text{ K}$

Remarks: H_2O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Correct symmetry is space group (225) $Fm-3m$ if sites Cs3 and Cs4 have the same occupancy.

References: [1] Ziegler B., Witzel M., Schwarten M., Babel D. (1999), Z. Naturforsch. B 54, 870-876.

216
cF64

$\text{Hg}_5\text{In}_2\text{Se}_8$	cF64	(216) $F-43m - ge^2ba$
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Hg₅In₂Se₈ [1]

Structural features: Close-packed Se layers in c stacking; Hg and In in tetrahedral voids. HgSe_4 and $(\text{Hg},\text{In})\text{Se}_4$ tetrahedra share vertices to form a 3D-framework.

Radaoutsan S.I. (1964) [1]

$\text{Hg}_5\text{In}_2\text{Se}_8$

$a = 1.18 \text{ nm}$, $V = 1.6430 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	24g	2.mm	0.0	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron In_2Hg_2
Hg2	16e	.3m	0.125	0.125	0.125		tetrahedron Se_4
M3	16e	.3m	0.625	0.625	0.625	0.75	tetrahedron Se_4
Se4	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron In_4

Se5	4a	-43m	0	0	0	tetrahedron Hg ₄
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$$M3 = 0.667\text{In} + 0.333\text{Hg}$$

Experimental: powder, Debye film, X-rays

Remarks: We took idealized atom coordinates from [2].

References: [1] Radaoutsan S.I. (1964), Rev. Roum. Phys. 9, 293-304. [2] Parthé E. (1972), Cristallochimie des structures tétraédriques, Gordon & Breach, Paris 1972, p. 285.

216
cF64
$$\text{Yb}_{0.88}\text{S} \qquad cF64 \qquad (216) F-43m - \text{gfdcba}$$
 $\mathbf{Yb}_{0.875}\mathbf{S}$ [1]

Structural features: Close-packed S layers in c stacking; Yb in octahedral voids. Vacancy derivative of NaCl with partly ordered vacancies.

Tomas A. et al. (1988) [1]

SYb_{0.88} $a = 1.125 \text{ nm}, V = 1.4238 \text{ nm}^3, Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Yb1	24g	2. <i>mm</i>	0.005	$1/4$	$1/4$	0.95	octahedron S ₆
S2	24 <i>f</i>	2. <i>mm</i>	0.234	0	0		octahedron Yb ₆
S3	4 <i>d</i>	-43 <i>m</i>	$3/4$	$3/4$	$3/4$		octahedron Yb ₆
S4	4 <i>c</i>	-43 <i>m</i>	$1/4$	$1/4$	$1/4$		octahedron Yb ₆
Yb5	4 <i>b</i>	-43 <i>m</i>	$1/2$	$1/2$	$1/2$	0.325	octahedron S ₆
Yb6	4 <i>a</i>	-43 <i>m</i>	0	0	0		octahedron S ₆

Transformation from published data: $-x, -y, -z$; origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.040

Remarks: Refinement in a NaCl-type subcell gave R = 0.04. Space group (225) *Fm-3m* was tested and rejected for the large cell.

References: [1] Tomas A., Robert M., Guittard M. (1988), Mater. Res. Bull. 23, 507-511.

216
cF76
$$\text{Ag}_{3.2}\text{Hg}_{2.4}\text{SiSe}_6 \quad cF76 \quad (216) F-43m - \text{fe}^3\text{a}$$

Ag_{3.2}Hg_{2.4}SiSe₆ [1]; "Ag₂HgGeSe₄" (see remark)

Structural features: Single SiSe₆ octahedra in a Cu-type (c.c.p.) arrangement.

Parasyuk O.V. et al. (2003) [1]

$$\text{Ag}_{3.09}\text{Hg}_{2.43}\text{Se}_6\text{Si}$$
$$a = 1.07108 \text{ nm}, V = 1.2288 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	24 <i>f</i>	2. <i>mm</i>	0.2654	0	0		7-vertex polyhedron Ag ₂ Hg ₄ Si
Hg2	16 <i>e</i>	.3 <i>m</i>	0.1195	0.1195	0.1195	0.301	7-vertex polyhedron SiSe ₃ Ag ₃
Ag3	16 <i>e</i>	.3 <i>m</i>	0.3668	0.3668	0.3668	0.773	trigonal prism Se ₃ Hg ₃
Hg4	16 <i>e</i>	.3 <i>m</i>	0.6724	0.6724	0.6724	0.306	octahedron Hg ₃ Se ₃
Si5	4 <i>a</i>	-43 <i>m</i>	0	0	0		fourcapped trigonal prism Hg ₄ Se ₆

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.095$

Remarks: Phase referred to as δ -(AgHgSeSi), homogeneity range $(\text{Ag}_8\text{SiSe}_6)_{100-x}(\text{Hg}_4\text{SiSe}_6)_x$, $x = 58 < x < 62$. Stated to be isotypic with so-called $\text{Ag}_2\text{HgGeSe}_4$ [2], for which the atom coordinates were not determined. Short interatomic distances for partly occupied site(s).

References: [1] Parasyuk O.V., Gulay L.D., Romanyuk Y.E., Olekseyuk I.D. (2003), J. Alloys Compd. 348, 157-166. [2] Haeuseler H., Himmrich M. (1989), Z. Naturforsch. B 44, 1035-1036.

216
cF76

$\text{Cu}_4\text{SnP}_{10}$	cF76	(216) $F-43m - ge^3a$
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$\text{Cu}_4\text{SnP}_{10}$ [1]

Structural features: Adamantane-type P_{10} units (cage with four 6-membered rings) in a Cu-type (c.c.p.) arrangement; (SnCu_3) tetrahedral clusters (substitutional disorder, distinct positions for Sn and Cu) and single Cu atoms in tetrahedral voids.

Hönle W., Von Schnering H.G. (1980) [1]

$\text{Cu}_4\text{P}_{10}\text{Sn}$

$a = 1.0267 \text{ nm}$, $V = 1.0823 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	24g	2.mm	0.0043	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron P_2Cu_2
P2	16e	.3m	0.1272	0.1272	0.1272		tetrahedron P_3Cu
Sn3	16e	.3m	0.5753	0.5753	0.5753	0.25	
Cu4	16e	.3m	0.62	0.62	0.62	0.75	
Cu5	4a	-43m	0	0	0		tetrahedron P_4

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.048$

Remarks: Average structure; an ordered model in space group (160) $R3m$ is proposed. Space group (225) $Fm-3m$ was tested and rejected ($R > 0.5$). Preliminary data in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Hönle W., Von Schnering H.G. (1980), Z. Kristallogr. 153, 339-350. [2] Goryunova N.A., Orlov V.M., Sokolova V.I., Shpenkov G.P., Tsvetkova E.V. (1970), Phys. Status Solidi A 3, 75-87.

216
cF76

$\text{Zr}_2\text{C}_{1.2}\text{H}_{0.8}$	cF76	(216) $F-43m - gfedba$
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$\text{ZrC}_{0.6}\text{H}_{0.4}$ [1]

Structural features: Close-packed Zr layers in c stacking; C in octahedral, H in tetrahedral voids (partial disorder for both).

Goretzki H. et al. (1965) [1]

$\text{C}_{1.19}\text{H}_{0.80}\text{Zr}_2$

$a = 0.934 \text{ nm}$, $V = 0.8148 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	24g	2.mm	0.0	$\frac{1}{4}$	$\frac{1}{4}$		monocapped trigonal prism H_2C_5
C2	24f	2.mm	0.25	0	0	0.68	8-vertex polyhedron H_2Zr_6
H3	16e	.3m	0.125	0.125	0.125	0.8	7-vertex polyhedron Zr_4C_3

C4	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.68	octahedron Zr ₆
Zr5	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron C ₆
Zr6	4a	-43m	0	0	0		fourcapped trigonal prism H ₄ C ₆

Transformation from published data (*F*23): origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, neutrons

Remarks: The description in space group (196) *F*23 in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Goretzki H., Ganglberger E., Nowotny H., Bittner H. (1965), Monatsh. Chem. 96, 1563-1566.

216
c*F*76

Cu ₆ PS ₄ (S _{0.5} Br _{0.5}) ₂	c <i>F</i> 76	(216) <i>F</i> -43m – hecba
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Cu₆PS₅Br α [1], argyrodite family

Structural features: S and Br form a tetrahedrally close-packed (MgCu₂-type) framework; P in tetrahedral, Cu in trigonal voids (partial disorder). Single PS₄ tetrahedra.

Kuhs W.F., Heger G. (1979) [1]

BrCu_{5.76}PS₅

a = 0.9745 nm, *V* = 0.9254 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	48 <i>h</i>	..m	0.20934	0.20934	0.0232	0.48	
S2	16 <i>e</i>	.3m	0.62267	0.62267	0.62267		
M3	4 <i>c</i>	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
P4	4 <i>b</i>	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron S ₄
M5	4 <i>a</i>	-43m	0	0	0		cuboctahedron Cu ₁₂

M3 = 0.645S + 0.355Br; M5 = 0.645Br + 0.355S

Experimental: single crystal, diffractometer, neutrons, *R* = 0.053, *T* = 298 K

Remarks: Phase stable at *T* > 268 K. Short interatomic distances for partly occupied site(s).

References: [1] Kuhs W.F., Heger G. (1979), Fast Ion Transp. Solids Electrodes Electrolytes, Proc. Int. Conf. 1979 1979, 233-236.

216
c*F*76

UO _{2.25}	c <i>F</i> 76	(216) <i>F</i> -43m – hedba
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U₄O₉ β [1]

Structural features: Close-packed U layers in c stacking; O mainly in tetrahedral, in part in octahedral voids (displaced towards a face or and edge).

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

O_{2.33}U

a = 0.544 nm, *V* = 0.1610 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>h</i>	..m	0.127	0.127	0.25	0.054	
O2	16 <i>e</i>	.3m	0.188	0.188	0.188	0.022	
U3	4 <i>d</i>	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		

O4	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.64
O5	4a	-43m	0	0	0	0.95

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

Experimental: single crystal, diffractometer, neutrons, $R = 0.036$, $T = 393$ K

Remarks: Phase stable at $T > 393$ K. Short interatomic distances for partly occupied site(s). Average structure. An alternative refinement in space group (215) $P-43m$ gave $R = 0.049$. The superstructure with 8-fold unit cell was refined in space group (220) $I-43d$.

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

216
cF84

$\text{Cr}_4\text{Al}_{13}\text{Si}_4$	cF84	(216) $F-43m - g\bar{f}e^2a$
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$\text{Cr}_4\text{Al}_{13}\text{Si}_4$ [1]

Structural features: Cr_4Si_4 tetrahedron stars (a Cr_4 inner tetrahedron, the faces of which are capped by the atoms of a Si_4 outer tetrahedron) embedded in an Al matrix. Interpenetrating $\text{Cr}(\text{Al}_6\text{Cr}_3\text{Si}_3)$ icosahedra.

Robinson K. (1953) [1]

$\text{Al}_{13}\text{Cr}_4\text{Si}_4$

$a = 1.0917$ nm, $V = 1.3011$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24g	2.mm	0.56	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron $\text{Cr}_2\text{Si}_2\text{Al}_8$
Al2	24f	2.mm	0.3103	0	0		tricapped pentagonal prism $\text{Cr}_2\text{Si}_2\text{Al}_9$
Si3	16e	.3m	0.126	0.126	0.126		bicapped square prism Al_7Cr_3
Cr4	16e	.3m	0.3421	0.3421	0.3421		icosahedron $\text{Si}_3\text{Al}_6\text{Cr}_3$
Al5	4a	-43m	0	0	0		tetrahedron Si_4

Experimental: single crystal, oscillation photographs, X-rays, $R = 0.120$

Remarks: Phase referred to as α -(CrAlSi).

References: [1] Robinson K. (1953), Acta Crystallogr. 6, 854-859.

216
cF84

$\text{Ru}_4\text{Pb}_4\text{O}_{13}$	cF84	(216) $F-43m - g\bar{f}e^2a$
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$\text{Pb}_2\text{Ru}_2\text{O}_{6.5}$ [1], pyrochlore family; $\text{Pb}_2\text{TiSbO}_{6.5}$ [2]

Structural features: RuO_6 octahedra share vertices to form a pyrochlore-type framework with channels along $\langle 110 \rangle$; additional O in Pb_4 tetrahedra. Derivative of $\text{Ca}_2\text{Nb}_2\text{O}_7$ with ordered arrangement of vacancies in the Pb_4 tetrahedra.

Beyerlein R.A. et al. (1984) [1]

$\text{O}_{13}\text{Pb}_4\text{Ru}_4$

$a = 1.02519$ nm, $V = 1.0775$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	2.mm	0.5528	$\frac{1}{4}$	$\frac{1}{4}$		non-colinear Ru_2
O2	24f	2.mm	0.3008	0	0		non-colinear Ru_2
Pb3	16e	.3m	0.1272	0.1272	0.1272		7-vertex polyhedron O_7
Ru4	16e	.3m	0.6254	0.6254	0.6254		octahedron O_6

O5 4a -43m 0 0 0 tetrahedron Pb₄

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.036$

Remarks: Space group (227) $Fd-3m$ was tested and rejected ($R_B = 0.061$).

References: [1] Beyerlein R.A., Horowitz H.S., Longo J.M., Leonowicz M.E., Jorgensen J.D., Rotella F.J. (1984), J. Solid State Chem. 51, 253-265. [2] Alonso J.A., Cascales C., Rasines I., Pannetier J. (1989), Acta Crystallogr. C 45, 3-7.

216
cF88

Ca₃Er₃Ge₂BO₁₃

cF88

(216) $F-43m - fe^3dcba$

Ca₃Er₃Ge₂BO₁₃ [1]

Structural features: Single BO₄ and GeO₄ tetrahedra in a CaF₂-type arrangement; additional O in (Ca,Er)₆ octahedra.

Chenavas J. et al. (1981) [1]

BCa₃Er_{2.64}Ge₂O₁₃Pb_{0.36}

$a = 1.0452$ nm, $V = 1.1418$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24f	2.mm	0.27193	0	0		7-vertex polyhedron O ₇
O2	16e	.3m	0.082	0.082	0.082		single atom B
O3	16e	.3m	0.3488	0.3488	0.3488		single atom Ge
O4	16e	.3m	0.6539	0.6539	0.6539		single atom Ge
Ge5	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		tetrahedron O ₄
Ge6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O ₄
O7	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Ca ₆
B8	4a	-43m	0	0	0		tetrahedron O ₄

M1 = 0.50Ca + 0.44Er + 0.06Pb

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.017$

Remarks: Small amounts of Pb are ignored in the chemical formulae given above.

References: [1] Chenavas J., Grey I.E., Guitel J.C., Joubert J.C., Marezio M. (1981), Acta Crystallogr. B 37, 1343-1346.

216
cF88

Mn₅Ni₂Bi₄

cF88

(216) $F-43m - gfe^2ba$

Mn₅Ni₂Bi₄ [1]

Structural features: Close-packed Bi layers in c stacking; part of Mn in octahedral voids, Ni and remaining Mn in tetrahedral voids.

Szytula A. et al. (1981) [1]

Bi₄Mn₅Ni₂

$a = 1.2161$ nm, $V = 1.7985$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Bi1	24g	2.mm	0.522	$\frac{1}{4}$	$\frac{1}{4}$		4-vertex polyhedron Ni ₂ Mn ₂

Mn2	24f	2.mm	0.286	0	0	single atom Bi
Ni3	16e	.3m	0.147	0.147	0.147	non-coplanar triangle Mn ₃
Mn4	16e	.3m	0.325	0.325	0.325	icosahedron Ni ₃ Mn ₆ Bi ₃
Bi5	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	octahedron Mn ₆
Bi6	4a	-43m	0	0	0	fourcapped trigonal prism Ni ₄ Mn ₆

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, diffractometer, neutrons, $R_B = 0.085$, $T = 293$ K

Remarks: Supersedes a partly disordered structure proposal in [2].

References: [1] Szytula A., Biriczycka H., Todorovic J. (1981), Solid State Commun. 38, 41-43. [2] Suits J.C., Street G.B., Lee K., Goodenough J.B. (1974), Phys. Rev. B: Solid State 10, 120-127.

216
cF88

$(Y_{0.2}Bi_{0.8})_2Sn_2O_7$	cF88	(216) $F-43m - gfe^2ca$
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(Bi_{1.6}Y_{0.4})Sn₂O₇ [1], pyrochlore family

Structural features: SnO₆ octahedra share vertices to form a pyrochlore-type framework with channels along $\langle 110 \rangle$; additional O in (Bi,Y)₄ tetrahedra. Distortions due to the electron lone-pair of Bi³⁺.

Kennedy I.J. et al. (1997) [1]

Bi_{1.60}O₇Sn₂Y_{0.40}

$a = 1.05332$ nm, $V = 1.1686$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	2.mm	0.546	$\frac{1}{4}$	$\frac{1}{4}$		non-colinear Sn ₂
O2	24f	2.mm	0.278	0	0		non-colinear Sn ₂
M3	16e	.3m	0.1266	0.1266	0.1266		square prism (cube) O ₈
Sn4	16e	.3m	0.6217	0.6217	0.6217		octahedron O ₆
O5	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron Bi ₄
O6	4a	-43m	0	0	0		tetrahedron Bi ₄

M3 = 0.8Bi + 0.2Y

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, Debye-Scherrer film, X-rays, $R_p = 0.035$

Remarks: Space group (227) $Fd-3m$ was tested and rejected based on the presence of additional reflections.

References: [1] Kennedy I.J., Kennedy B.J., Hunter B.A., Vogt T. (1997), J. Solid State Chem. 131, 317-325.

216
cF96

$[NH_4](Nb_{0.5}W_{0.5})_2O_6$	cF96	(216) $F-43m - gfe^3$
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NH₄NbWO₆ [1]

Structural features: (Nb,W)O₆ octahedra share vertices to form a pyrochlore-type framework; NH₄ tetrahedra in channels along $\langle 110 \rangle$ (disorder).

Perottoni C.A. et al. (1998) [1]

H₄NNbO₆W

$a = 1.03755$ nm, $V = 1.1169$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	2.mm	0.555	1/4	1/4		non-colinear Nb ₂
O2	24f	2.mm	0.316	0	0		non-colinear Nb ₂
(NH ₄)3	16e	.3m	0.011	0.011	0.011	0.25	
(NH ₄)4	16e	.3m	0.297	0.297	0.297	0.25	
M5	16e	.3m	0.629	0.629	0.629		octahedron O ₆

M5 = 0.5Nb + 0.5W

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

Experimental: powder, diffractometer, X-rays, R_p = 0.052

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

References: [1] Perottoni C.A., Haines J., Da Jornada J.A.H. (1998), J. Solid State Chem. 141, 537-545.

216
cF100

Fe_{0.67}Ni[CN]₄[H₂O]_{3.33} cF100 (216) F-43m – f³ecba

Ni₃[Fe(CN)₆]₂·10H₂O [1]

Structural features: FeC₆ (67% occupancy) and Ni(N₂OH₂)₆ octahedra (distinct positions for N and O) are interconnected via C-N bonds (cyanide units) to form a 3D-framework with disordered vacancies; additional H₂O in voids.

Ratuszna A. et al. (1995) [1]

C₄Fe_{0.67}H_{6.66}N₄NiO_{3.33}

a = 1.0229 nm, V = 1.0703 nm³, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24f	2.mm	0.18	0	0	0.667	
(OH ₂)2	24f	2.mm	0.2817	0	0	0.333	
N3	24f	2.mm	0.2998	0	0	0.667	
(OH ₂)4	16e	.3m	0.2045	0.2045	0.2045	0.167	
(OH ₂)5	4c	-43m	1/4	1/4	1/4	0.333	
Ni6	4b	-43m	1/2	1/2	1/2		octahedron N ₆
M7	4a	-43m	0	0	0		octahedron C ₆

M7 = 0.667Fe + 0.333OH₂

Experimental: powder, diffractometer, X-rays, wR_p = 0.026

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] Ratuszna A., Juszczak S., Matecki G. (1995), Powder Diffr. 10, 300-305.

216
cF100

Mo₃Ni₂P_{1.18} cF100 (216) F-43m – gfe³a

Mo₃Ni₂P_{1.18} [1]

Structural features: P(Mo₆Ni₆) icosahedra share atoms to form a 3D-framework; additional P in octahedral voids.

Oryshchyn S.V. et al. (2001) [1]

 $\text{Mo}_3\text{Ni}_2\text{P}_{1.17}$ $a = 1.0846 \text{ nm}$, $V = 1.2759 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mo1	24g	2.mm	0.55532	$\frac{1}{4}$	$\frac{1}{4}$		14-vertex polyhedron $\text{Ni}_4\text{P}_2\text{Mo}_8$
Mo2	24f	2.mm	0.19448	0	0		single atom P
Ni3	16e	.3m	0.16826	0.16826	0.16826		pseudo Frank-Kasper $\text{P}_4\text{Ni}_3\text{Mo}_6$
P4	16e	.3m	0.3771	0.3771	0.3771		icosahedron Ni_6Mo_6
Ni5	16e	.3m	0.5809	0.5809	0.5809		icosahedron $\text{P}_3\text{Ni}_3\text{Mo}_6$
P6	4a	-43m	0	0	0	0.67	octahedron Mo_6

Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.032$

Remarks: Space group (227) $Fd-3m$ was tested and rejected based on the presence of weak additional reflections. Refinements of the occupancy at the centers of the Mo_6 octahedra showed no significant deviation from zero. The absence of oxygen was confirmed by electron microprobe analysis.

References: [1] Oryshchyn S.V., Le Sénéchal C., Députier S., Bauer J., Guérin R., Akselrud L.G. (2001), J. Solid State Chem. 160, 156-166.

216
cF108

$\text{Na}_{11}\text{Ca}_{6.5}\text{P}_8$	<i>cF108</i>	(216) $F-43m - \text{gfe}^3\text{dca}$
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 $\text{Na}_{22}\text{Ca}_{13}\text{P}_{16}$ [1]

Structural features: Close-packed P layers in c stacking; part of Na in octahedral, Ca and remaining Na in tetrahedral voids.

Cardoso Gil R.H. et al. (1998) [1]

 $\text{Ca}_{6.51}\text{Na}_{11}\text{P}_8$ $a = 1.3824 \text{ nm}$, $V = 2.6418 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ca1	24g	2.mm	0.5093	$\frac{1}{4}$	$\frac{1}{4}$	0.8	icosahedron $\text{P}_4\text{Ca}_2\text{Na}_6$
Na2	24f	2.mm	0.2273	0	0		pseudo Frank-Kasper $\text{P}_4\text{Na}_3\text{Ca}_4$
P3	16e	.3m	0.1311	0.1311	0.1311		square prism (cube) Ca_4Na_4
Na4	16e	.3m	0.4148	0.4148	0.4148		16-vertex Frank-Kasper $\text{P}_6\text{Na}_6\text{Ca}_4$
P5	16e	.3m	0.6242	0.6242	0.6242		bicapped square prism Ca_4Na_6
Ca6	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.71	fourcapped trigonal prism P_4Ca_6
Ca7	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{P}_4\text{Ca}_6\text{Na}_4$
Na8	4a	-43m	0	0	0		fourcapped trigonal prism P_4Na_6

Experimental: single crystal, diffractometer, X-rays, $wR = 0.035$, $T = 293 \text{ K}$

References: [1] Cardoso Gil R.H., Carrillo Cabrera W., Somer M., Peters K., Von Schnering H.G. (1998), Z. Kristallogr., New Cryst. Struct. 213, 9.

216
cF108

$\text{CsLi}[\text{MoO}_4]$	<i>cF108</i>	(216) $F-43m - \text{icba}$
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 CsLiMoO_4 [1]

Structural features: MoO₄ tetrahedra (orientational disorder) in a Cu-type (c.c.p) arrangement; Cs in "octahedral", Li in "tetrahedral" voids.

Klevtsova P.F. et al. (1980) [1]

CsLiMoO_{4.01}

$a = 0.8318 \text{ nm}$, $V = 0.5755 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96i	1	0.101	0.112	0.148	0.167	
Li2	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Cs3	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Mo4	4a	-43m	0	0	0		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.040$

Remarks: A similar model with O in Wyckoff position 16e was tested and rejected ($R = 0.041$, $B(O) = 0.0729 \text{ nm}^2$). Short interatomic distances for partly occupied site(s).

References: [1] Klevtsova P.F., Klevtsov P.V., Alexandrov K.S. (1980), Dokl. Akad. Nauk SSSR 255, 1379-1382.

216
cF112

AuTa ₅ S	cF112	(216) $F-43m - gfe^4$
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AuTa₅S [1]

Structural features: Ta(Ta₉Au₃) icosahedra share atoms to form a 3D-framework; S in octahedral (Ta₆) voids. Alternatively: 26-atom γ brass-type nested polyhedra units (an inner Au₄ tetrahedron surrounded by a Ta₄ outer tetrahedron, a Ta₆ octahedron and a Ta₁₂ cuboctahedron) in a Cu-type (c.c.p.) arrangement share vertices of the cuboctahedra to form a 3D-framework; S and additional Ta in voids.

Harbrecht B. et al. (1998) [1]

AuSTa₅

$a = 1.25082 \text{ nm}$, $V = 1.9570 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ta1	24g	2.mm	0.0302	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron S ₂ Ta ₈ Au ₂
Ta2	24f	2.mm	0.1975	0	0		16-vertex polyhedron S ₂ Au ₂ Ta ₁₂
S3	16e	.3m	0.1324	0.1324	0.1324		octahedron Ta ₆
Ta4	16e	.3m	0.3982	0.3982	0.3982		15-vertex Frank-Kasper Ta ₁₂ S ₃
Ta5	16e	.3m	0.6164	0.6164	0.6164		icosahedron Ta ₉ Au ₃
Au6	16e	.3m	0.8313	0.8313	0.8313		icosahedron Ta ₉ Au ₃

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.014$

References: [1] Harbrecht B., Wagner V., Pietzonka C. (1998), J. Solid State Chem. 139, 45-51.

216
cF112

K ₂ Zn[GeO ₄]	cF112	(216) $F-43m - idcba$
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K₂ZnGeO₄ β [1]

Structural features: GeO_4 and ZnO_4 tetrahedra share vertices (split O site) to form a β cristobalite-type framework; K in voids.

Colbeau Justin C. et al. (1997) [1]

$\text{GeK}_2\text{O}_{4.01}\text{Zn}$

$a = 0.80254 \text{ nm}$, $V = 0.5169 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96i	1	0.0742	0.1041	0.1893	0.167	
K2	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		
Zn3	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
K4	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Ge5	4a	-43m	0	0	0		

Experimental: powder, diffractometer, neutrons, $R_p = 0.019$, $T = 1153 \text{ K}$

Remarks: Phase stable at $T > 1049 \text{ K}$. Short interatomic distances for partly occupied site(s). A model for local order is proposed in space group (82) $I-4$.

References: [1] Colbeau Justin C., Wallez G., Elfakir A., Querton M., Suard E. (1997), J. Solid State Chem. 134, 59-66.

216
 $cF116$

$\text{Tb}_5\text{Rh}_6\text{Sn}_{17}$	$cF116$	$(216) F-43m - hfe^2dca$
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TbRh_{1.1}Sn_{3.6} [1]

Structural features: RhSn_6 trigonal prisms share vertices to form a 3D-framework; Tb and additional Sn in larger voids.

Vandenberg J.M. (1980) [1]

$\text{Rh}_6\text{Sn}_{17}\text{Tb}_5$

$a = 1.3774 \text{ nm}$, $V = 2.6132 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	48h	..m	0.178	0.178	0.0		14-vertex Frank-Kasper $\text{Rh}_2\text{Sn}_9\text{Tb}_3$
Rh2	24f	2.mm	0.26	0	0		tricapped trigonal prism Sn_6Tb_3
Tb3	16e	.3m	0.36	0.36	0.36		pseudo Frank-Kasper $\text{Sn}_{10}\text{Rh}_3$
Sn4	16e	.3m	0.59	0.59	0.59		16-vertex Frank-Kasper $\text{Rh}_3\text{Tb}_3\text{Sn}_{10}$
Sn5	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.5	16-vertex Frank-Kasper Sn_{16}
Sn6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.5	16-vertex Frank-Kasper $\text{Tb}_4\text{Sn}_{12}$
Tb7	4a	-43m	0	0	0		18-vertex polyhedron $\text{Sn}_{12}\text{Rh}_6$

Experimental: powder, Guinier-Huber, X-rays

Remarks: Referred to as phase III in the literature. A related model with a different distribution of Sn over the three 4-fold Wyckoff positions not occupied by Tb (composition $\text{Tb}_5\text{Rh}_6\text{Sn}_{18}$) was tested and rejected. In [1] the Wyckoff position of the Rh site is misprinted as 24e instead of 24f.

References: [1] Vandenberg J.M. (1980), Mater. Res. Bull. 15, 835-847.

216
 $cF124$

$\text{Cu}_6\text{PS}_5\text{Br}$	$cF124$	$(216) F-43m - h^2ecba$
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Cu₆PS₅Br α [1], argyrodite family

Structural features: S and Br form a tetrahedrally close-packed (MgCu₂-type) framework; P in tetrahedral voids, Cu in tetrahedral and trigonal voids (partial disorder). Single PS₄ tetrahedra.

Kuhs W.F., Heger G. (1979) [1]

BrCu₆PS₅

$a = 0.9745 \text{ nm}$, $V = 0.9254 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	48h	..m	0.19425	0.19425	0.02015	0.25	
Cu2	48h	..m	0.23823	0.23823	0.02277	0.25	
S3	16e	.3m	0.6218	0.6218	0.6218		
M4	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
P5	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron S ₄
M6	4a	-43m	0	0	0		cuboctahedron Cu ₁₂

M4 = 0.87S + 0.13Br; M6 = 0.87Br + 0.13S

Experimental: single crystal, diffractometer, neutrons, R = 0.053, T = 298 K

Remarks: Phase stable at T > 268 K. Short interatomic distances for partly occupied site(s).

References: [1] Kuhs W.F., Heger G. (1979), Fast Ion Transp. Solids Electrodes Electrolytes, Proc. Int. Conf. 1979 1979, 233-236.

216
cF124

Mg ₅ Pd ₁₀ Si ₁₆	cF124	(216) <i>F</i> -43m – hfe ³ a
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Mg₅Pd₁₀Si₁₆ [1]

Structural features: MgPd₁₀ units (a central Mg atom surrounded by an adamantane-type cage with four 6-membered rings) in a Cu-type (c.c.p.) arrangement; Si₄ tetrahedra in "octahedral", Si₁₂ truncated tetrahedra and Mg₄ tetrahedra in "tetrahedral" voids.

Lorenz P., Jung W. (2002) [1]

Mg₅Pd₁₀Si₁₆

$a = 1.25881 \text{ nm}$, $V = 1.9947 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	48h	..m	0.18414	0.18414	0.9553		pentagonal pyramid Si ₃ Pd ₃
Pd2	24f	2.mm	0.25827	0	0		pseudo Frank-Kasper Si ₆ Pd ₂ Mg ₃
Pd3	16e	.3m	0.13009	0.13009	0.13009		bicapped square prism Si ₃ Mg ₄ Pd ₃
Mg4	16e	.3m	0.351	0.351	0.351		18-vertex polyhedron Pd ₆ Si ₉ Mg ₃
Si5	16e	.3m	0.5703	0.5703	0.5703		trigonal prism Pd ₃ Si ₃
Mg6	4a	-43m	0	0	0		22-vertex polyhedron Pd ₁₀ Si ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.017

References: [1] Lorenz P., Jung W. (2002), Z. Naturforsch. B 57, 1346-1352.

216
cF124

Ag ₇ GeS ₅ I	cF124	(216) <i>F</i> -43m – hgfedca
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Ag₇GeS₅I [1], argyrodite family

Structural features: S and I form a tetrahedrally close-packed (MgCu₂-type) framework; Ge in tetrahedral, Ag mainly in trigonal voids (partial disorder). Single GeS₄ tetrahedra.

Nagel A., Range K.J. (1978) [1]

Ag₇GeS₅

$a = 1.0722$ nm, $V = 1.2326$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	48h	..m	0.15	0.15	0.0	0.056	
Ag2	24g	2.mm	0.033	$\frac{1}{4}$	$\frac{1}{4}$	0.054	
Ag3	24f	2.mm	0.25	0	0		non-coplanar square Ag ₄
S4	16e	.3m	0.375	0.375	0.375		7-vertex polyhedron Ag ₆ Ge
I5	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		
Ge6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		fourcapped trigonal prism S ₄ Ag ₆
S7	4a	-43m	0	0	0		18-vertex polyhedron Ag ₁₈

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays

Remarks: Short interatomic distances for partly occupied site(s). On page 1463 of [1] the occupancy of the Ge site is misprinted as 2.4 atoms per cell instead of 4 atoms per cell (from the description of the structure).

References: [1] Nagel A., Range K.J. (1978), Z. Naturforsch. B 33, 1461-1464.

216
cF136

Na_{0.01}Ca_{1.04}Mn_{0.07}(Ti_{0.38}Fe_{0.09}Al_{0.03}Sb_{0.50})₂Sb_{0.65}O₆[OH]_{0.91} cF136
(216) $F\text{-}43m$ – hgfe²ca

(Ca_{1.04}Mn_{0.07}Na_{0.01})Sb_{0.65}(Sb_{0.99}Ti_{0.76}Fe_{0.19}Al_{0.06})O₆(OH)_{0.91} [1], lewisite, pyrochlore family

Structural features: (Sb³⁺, Ti, Fe³⁺, Al)O₆ octahedra share vertices to form a pyrochlore-type framework with channels along $\langle 110 \rangle$.

Rouse R.C. et al. (1998) [1]

Al_{0.06}Ca_{1.04}Fe_{0.19}H_{0.91}Mn_{0.07}Na_{0.01}O_{6.91}Sb_{1.64}Ti_{0.76}

$a = 1.0277$ nm, $V = 1.0854$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	..m	0.1418	0.1418	0.0915	0.147	
O2	24g	2.mm	0.5546	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron Sb ₂ Ca ₂
O3	24f	2.mm	0.2988	0	0		non-colinear Sb ₂
M4	16e	.3m	0.122	0.122	0.122	0.442	
M5	16e	.3m	0.62522	0.62522	0.62552		octahedron O ₆
(OH)6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.91	
(OH)7	4a	-43m	0	0	0	0.91	

M1 = 0.5868Ca + 0.3672Sb + 0.0388Mn + 0.0072Na; M4 = 0.5868Ca + 0.3672Sb + 0.0388Mn + 0.0072Na; M5 = 0.495Sb + 0.380Ti + 0.095Fe + 0.030Al

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.014$, $T = 297$ K

Remarks: Natural specimen from Tripui, Ouro Preto, Minas Gerais. Composition Ca_{8.31}Na_{0.10}Fe_{1.53}Mn_{0.55}Ti_{6.07}Al_{0.44}Sb_{13.16}O_x from electron microprobe analysis, no F detected. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space groups (196) $F23$ and (227) $Fd\text{-}3m$ were tested and rejected.

References: [1] Rouse R.C., Dunn P.J., Peacor D.R., Wang L. (1998), J. Solid State Chem. 141, 562-569.

216
cF140

Cu_7PSe_6	<i>cF140</i>	(216) <i>F-43m</i> – $\text{h}^2\text{e}^2\text{cba}$
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$\text{Cu}_7\text{PSe}_6 \gamma$ [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu_2 -type) framework; P in tetrahedral, Cu in tetrahedral, trigonal and linear voids (disorder). Single PSe_4 tetrahedra.

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

Cu_7PSe_6

$a = 1.0113 \text{ nm}$, $V = 1.0343 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	48 <i>h</i>	<i>..m</i>	0.1713	0.1713	0.0173	0.314	
Cu2	48 <i>h</i>	<i>..m</i>	0.234	0.234	0.0257	0.179	
Cu3	16 <i>e</i>	<i>.3m</i>	0.1214	0.1214	0.1214	0.27	non-coplanar triangle Cu_3
Se4	16 <i>e</i>	<i>.3m</i>	0.62576	0.62576	0.62576		
Se5	4 <i>c</i>	<i>-43m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
P6	4 <i>b</i>	<i>-43m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Se_4
Se7	4 <i>a</i>	<i>-43m</i>	0	0	0		tetrahedron Cu_4

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.020$, $T = 353 \text{ K}$

Remarks: Phase stable at $T > 320 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Gaudin E., Boucher F., Petricek V., Taulelle F., Evain M. (2000), Acta Crystallogr. B 56, 402-408.

216
cF144

$\text{ReAsSBrNF}_6[\text{CO}]_5$	<i>cF144</i>	(216) <i>F-43m</i> – hg^2feca
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$[\text{Re}(\text{CO})_5(\text{NSBr})]\text{AsF}_6$ [1]

Structural features: $\text{Re}([\text{CO}]_5[\text{NSBr}])$ octahedral units ($\text{Re}(\text{C}_5\text{N})$ octahedron, linear Re-C-O segments, non-linear NSBr units, substitutional disorder of ligands) and AsF_6 octahedra in a sphalerite-type arrangement.

Ruf C. et al. (1997) [1]

$\text{AsBrC}_5\text{F}_6\text{NO}_5\text{ReS}$

$a = 1.1264 \text{ nm}$, $V = 1.4292 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	48 <i>h</i>	<i>..m</i>	0.1943	0.1943	0.5347	0.083	
M2	24 <i>g</i>	<i>2.mm</i>	0.0701	$\frac{1}{4}$	$\frac{1}{4}$		
O3	24 <i>g</i>	<i>2.mm</i>	0.5306	$\frac{1}{4}$	$\frac{1}{4}$	0.833	
F4	24 <i>f</i>	<i>2.mm</i>	0.1527	0	0		single atom As
Br5	16 <i>e</i>	<i>.3m</i>	0.5376	0.5376	0.5376	0.25	
Re6	4 <i>c</i>	<i>-43m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron C_6
As7	4 <i>a</i>	<i>-43m</i>	0	0	0		octahedron F_6

$M2 = 0.833\text{C} + 0.167\text{N}$

Transformation from published data: $-x, -y, -z$; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.019$, $T = 173$ K

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

References: [1] Ruf C., Lork E., Behrens U., Mews R. (1997), *Z. Anorg. Allg. Chem.* 623, 444-448.

216
cF148

$\text{Ag}_7\text{GeSe}_5\text{I}$	<i>cF148</i>	(216) <i>F-43m</i> – $\text{h}^2\text{e}^3\text{d}$
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Ag₇GeSe₅I [1], argyrodite family

Structural features: Se and I form a tetrahedrally close-packed (MgCu₂-type) framework (split sites); Ge in Se₄ tetrahedral voids, Ag in Se₃I tetrahedral voids (in part displaced towards the Se₃ face, disorder). Single GeSe₄ tetrahedra.

Aldon L. et al. (2001) [1]

$\text{Ag}_7\text{GeISe}_5$

$a = 1.09864$ nm, $V = 1.3261$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	48h	..m	0.01	0.01	0.2161	0.252	
Ag2	48h	..m	0.0749	0.0749	0.2335	0.331	
Se3	16e	.3m	0.0204	0.0204	0.0204	0.25	
I4	16e	.3m	0.2693	0.2693	0.2693	0.25	
Se5	16e	.3m	0.62701	0.62701	0.62701		
Ge6	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		tetrahedron Se ₄

Transformation from published data: $-x, -y, -z$; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, neutrons, $R = 0.036$, $T = 293$ K

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

References: [1] Aldon L., Belin R., Pontillon Y. (2001), *Z. Kristallogr., New Cryst. Struct.* 216, 181-182.

216
cF148

Li_7IN_2	<i>cF148</i>	(216) <i>F-43m</i> – h^2fedca
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Li₇N₂I [1]

Structural features: I and N form a tetrahedrally close-packed MgCu₂-type framework; Li in tetrahedral, trigonal and approximately linear voids.

Marx R. (1998) [1]

ILi_7N_2

$a = 1.0388$ nm, $V = 1.1210$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	..m	0.169	0.169	0.107	0.083	
Li2	48h	..m	0.2284	0.2284	0.0377	0.5	
Li3	24f	2.mm	0.3246	0	0		non-colinear N ₂
N4	16e	.3m	0.36882	0.36882	0.36882		
I5	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		
Li6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
I7	4a	-43m	0	0	0		

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_B = 0.041$

Remarks: Short interatomic distances for partly occupied site(s). Refinement of an alternative model considering seven Li sites gave $R_B = 0.029$. In table II of [1] the Wyckoff positions of former I1, I2, Li1 and Li3 are misprinted as *4a*, *4c*, *4b* and *24f* instead of *4b*, *4d*, *4a* and *24g*, respectively.

References: [1] Marx R. (1998), Eur. J. Solid State Inorg. Chem. 35, 197-209.

216
cF152

Ag_7PSe_6	<i>cF152</i>	(216) <i>F-43m</i> – h^2e^3da
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Ag_7PSe_6 γ [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu_2 -type) framework; P in tetrahedral, Ag in tetrahedral, trigonal and linear voids (disorder). Single PSe_4 tetrahedra (split Se site).

Evain M. et al. (1998) [1]

$\text{Ag}_{7.01}\text{PSe}_6$

$a = 1.0838 \text{ nm}$, $V = 1.2731 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	48 <i>h</i>	.. <i>m</i>	0.0308	0.0308	0.2297	0.261	
Ag2	48 <i>h</i>	.. <i>m</i>	0.0964	0.0964	0.234	0.25	
Ag3	16 <i>e</i>	.3 <i>m</i>	0.13	0.13	0.13	0.22	
Se4	16 <i>e</i>	.3 <i>m</i>	0.2702	0.2702	0.2702	0.25	
Se5	16 <i>e</i>	.3 <i>m</i>	0.63158	0.63158	0.63158		
P6	4 <i>d</i>	-43 <i>m</i>	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		tetrahedron Se_4
Se7	4 <i>a</i>	-43 <i>m</i>	0	0	0		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.033$, $T = 473 \text{ K}$

Remarks: Phase stable at $T > 453 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Evain M., Gaudin E., Boucher F., Petricek V., Taulelle F. (1998), Acta Crystallogr. B 54, 376-383.

216
cF160

$[\text{NH}_4]_2\text{Re}_2\text{S}_{11}[\text{H}_2\text{O}]$	<i>cF160</i>	(216) <i>F-43m</i> – h^2fe^2da
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$(\text{NH}_4)_4\text{Re}_4\text{S}_{22} \cdot 2\text{H}_2\text{O}$ [1]; $\text{K}_4\text{Pt}_4\text{S}_{22} \cdot 4\text{H}_2\text{O}$ [2]

Structural features: Re_4S_{22} units consisting of four ReS_6 octahedra interconnected via common edges (central Re_4S_4 cube) and additional S atoms (S-S-S bridges). Three finite S_3 chains for two single S.

Müller A. et al. (1987) [1]

$\text{H}_{10}\text{N}_2\text{ORe}_2\text{S}_{11}$

$a = 1.5203 \text{ nm}$, $V = 3.5139 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	48 <i>h</i>	.. <i>m</i>	0.1698	0.1698	0.024		non-coplanar triangle S_2Re
S2	48 <i>h</i>	.. <i>m</i>	0.2171	0.2171	0.538	0.5	non-coplanar triangle S_3
M3	24 <i>f</i>	2.. <i>mm</i>	0.3476	0	0	0.667	bicapped hexagonal prism $(\text{NH}_4)_4\text{S}_{10}$
Re4	16 <i>e</i>	.3 <i>m</i>	0.1856	0.1856	0.1856		tricapped trigonal prism S_6Re_3
S5	16 <i>e</i>	.3 <i>m</i>	0.3355	0.3355	0.3355		non-coplanar triangle Re_3
$(\text{NH}_4)_6$	4 <i>d</i>	-43 <i>m</i>	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		12-vertex polyhedron S_{12}

(NH₄)₇ 4a -43m 0 0 0 cuboctahedron S₁₂

M3 = 0.5NH₄ + 0.5OH₂

Transformation from published data: -x,-y,-z; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.040, T = 294 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. Similar units in (NH₄)₂Re₂S₁₁·(0.3NH₄Cl 0.7H₂O) [3] (same space group, atom coordinates of NH₄ units not determined).

References: [1] Müller A., Krickemeyer E., Bögger H. (1987), Z. Anorg. Allg. Chem. 554, 61-78. [2] Kim K.H., Kanatzidis M.G. (1993), Inorg. Chem. 32, 4161-4163. [3] Müller A., Krickemeyer E., Bögger H. (1986), Angew. Chem. Int. Ed. Engl. 25, 272-273.

216
cF168

Ba₃Zn₅In₂O₁₁ cF168 (216) *F*-43m – hgfe⁴ba

Ba₃In₂Zn₅O₁₁ [1]

Structural features: In₄O₁₆ units consisting of four edge-linked InO₆ octahedra (central In₄O₄ cube) and ZnO₄ tetrahedra (interconnected tetrahedral units formed by ten vertex-linked tetrahedra) share vertices to form a 3D-framework; OBa₆ octahedra in voids.

Scheikowski M., Müller Buschbaum H. (1993) [1]

Ba₃In₂O₁₁Zn₅

a = 1.33588 nm, *V* = 2.3840 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48h	..m	0.165	0.165	0.502		coplanar triangle Zn ₂ In
Zn2	24g	2.mm	0.0803	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O ₄
Ba3	24f	2.mm	0.2052	0	0		pseudo Frank-Kasper O ₆ Zn ₂
O4	16e	.3m	0.157	0.157	0.157		non-coplanar triangle Zn ₃
Zn5	16e	.3m	0.4171	0.4171	0.4171		tetrahedron O ₄
In6	16e	.3m	0.665	0.665	0.665		octahedron O ₆
O7	16e	.3m	0.83	0.83	0.83		non-coplanar triangle In ₃
O8	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Zn ₄
O9	4a	-43m	0	0	0		octahedron Ba 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, wR = 0.040

References: [1] Scheikowski M., Müller Buschbaum H. (1993), Z. Anorg. Allg. Chem. 619, 559-562.

216
cF172

Ag₇GeS₅I cF172 (216) *F*-43m – h³ecba

Ag₇GeS₅I [1], argyrodite family

Structural features: S and I form a tetrahedrally close-packed (MgCu₂-type) framework; Ge in S₄ tetrahedral voids, Ag in S₃I tetrahedral voids (in part displaced towards the S₃ face, disorder). Single GeS₄ tetrahedra.

Cros B. et al. (1986) [1]

Ag_{7.01}GeIS₅

a = 1.07116 nm, *V* = 1.2290 nm³, *Z* = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	48h	..m	0.166	0.166	0.0096	0.194	
Ag2	48h	..m	0.196	0.196	0.0124	0.05	
Ag3	48h	..m	0.2368	0.2368	0.0263	0.34	
S4	16e	.3m	0.6195	0.6195	0.6195		single atom Ge
S5	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ge6	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron S ₄
I7	4a	-43m	0	0	0		cuboctahedron Ag ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.075, T = 173 K

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

References: [1] Cros B., Laqibi M., Peytavin S., Ribes M. (1986), Rev. Chim. Miner. 23, 796-809.

216
cF172

Cd _{3.25} PS _{5.5} I _{0.5}	cF172	(216) <i>F</i> -43m – ihecba
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Cd₁₃P₄S₂₂I₂ [1], argyrodite family

Structural features: S and I form a tetrahedrally close-packed (MgCu₂-type) framework; P in tetrahedral, Cd in tetrahedral and trigonal voids (disorder). Single PS₄ tetrahedra.

Bubenzer A. et al. (1976) [1]

Cd_{3.26}I_{0.50}PS_{5.50}

$a = 0.9969$ nm, $V = 0.9907$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	96i	1	0.047	0.126	0.2	0.042	
Cd2	48h	..m	0.178	0.178	0.018	0.188	
S3	16e	.3m	0.6186	0.6186	0.6186		single atom P
M4	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
P5	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron S ₄
M6	4a	-43m	0	0	0		

M4 = 0.75S + 0.25I; M6 = 0.75S + 0.25I

Experimental: single crystal, diffractometer, X-rays, R = 0.065, T = 293 K

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

References: [1] Bubenzer A., Nitsche R., Grieshaber E. (1976), Acta Crystallogr. B 32, 2825-2829.

216
cF180

In ₂ Te ₃	cF180	(216) <i>F</i> -43m – h ² gfe ² a
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In₂Te₃ α [2]

Structural features: Close-packed Te layers in c stacking, In in tetrahedral voids. InTe₄ tetrahedra share vertices to form a 3D-framework; additional Te in voids. Vacancy derivative of ZnS (sphalerite).

Zaslavskii A.I., Sergeeva V.M. (1961) [1]

In₂Te₃

$a = 1.85$ nm, $V = 6.3316$ nm³, $Z = 36$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	48h	..m	0.08333	0.08333	0.25		tetrahedron Te ₄
Te2	48h	..m	0.16667	0.16667	0.0		non-coplanar triangle In ₃
In3	24g	2.mm	0.58333	1/4	1/4		tetrahedron Te ₄
Te4	24f	2.mm	0.33333	0	0		non-collinear In ₂
Te5	16e	.3m	0.33333	0.33333	0.33333		non-coplanar triangle In ₃
Te6	16e	.3m	0.66667	0.66667	0.66667		non-coplanar triangle In ₃
Te7	4a	-43m	0	0	0		cuboctahedron Te ₁₂

Transformation from published data: -x,-y,-z; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, Laue photographs, X-rays

Remarks: Phase stable at T < 793-893 K. Idealized coordinates. Preliminary data in [3].

References: [1] Zaslavskii A.I., Sergeeva V.M. (1961), Sov. Phys. Solid State (Engl. Transl.) 2, 2556-2561. [2] Zhuze V.P., Zaslavskii A.I., Petrusovich V.A., Sergeeva V.M., Smirnov I.A., Shelykh A.I. (1961), Proc. Int. Conf. Semicond. Phys. 1961, 871-881. [3] Inuzuka H., Sugaike S. (1954), Proc. Jpn. Acad. 30, 383-386.

216
cF192

TmNi ₂	cF192	(216) <i>F</i> -43m – h ² ge ⁴ ba
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TmNi₂ rt [1]; Y_{0.95}Ni₂ [2]

Structural features: Deformation derivative of MgCu₂ (cubic Laves phase). Tm(Ni₁₂Tm₄) Friauf polyhedra (Ni₁₂ truncated tetrahedron + Tm₄ tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. Tetrahedrally close-packed structure (Frank-Kasper phase).

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

Ni₂Tm

a = 1.41930 nm, *V* = 2.8591 nm³, *Z* = 64

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	48h	..m	0.0677	0.0677	0.3167		icosahedron Ni ₆ Tm ₆
Ni2	48h	..m	0.0678	0.0678	0.8195		icosahedron Ni ₆ Tm ₆
Tm3	24g	2.mm	0.0132	1/4	1/4		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Tm4	16e	.3m	0.1210	0.1210	0.1210		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Ni5	16e	.3m	0.3092	0.3092	0.3092		icosahedron Ni ₆ Tm ₆
Tm6	16e	.3m	0.6276	0.6276	0.6276		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Ni7	16e	.3m	0.8160	0.8160	0.8160		icosahedron Ni ₆ Tm ₆
Tm8	4b	-43m	1/2	1/2	1/2		16-vertex Frank-Kasper Ni ₁₂ Tm ₄
Tm9	4a	-43m	0	0	0		16-vertex Frank-Kasper Ni ₁₂ Tm ₄

Experimental: powder, diffractometer, neutrons, R_B = 0.079, T = 300 K

Remarks: No evidence for Tm deficiency.

References: [1] Deutz A.F., Helmholdt R.B., Moleman A.C., De Mooij D.B., Buschow K.H.J. (1989), J. Less-Common Met. 153, 259-266. [2] Latroche M., Paul Boncour V., Percheron Guégan A., Achard J.C. (1990), J. Less-Common Met. 161, L27-L31.

216
cF220

Ag ₈ GeTe ₆	cF220	(216) <i>F</i> -43m – ih ² ecba
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Ag₈GeTe₆ γ (see remark), argyrodite family; Ag₈SiTe₆ γ [2]; Ag₇TaS₆ [3]

Structural features: Te forms a tetrahedrally close-packed (MgCu₂-type) framework; Ge in tetrahedral voids, Ag distributed over several sites of low coordination (partial disorder). Single GeTe₄ tetrahedra. See Fig. II.19.

Boucher F. et al. (1993) [1]

Ag_{7.94}GeTe₆

$a = 1.15656 \text{ nm}$, $V = 1.5471 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	96i	1	0.051	0.085	0.207	0.041	
Ag2	48h	$\dots m$	0.1645	0.1645	0.011	0.33	
Ag3	48h	$\dots m$	0.214	0.214	0.0266	0.25	
Te4	16e	$\dots 3m$	0.62731	0.62731	0.62731		
Te5	4c	$\dots 43m$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ge6	4b	$\dots 43m$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Te ₄
Te7	4a	$\dots 43m$	0	0	0		

Transformation from published data: $-x, -y, -z$; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.036$, $T = 293 \text{ K}$

Remarks: We changed the y -coordinate of former Ag(1) from 0.415 to 0.4145 and the y - and z -coordinates of former Te(1) from 0.6227 to 0.62269 to be in agreement with Wyckoff positions 48h and 16e, respectively. Short interatomic distances for partly occupied site(s). Ionic conductivity is explained by diffusion via a third tetrahedral site for which, however, no significant electron density was detected. Supersedes structure proposals with different distribution of Ag in the same space group ([5], [6]) and in space group (146) $R3$ [7]. Preliminary data for Ag₇TaS₆ in [4].

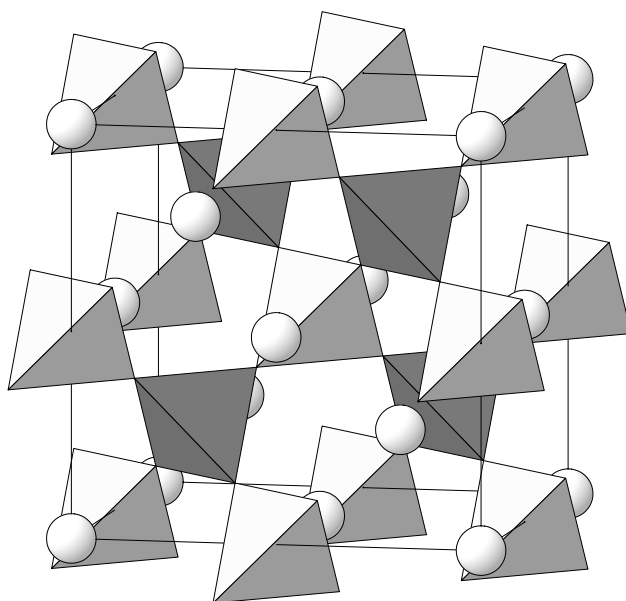


Fig. II.19. **Ag₈GeTe₆**

Arrangement of GeTe₄ (dark) and Te₄ (light) tetrahedra and additional Te atoms.

References: [1] Boucher F., Evain M., Brec R. (1993), J. Solid State Chem. 107, 332-346. [2] Boucher F., Evain M., Brec R. (1992), J. Solid State Chem. 100, 341-355. [3] Wada H., Onoda M. (1991), J. Less-Common Met. 175, 209-217. [4] Wada H. (1991), Bull. Chem. Soc. Jpn. 64, 2022-2023. [5] Rysanek N., Laruelle P., Katty A. (1976), Acta Crystallogr. B 32, 692-696. [6] Nagel A., Range K.J. (1978), Z. Naturforsch. B 33, 1461-1464. [7] Unterrichter J.V., Range K.J. (1978), Z. Naturforsch. B 33, 866-872.

Ag ₉ GaSe ₆	cF220	(216) <i>F</i> -43 <i>m</i> – ih ² ecba
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Ag₉GaSe₆ α [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu₂-type) framework; Ga in tetrahedral, Ag in tetrahedral and trigonal voids (disorder). Single GaSe₄ tetrahedra.

Deloume J.P., Faure R. (1981) [1]

Ag₉GaSe₆

$a = 1.1126$ nm, $V = 1.3773$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	96 <i>i</i>	1	0.129	0.34	0.573	0.125	
Ag2	48 <i>h</i>	.. <i>m</i>	0.169	0.169	0.031	0.25	
Ag3	48 <i>h</i>	.. <i>m</i>	0.232	0.232	0.029	0.25	
Se4	16 <i>e</i>	.3 <i>m</i>	0.623	0.623	0.623		
Se5	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ga6	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Se ₄
Se7	4 <i>a</i>	-43 <i>m</i>	0	0	0		

Experimental: single crystal, diffractometer, X-rays, $R = 0.063$, $T = 293$ K

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

References: [1] Deloume J.P., Faure R. (1981), J. Solid State Chem. 36, 112-117.

Ag _{6.4} Hg _{0.8} SiSe ₆	cF220	(216) <i>F</i> -43 <i>m</i> – ih ² ecba
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Ag_{6.4}Hg_{0.8}SiSe₆ [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu₂-type) framework; Si and Hg in tetrahedral, Ag mainly in trigonal voids (disorder). Single SiSe₄ tetrahedra.

Parasyuk O.V. et al. (2003) [1]

Ag_{6.25}Hg_{0.83}Se₆Si

$a = 1.08806$ nm, $V = 1.2881$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	96 <i>i</i>	1	0.0037	0.1377	0.1729	0.137	
Hg2	48 <i>h</i>	.. <i>m</i>	0.1991	0.1991	0.0273	0.069	
Ag3	48 <i>h</i>	.. <i>m</i>	0.2355	0.2355	0.0342	0.247	
Se4	16 <i>e</i>	.3 <i>m</i>	0.6185	0.6185	0.6185		single atom Si
Se5	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Si6	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Se ₄
Se7	4 <i>a</i>	-43 <i>m</i>	0	0	0		

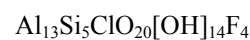
Transformation from published data: -*x*, -*y*, -*z*; origin shift $\frac{3}{4}$ $\frac{3}{4}$ $\frac{3}{4}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.083$

Remarks: Phase referred to as β-(AgHgSeSi), homogeneity range (Ag₈SiSe₆)_{100-x}(Hg₄SiSe₆)_x, $12 < x < 21$. Short interatomic distances for partly occupied site(s). In table 2 of [1] the Wyckoff position of former Ag2 is misprinted as 98*i* instead of 96*i*.

References: [1] Parasyuk O.V., Gulay L.D., Romanyuk Y.E., Olekseyuk I.D. (2003), J. Alloys Compd. 348, 157-166.

216
cF228



cF228

(216) $F\bar{4}3m - h^3ge^3dba$

$\text{Al}_{13}\text{Si}_5\text{O}_{20}(\text{OH},\text{F})_{18}\text{Cl}$ [2], zunyite, Strukturbericht notation S0_8

Structural features: $\text{AlAl}_{12}(\text{O},\text{OH})_{40}$ Keggin units (twelve edge- and vertex-linked $\text{Al}(\text{O},\text{OH},\text{F})_6$ octahedra sharing vertices with a central AlO_4 tetrahedron) in a Cu-type (c.c.p.) arrangement and Si_5O_{16} units (a central SiO_4 tetrahedron sharing vertices with four surrounding tetrahedra) share atoms to form a 3D-framework. See Fig. II.20.

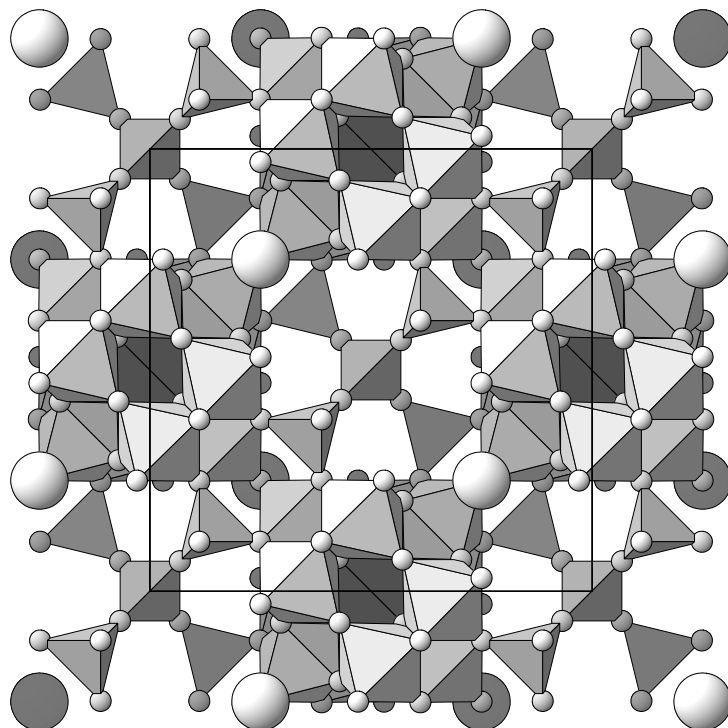
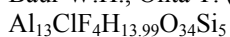


Fig. II.20. **$\text{Al}_{13}\text{Si}_5\text{O}_{20}\text{Cl}(\text{OH},\text{F})_{18}$**

Arrangement of AlO_4 (dark) and SiO_4 (light) tetrahedra, $\text{Al}(\text{O}_3(\text{OH},\text{F})_3)$ octahedra (O and F atoms small) and Cl atoms (large) (Al atoms at $x = 0, \pm 0.02$ and ± 0.16 , Si atoms at $x = 0$ and ± 0.14 , Cl atoms at $x = \pm 1/4$).

Baur W.H., Ohta T. (1982) [1]



$a = 1.38654 \text{ nm}$, $V = 2.6656 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	$\bar{3}m$	0.0713	0.0713	0.70399		non-colinear Al_2
O2	48h	$\bar{3}m$	0.11166	0.11166	0.24848		non-coplanar triangle SiAl_2
Al3	48h	$\bar{3}m$	0.16444	0.16444	0.4833		octahedron O_6
O4	24g	$2\bar{3}m$	0.52949	$1/4$	$1/4$		non-colinear Al_2
O5	16e	$\bar{3}m$	0.06757	0.06757	0.06757		colinear Si_2
Si6	16e	$\bar{3}m$	0.1357	0.1357	0.1357		tetrahedron O_4
O7	16e	$\bar{3}m$	0.42522	0.42522	0.42522		tetrahedron Al_4
Cl8	4d	$\bar{4}3m$	$3/4$	$3/4$	$3/4$		octahedron O_6
Al9	4b	$\bar{4}3m$	$1/2$	$1/2$	$1/2$		tetrahedron O_4
Si10	4a	$\bar{4}3m$	0	0	0		tetrahedron O_4

H11	48h	..m	0.022	0.022	0.72	0.333
H12	48h	..m	0.06	0.06	0.77	0.333
H13	24g	2.mm	0.586	$\frac{1}{4}$	$\frac{1}{4}$	

M1 = 0.667O + 0.333F

Transformation from published data: -x,-y,-z; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.016, T = 293 K

Remarks: Natural specimen from Quartzsite, Yuma County, Arizona. Composition $\text{Na}_{0.04}\text{Al}_{13.05}\text{Fe}_{0.005}\text{Si}_{4.95}\text{O}_x(\text{OH})_y\text{F}_{4.1}\text{Cl}_{0.92}$ from electron microprobe analysis. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The data from [3] are quoted in [4].

References: [1] Baur W.H., Ohta T. (1982), Acta Crystallogr. B 38, 390-401. [2] Pauling L. (1933), Z. Kristallogr. 84, 442-452. [3] Barclay Kamb W. (1960), Acta Crystallogr. 13, 15-24. [4] Yang Q.B., Andersson S. (1987), Acta Crystallogr. B 43, 1-14.

216
cF232

$\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$	cF232	(216) $F-43m - h^2gfe^5da$
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$\text{Ca}_{12}\text{Be}_{17}\text{O}_{29}$ [1]

Structural features: BeO_4 tetrahedra and BeO_3 trigonal units share vertices to form a 3D-framework with channels along $\langle 100 \rangle$.

Harris L.A., Yakel H.L. (1966) [1]

$\text{Be}_{17}\text{Ca}_{12}\text{O}_{29}$

$a = 1.4023 \text{ nm}$, $V = 2.7575 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	..m	0.11211	0.11211	0.74745		non-colinear Be_2
O2	48h	..m	0.11431	0.11431	0.24819		non-colinear Be_2
Ca3	24g	2.mm	0.00404	$\frac{1}{4}$	$\frac{1}{4}$		square prism (cube) O_8
Ca4	24f	2.mm	0.20682	0	0		6-vertex polyhedron O_6
O5	16e	.3m	0.06856	0.06856	0.06856		colinear Be_2
Be6	16e	.3m	0.13616	0.13616	0.13616		tetrahedron O_4
Be7	16e	.3m	0.34346	0.34346	0.34346		non-coplanar triangle O_3
Be8	16e	.3m	0.66316	0.66316	0.66316		non-coplanar triangle O_3
Be9	16e	.3m	0.82609	0.82609	0.82609		tetrahedron O_4
O10	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		square prism (cube) Be_8
Be11	4a	-43m	0	0	0		tetrahedron O_4

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

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.066

References: [1] Harris L.A., Yakel H.L. (1966), Acta Crystallogr. 20, 295-301.

216
cF240

$\text{Na}_2\text{AlSiO}_{4.5}$	cF240	(216) $F-43m - i^2e^2dcba$
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$\text{Na}_2\text{Al}_4\text{Si}_4\text{O}_{18}$ [1], carnegieite

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a cristobalite-type framework (Al and Si form a sphalerite-type substructure); disordered arrangement of Na_2O in voids.

Borchert W., Keidel J. (1947) [1]

$\text{AlNa}_{1.99}\text{O}_{4.50}\text{Si}$

$a = 0.7273 \text{ nm}$, $V = 0.3847 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	96i	1	0.05	0.11	0.17	0.033	
O2	96i	1	0.11	0.17	0.55	0.167	
O3	16e	.3m	0.06	0.06	0.06	0.062	
O4	16e	.3m	0.31	0.31	0.31	0.062	
Al5	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		
Na6	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Si7	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Na8	4a	-43m	0	0	0	0.2	

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

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

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

References: [1] Borchert W., Keidel J. (1947), Beitr. Mineral. Petrogr. 1, 17-30.

216
cF264

$\text{Cu}_6\text{PS}_5\text{Br}$	cF264	(216) $F-43m - h^4ge^2dcba$
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$\text{Cu}_6\text{PS}_5\text{Br}$ [1], argyrodite family

Structural features: S and Br form a tetrahedrally close-packed (MgCu_2 -type) framework; P in tetrahedral voids (partial disorder), Cu distributed over several sites in low coordination (high degree of disorder). Single PS_4 tetrahedra.

Kuhs W.F. et al. (1978) [1]

BrCu_6PS_5

$a = 0.9728 \text{ nm}$, $V = 0.9206 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	48h	..m	0.0145	0.0145	0.227	0.245	
Cu2	48h	..m	0.046	0.046	0.769	0.018	
Cu3	48h	..m	0.056	0.056	0.229	0.105	
Cu4	48h	..m	0.07	0.07	0.263	0.068	
Cu5	24g	2.mm	0.509	$\frac{1}{4}$	$\frac{1}{4}$	0.084	
Cu6	16e	.3m	0.108	0.108	0.108	0.065	
S7	16e	.3m	0.6286	0.6286	0.6286		
P8	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.85	fourcapped trigonal prism S_4Cu_6
M9	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
P10	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.15	tetrahedron S_4
M11	4a	-43m	0	0	0		tetrahedron Cu_4

$\text{M9} = 0.84\text{Br} + 0.16\text{S}$; $\text{M11} = 0.84\text{S} + 0.16\text{Br}$

Transformation from published data: $-x, -y, -z$; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.043$

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

References: [1] Kuhs W.F., Nitsche R., Scheunemann K. (1978), Acta Crystallogr. B 34, 64-70.

216
cF268

Li ₇ IN ₂	cF268	(216) <i>F</i> -43 <i>m</i> – h ⁴ gfedca
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Li₇N₂I [1]

Structural features: I and N form a tetrahedrally close-packed MgCu₂-type framework; Li distributed over several sites in low coordination (high degree of disorder).

Marx R. (1998) [1]

ILi₇N₂ $a = 1.0388 \text{ nm}$, $V = 1.1210 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	48 <i>h</i>	.. <i>m</i>	0.1602	0.1602	0.1297	0.083	
Li2	48 <i>h</i>	.. <i>m</i>	0.2011	0.2011	0.0599	0.083	
Li3	48 <i>h</i>	.. <i>m</i>	0.2195	0.2195	0.0416	0.167	
Li4	48 <i>h</i>	.. <i>m</i>	0.2367	0.2367	0.0338	0.167	
Li5	24 <i>g</i>	2.. <i>mm</i>	0.032	¹ / ₄	¹ / ₄	0.167	
Li6	24 <i>f</i>	2.. <i>mm</i>	0.3249	0	0		non-collinear N ₂
N7	16 <i>e</i>	.3 <i>m</i>	0.36882	0.36882	0.36882		
I8	4 <i>d</i>	-43 <i>m</i>	³ / ₄	³ / ₄	³ / ₄		
Li9	4 <i>c</i>	-43 <i>m</i>	¹ / ₄	¹ / ₄	¹ / ₄		
I10	4 <i>a</i>	-43 <i>m</i>	0	0	0		

Transformation from published data: origin shift ³/₄ ³/₄ ³/₄Experimental: powder, diffractometer, neutrons, time-of-flight, R_B = 0.029

Remarks: Short interatomic distances for partly occupied site(s). Refinement of an alternative model considering two Li sites gave R_B = 0.041. In tables II and V of [1] the Wyckoff positions of former I(1), I(2), Li(1), Li(3), and Li(4) are misprinted as 4*a*, 4*c*, 4*b*, 24*f*, and 16*e*, instead of 4*b*, 4*d*, 4*a*, 24*g*, and 48*h*, respectively.

References: [1] Marx R. (1998), Eur. J. Solid State Inorg. Chem. 35, 197-209.

216
cF284

Ag ₁₈ Tl ₄ Te ₁₁	cF284	(216) <i>F</i> -43 <i>m</i> – h ⁴ g ² e ² cba
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Tl₄Ag₁₈Te₁₁ [1]

Structural features: Tl₇Te₅₆ units (a TlTe₈ cube sharing faces with six surrounding TlTe₈ square antiprisms) share atoms to form a 3D-framework; additional Tl in large voids (displaced towards a square face, disorder).

Moreau J.M. et al. (1992) [1]

Ag₁₈Te₁₁Tl₄ $a = 1.8717 \text{ nm}$, $V = 6.5571 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	48 <i>h</i>	.. <i>m</i>	0.0581	0.0581	0.245		9-vertex polyhedron Te ₄ Ag ₅
Te2	48 <i>h</i>	.. <i>m</i>	0.0915	0.0915	0.7456		10-vertex polyhedron Ag ₆ Tl ₄
Ag3	48 <i>h</i>	.. <i>m</i>	0.1139	0.1139	0.5058		pseudo Frank-Kasper Ag ₆ Te ₄ Tl
Ag4	48 <i>h</i>	.. <i>m</i>	0.1219	0.1219	0.9908		pseudo Frank-Kasper Te ₄ Ag ₆ Tl
Tl5	24 <i>g</i>	2.. <i>mm</i>	0.0195	¹ / ₄	¹ / ₄		pseudo Frank-Kasper Ag ₈ Tl ₂ Te ₈
Tl6	24 <i>g</i>	2.. <i>mm</i>	0.671	¹ / ₄	¹ / ₄	0.167	non-coplanar square Tl ₄
Te7	16 <i>e</i>	.3 <i>m</i>	0.1396	0.1396	0.1396		6-vertex polyhedron Ag ₆

Te8	16e	.3m	0.357	0.357	0.357	pseudo Frank-Kasper Ag ₆ Tl ₄ Te ₃
Tl9	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	square prism (cube) Te ₈
Te10	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	cuboctahedron Ag ₁₂
Te11	4a	-43m	0	0	0	cuboctahedron Ag ₁₂

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.070

Remarks: Preliminary data in [3]. Supersedes a refinement in space group (225) *Fm-3m* where the partly occupied Tl site was not detected [2] (Tl₇Ag₃₆Te₂₂). Short interatomic distances for partly occupied site(s).

References: [1] Moreau J.M., Allemand J., Brun G., Liautard B. (1992), J. Alloys Compd. 178, 85-90. [2] Klepp K.O. (1983), Z. Kristallogr. 162, 136-137. [3] Moreau J.M., Allemand J. (1991), Coll. Abs. X Int. Conf. Solid Compd. Trans. El., Muenster 1991, P-146.

216
cF292

Ag ₇ GeS ₅ I	cF292	(216) <i>F-43m</i> – h ⁵ fecba
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Ag₇GeS₅I [1], argyrodite family

Structural features: S and I form a tetrahedrally close-packed (MgCu₂-type) framework; Ge in tetrahedral voids, Ag distributed over several sites in low coordination (disorder). Single GeS₄ tetrahedra.

Nagel A., Range K.J. (1979) [1]

Ag_{6.97}GeIS₅

a = 1.0722 nm, *V* = 1.2326 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	48h	..m	0.098	0.098	0.255	0.021	
Ag2	48h	..m	0.116	0.116	0.309	0.035	
Ag3	48h	..m	0.1747	0.1747	0.0094	0.113	
Ag4	48h	..m	0.2095	0.2095	0.0255	0.129	
Ag5	48h	..m	0.2347	0.2347	0.0233	0.256	
Ag6	24f	2..mm	0.283	0	0	0.054	
S7	16e	.3m	0.6195	0.6195	0.6195		4-vertex polyhedron Ag ₃ Ge
S8	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ge9	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		fourcapped trigonal prism S ₄ Ag ₆
I10	4a	-43m	0	0	0		cuboctahedron Ag ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.072

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

References: [1] Nagel A., Range K.J. (1979), Z. Naturforsch. B 34, 360-362.

216
cF296

Ce ₃ Pt ₂₃ Ge ₁₁	cF296	(216) <i>F-43m</i> – h ² gf ² e ⁸
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Ce₃Pt₂₃Ge₁₁ [1]

Structural features: GePt₇ polyhedra (trigonal prism, one additional atom capping a trigonal face) and GePt₈ cubes share atoms to form a 3D-framework; Ce in large voids.

Gribanov A.V. et al. (1993) [1]

 $\text{Ce}_3\text{Ge}_{11.92}\text{Pt}_{22.08}$ $a = 1.71833 \text{ nm}$, $V = 5.0736 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pt1	48h	..m	0.0841	0.0841	0.2479		bicapped square prism $\text{Ge}_3\text{Pt}_5\text{Ce}_2$
M2	48h	..m	0.0847	0.0847	0.7541		bicapped square prism $\text{Ge}_3\text{Pt}_5\text{Ce}_2$
Ce3	24g	2.mm	0.0018	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex polyhedron $\text{Pt}_{12}\text{Ge}_4$
Pt4	24f	2.mm	0.1281	0	0		13-vertex polyhedron Ge_5Pt_8
Ge5	24f	2.mm	0.3285	0	0		square prism (cube) Pt_8
Ge6	16e	.3m	0.1075	0.1075	0.1075		7-vertex polyhedron Pt_7
Pt7	16e	.3m	0.1927	0.1927	0.1927		fourcapped trigonal prism Ge_4Pt_6
Ge8	16e	.3m	0.3357	0.3357	0.3357		7-vertex polyhedron Pt_7
Pt9	16e	.3m	0.4139	0.4139	0.4139		fourcapped trigonal prism Ge_4Pt_6
Pt10	16e	.3m	0.5787	0.5787	0.5787		fourcapped trigonal prism Ge_4Pt_6
Ge11	16e	.3m	0.6672	0.6672	0.6672		7-vertex polyhedron Pt_7
Pt12	16e	.3m	0.8098	0.8098	0.8098		fourcapped trigonal prism Ge_4Pt_6
M13	16e	.3m	0.8962	0.8962	0.8962		7-vertex polyhedron Pt_7

 $\text{M2} = 0.78\text{Pt} + 0.22\text{Ge}$; $\text{M13} = 0.80\text{Ge} + 0.20\text{Pt}$ Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.074$

Remarks: Supersedes a refinement of so-called $\text{Ce}_{7.5}\text{Pt}_{62.5}\text{Ge}_{30}$ with ~281 atoms in the unit cell [2]. In [2] the x -coordinate of former Pt(3) is misprinted as 0.6421 instead of 0.9421 and the y -coordinate of former Pt(7) as equal to x instead of equal to z (from similarity with related structures, interatomic distances closer to expected ones).

References: [1] Gribanov A.V., Seropegin Y.D., Bodak O.I., Pavlyuk V.V., Akselrud L.G., Nikiforov V.N., Velikhovskii A.A. (1993), J. Alloys Compd. 202, 133-136. [2] Gribanov A.V., Sologub O.L., Salamakha P.S., Seropegin Y.D., Bodak O.I. (1992), Tezisy Dokl. Sov. Kristallokhim. Neorg. Koord. Soeden. 6th 1992, 172.

216
cF312

Ag_8GeTe_6	cF312	(216) $F-43m - ih^3fe^2dcba$
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 $\text{Ag}_8\text{GeTe}_6 \gamma$ [1], argyrodite family

Structural features: Te forms a tetrahedrally close-packed (MgCu_2 -type) framework; Ge in tetrahedral voids, Ag distributed over several sites in low coordination (high degree of disorder). Single GeTe_4 tetrahedra.

Geller S. (1979) [1]

 $\text{Ag}_{7.96}\text{GeTe}_6$ $a = 1.158 \text{ nm}$, $V = 1.5528 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	96i	1	0.067	0.104	0.22	0.06	
Ag2	48h	..m	0.071	0.071	0.238	0.36	
Ag3	48h	..m	0.105	0.105	0.3	0.022	
Ag4	48h	..m	0.213	0.213	0.037	0.069	
Ag5	24f	2.mm	0.213	0	0	0.104	
Ag6	16e	.3m	0.379	0.379	0.379	0.065	
Te7	16e	.3m	0.6233	0.6233	0.6233		

Ge8	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	0.222	tetrahedron Te ₄
Te9	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ag10	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		square prism (cube) Ag ₄ Te ₄
Te11	4a	-43m	0	0	0		octahedron Ag ₆

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

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

References: [1] Geller S. (1979), Z. Kristallogr. 149, 31-47.

216
cF316

Na _{2.5} Zn ₄ Y _{3.5} Ti ₁₂ FeO ₃₁ [OH] ₂ F ₈	cF316	(216) <i>F</i> -43m – h ⁴ g ² fe ³ a
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(Y,Na)₆(Zn,Fe)₅Ti₁₂O₂₉(O,F)₁₀F₄ [1], murataite

Structural features: ZnTi₁₂O₄₀ (partial substitution ignored) Keggin units (twelve edge- and vertex-linked TiO₆ octahedra sharing vertices with a central ZnO₄ tetrahedron) in a Cu-type (c.c.p.) arrangement share atoms to form a 3D-arrangement.

Ercit T.S., Hawthorne F.C. (1995) [1]

Ca_{0.33}Er_{1.14}F_{7.58}FeH_{1.22}Mn_{0.21}Na_{4.06}Nb_{1.56}O_{32.06}Si_{0.11}Ti_{9.56}Y_{2.22}Zn_{2.81}
 $a = 1.4886$ nm, $V = 3.2986$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	..m	0.0729	0.0729	0.7976		non-colinear Ti ₂
O2	48h	..m	0.1038	0.1038	0.242	0.72	non-coplanar triangle ZnTi ₂
F3	48h	..m	0.106	0.106	0.585	0.333	
M4	48h	..m	0.1629	0.1629	0.0087		octahedron O ₆
O5	24g	2.mm	0.233	$\frac{1}{4}$	$\frac{1}{4}$	0.167	
M6	24g	2.mm	0.515	$\frac{1}{4}$	$\frac{1}{4}$		non-colinear Ti ₂
M7	24f	2.mm	0.3188	0	0		
O8	16e	.3m	0.0738	0.0738	0.0738		tetrahedron ZnTi ₃
M9	16e	.3m	0.3278	0.3278	0.3278		
M10	16e	.3m	0.421	0.421	0.421		
M11	4a	-43m	0	0	0		tetrahedron O ₄

M4 = 0.76Ti + 0.13Nb + 0.11Na; M6 = 0.64O + 0.27F + 0.09OH; M7 = 0.37Y + 0.35Na + 0.19Er + 0.055Ca + 0.035Mn; M9 = 0.48Zn + 0.25Fe + 0.16Na + 0.11Ti; M10 = 0.49F + 0.34O + 0.17OH; M11 = 0.89Zn + 0.11Si

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.047

Remarks: Natural specimen from St. Peters Dome area, Colorado. Composition Y_{2.24}Gd_{0.03}Tb_{0.02}Dy_{0.28}Ho_{0.10}Er_{0.30}Tm_{0.05}Yb_{0.32}Lu_{0.05}Na_{3.97}Zn_{2.81}Fe_{1.01}Ca_{0.33}Mn_{0.21}Ti_{9.61}Sn_{0.04}Nb_{1.53}Si_{0.11}O_{32.11}(OH)_{1.23}F_{7.55} from electron microprobe analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. We assume that in table 3 of [1] the occupancy of former O2 is misprinted as 0.82 instead of 0.72 (from the description of the structure).

References: [1] Ercit T.S., Hawthorne F.C. (1995), Can. Mineral. 33, 1223-1229.

216
cF332

NaAl ₁₂ Ga[SO ₄] ₄ O ₄ [OH] ₂₄ [H ₂ O] ₃₂	cF332	(216) <i>F</i> -43m – h ⁵ ge ⁴ b
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Na[GaO₄Al₁₂(OH)₂₄(H₂O)₁₂](SO₄)₄·~20H₂O [1]

Structural features: GaAl₁₂O₄(OH)₂₄(H₂O)₁₂ Keggin units (twelve edge-linked Al(O,OH,OH₂)₆ octahedra sharing vertices with a central GaO₄ tetrahedron) in a Cu-type (c.c.p.) arrangement; additional H₂O and SO₄ tetrahedra between the units.

Görz H. et al. (1991) [1]



$a = 1.7861 \text{ nm}$, $V = 5.6979 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	48h	..m	0.0453	0.0453	0.3205		non-colinear Al ₂
Al2	48h	..m	0.0571	0.0571	0.6729		octahedron (OH) ₄ (OH ₂)O
(OH ₂)3	48h	..m	0.0686	0.0686	0.7817		single atom Al
O4	48h	..m	0.1321	0.1321	0.0361		single atom S
(OH)5	48h	..m	0.1605	0.1605	0.5539		non-colinear Al ₂
(OH ₂)6	24g	2.mm	0.0368	$\frac{1}{4}$	$\frac{1}{4}$		square antiprism (OH) ₂ O ₄ (OH ₂) ₂
S7	16e	.3m	0.1173	0.1173	0.1173		tetrahedron O ₄
O8	16e	.3m	0.1647	0.1647	0.1647		single atom S
(OH ₂)9	16e	.3m	0.3388	0.3388	0.3388		tricapped trigonal prism (OH) ₃ O ₃ (OH ₂) ₃
O10	16e	.3m	0.5611	0.5611	0.5611		tetrahedron GaAl ₃
Ga11	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron O ₄

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.081$

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

References: [1] Görz H., Schönherr S., Pertlik F. (1991), Monatsh. Chem. 122, 759-764.

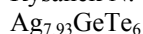
216
cF336

Ag ₈ GeTe ₆	<i>cF336</i>	(216) <i>F-43m</i> – <i>h</i> ⁶ <i>fecb</i>
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Ag₈GeTe₆ γ [1], argyrodite family

Structural features: Te forms a tetrahedrally close-packed (MgCu₂-type) framework (splitting of one site); Ge in tetrahedral voids, Ag distributed over several sites in low coordination (high degree of disorder). Single GeTe₄ tetrahedra.

Rysanek N. et al. (1976) [1]



$a = 1.1566 \text{ nm}$, $V = 1.5472 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	48h	..m	0.076	0.076	0.231	0.31	
Ag2	48h	..m	0.102	0.102	0.306	0.1	
Ag3	48h	..m	0.11	0.11	0.29	0.041	
Ag4	48h	..m	0.192	0.192	0.032	0.04	
Ag5	48h	..m	0.213	0.213	0.044	0.135	
Ag6	48h	..m	0.219	0.219	0.843	0.035	
Te7	24f	2.mm	0.045	0	0	0.167	
Te8	16e	.3m	0.627	0.627	0.627		
Te9	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Ge10	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, photographs, X-rays, $R = 0.074$

Remarks: Phase stable at $T > 244$ K. Short interatomic distances for partly occupied site(s). In table 2 of [1] the x - and y -coordinates of former Ag(2,1) are misprinted as 0.11 instead of 0.14 (checked on interatomic distances).

References: [1] Rysanek N., Laruelle P., Katty A. (1976), Acta Crystallogr. B 32, 692-696.

216
cF348

$\text{NaAl}_{13}[\text{SO}_4]_4\text{O}_4[\text{OH}]_{24}[\text{H}_2\text{O}]_{22}$	<i>cF348</i>	(216) <i>F-43m</i> – h^5fe^5c
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$\text{Na}[\text{AlO}_4\text{Al}_{12}(\text{OH})_{24}(\text{H}_2\text{O})_{12}](\text{SO}_4)_4 \cdot 10\text{H}_2\text{O}$ (see remark)

Structural features: $\text{AlAl}_{12}\text{O}_4(\text{OH})_{24}(\text{H}_2\text{O})_{12}$ Keggin units (twelve edge-linked $\text{Al}(\text{O},\text{OH},\text{OH}_2)_6$ octahedra sharing vertices with a central AlO_4 tetrahedron) in a Cu-type (c.c.p.) arrangement; additional H_2O , Na and SO_4 tetrahedra between the units.

Kiricsi I. et al. (1997) [1]

$\text{Al}_{13}\text{H}_{68}\text{NaO}_{66}\text{S}_4$

$a = 1.7856$ nm, $V = 5.6931$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	48 <i>h</i>	.. <i>m</i>	0.0899	0.0899	0.1969		non-colinear Al_2
O2	48 <i>h</i>	.. <i>m</i>	0.1166	0.1166	0.7111		single atom S
(OH ₂)3	48 <i>h</i>	.. <i>m</i>	0.182	0.182	0.9687		single atom Al
Al4	48 <i>h</i>	.. <i>m</i>	0.1931	0.1931	0.0774		octahedron $(\text{OH})_4(\text{OH}_2)\text{O}$
(OH)5	48 <i>h</i>	.. <i>m</i>	0.2037	0.2037	0.43		non-colinear Al_2
(OH ₂)6	24 <i>f</i>	2.. <i>mm</i>	0.2872	0	0		square antiprism $(\text{OH})_2\text{O}_4(\text{OH}_2)_2$
Na7	16 <i>e</i>	3.. <i>m</i>	0.0638	0.0638	0.0638	0.25	non-coplanar triangle $(\text{OH})_3$
O8	16 <i>e</i>	3.. <i>m</i>	0.1908	0.1908	0.1908		tetrahedron Al_4
(OH ₂)9	16 <i>e</i>	3.. <i>m</i>	0.4111	0.4111	0.4111		tricapped trigonal prism $(\text{OH})_3\text{O}_3(\text{OH}_2)_3$
O10	16 <i>e</i>	3.. <i>m</i>	0.5848	0.5848	0.5848		single atom S
S11	16 <i>e</i>	3.. <i>m</i>	0.6324	0.6324	0.6324		tetrahedron O_4
Al12	4 <i>c</i>	-43 <i>m</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O_4

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.058$, $T = 298$ K

Remarks: We assigned OH and H_2O in agreement with [2] ($\text{Na}[\text{GaO}_4\text{Al}_{12}(\text{OH})_{24}(\text{H}_2\text{O})_{12}](\text{SO}_4)_4 \cdot \sim 20\text{H}_2\text{O}$). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kiricsi I., Millini R., O'Neil Parker W. Jr. (1997), Inorg. Chem. 36, 571-575. [2] Görz H., Schönherr S., Pertlik F. (1991), Monatsh. Chem. 122, 759-764.

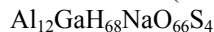
216
cF348

$\text{NaAl}_{12}\text{Ga}[\text{SO}_4]_4\text{O}_4[\text{OH}]_{24}[\text{H}_2\text{O}]_{22}$	<i>cF348</i>	(216) <i>F-43m</i> – h^5fe^5c
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$\text{Na}[\text{GaO}_4\text{Al}_{12}(\text{OH})_{24}(\text{H}_2\text{O})_{12}](\text{SO}_4)_4 \cdot 10\text{H}_2\text{O}$ [1]

Structural features: $\text{GaAl}_{12}\text{O}_4(\text{OH})_{24}(\text{H}_2\text{O})_{12}$ Keggin units (twelve edge-linked $\text{Al}(\text{O},\text{OH},\text{OH}_2)_6$ octahedra sharing vertices with a central GaO_4 tetrahedron) in a Cu-type (c.c.p.) arrangement; additional H_2O , Na and SO_4 tetrahedra between the units. See Fig. II.21.

Kiricsi I. et al. (1997) [1]



$$a = 1.7869 \text{ nm}, V = 5.7056 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	48h	..m	0.0892	0.0892	0.1967		non-colinear Al ₂
O2	48h	..m	0.1182	0.1182	0.714		single atom S
(OH ₂)3	48h	..m	0.1826	0.1826	0.9682		single atom Al
Al4	48h	..m	0.193	0.193	0.077		octahedron (OH) ₄ (OH ₂)O
(OH)5	48h	..m	0.2041	0.2041	0.4291		non-colinear Al ₂
(OH ₂)6	24f	2.mm	0.2904	0	0		square antiprism (OH) ₂ O ₄ (OH ₂) ₂
Na7	16e	.3m	0.0625	0.0625	0.0625	0.25	non-coplanar triangle (OH) ₃
O8	16e	.3m	0.1893	0.1893	0.1893		tetrahedron GaAl ₃
(OH ₂)9	16e	.3m	0.4115	0.4115	0.4115		tricapped trigonal prism (OH) ₃ O ₃ (OH ₂) ₃
O10	16e	.3m	0.5852	0.5852	0.5852		single atom S
S11	16e	.3m	0.6327	0.6327	0.6327		tetrahedron O ₄
Ga12	4c	-43m	1/4	1/4	1/4		tetrahedron O ₄

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.055, T = 298 K

Remarks: Na was not located in [2]. We assigned OH and H₂O in agreement with this reference. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

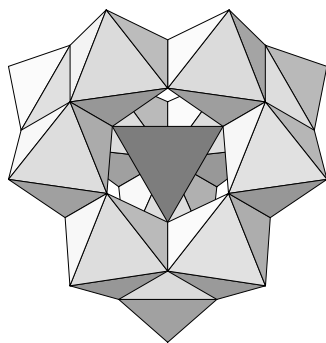


Fig. II.21. **Na[GaO₄Al₁₂(OH)₂₄ – (H₂O)₁₂](SO₄)₄·10H₂O**

Keggin unit: a central GaO₄ tetrahedron (dark) surrounded by twelve AlO₆ octahedra (light).

References: [1] Kiricsi I., Millini R., O'Neil Parker W. Jr. (1997), Inorg. Chem. 36, 571-575. [2] Görz H., Schönherr S., Pertlik F. (1991), Monatsh. Chem. 122, 759-764.

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cF348



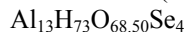
cF348

(216) *F*-43m – h⁵ge⁵a



Structural features: $\text{AlAl}_{12}\text{O}_4(\text{OH})_{24}(\text{H}_2\text{O})_{12}$ Keggin units (twelve edge-linked $\text{Al}(\text{O},\text{OH},\text{OH}_2)_6$ octahedra sharing vertices with a central AlO_4 tetrahedron) in a Cu-type (c.c.p.) arrangement; additional H₂O and SeO₄ tetrahedra between the units.

Johansson G. (1963) [1]



$$a = 1.801 \text{ nm}, V = 5.8417 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	48h	..m	0.0459	0.0459	0.8232		non-colinear Al ₂
Al2	48h	..m	0.0566	0.0566	0.1719		octahedron (OH) ₄ (OH ₂)O
(OH ₂)3	48h	..m	0.0692	0.0692	0.2772		single atom Al
O4	48h	..m	0.138	0.138	0.532		single atom Se
(OH)5	48h	..m	0.1582	0.1582	0.0527		non-colinear Al ₂
(OH ₂)6	24g	2.mm	0.54	¹ / ₄	¹ / ₄		8-vertex polyhedron O ₄ (OH) ₂ (OH ₂) ₂
O7	16e	.3m	0.0587	0.0587	0.0587		tetrahedron Al ₄
(OH ₂)8	16e	.3m	0.31	0.31	0.31	0.625	octahedron (OH ₂) ₆
Se9	16e	.3m	0.6183	0.6183	0.6183		tetrahedron O ₄
O10	16e	.3m	0.672	0.672	0.672		single atom Se
(OH ₂)11	16e	.3m	0.837	0.837	0.837		tricapped trigonal prism O ₃ (OH) ₃ (OH ₂) ₃
Al12	4a	-43m	0	0	0		tetrahedron O ₄

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

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.111

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

References: [1] Johansson G. (1963), Ark. Kemi 20, 305-319. [2] Johansson G. (1960), Acta Chem. Scand. 14, 771-773.

216
cF392

Zn ₃₀ (Zn _{0.56} Pt _{0.44}) ₁₁ Pt ₆	cF392	(216) <i>F</i> -43m – h ⁴ gf ² e ⁸
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Pt₃Zn₁₀ [1]

Structural features: Three kinds of γ brass-related nested polyhedra units; the octahedron is missing in one kind of unit, one tetrahedron in another kind of unit (disorder).

Johansson A., Westman S. (1970) [1]

Pt_{10.83}Zn_{36.17}

a = 1.81128 nm, V = 5.9423 nm³, Z = 8

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	48h	..m	0.0950	0.0950	0.7716		14-vertex Frank-Kasper Pt ₃ Zn ₁₁
Zn2	48h	..m	0.1001	0.1001	0.2704		15-vertex Frank-Kasper Zn ₁₀ Pt ₅
Zn3	48h	..m	0.1565	0.1565	0.0201		14-vertex Frank-Kasper Pt ₅ Zn ₉
Zn4	48h	..m	0.1612	0.1612	0.5091		icosahedron Zn ₉ Pt ₃
M5	24g	2.mm	0.0694	¹ / ₄	¹ / ₄		icosahedron Zn ₁₀ Pt ₂
M6	24f	2.mm	0.1796	0	0		pseudo Frank-Kasper Zn ₁₁ Pt ₂
M7	24f	2.mm	0.3237	0	0		pseudo Frank-Kasper Pt ₃ Zn ₁₀
Zn8	16e	.3m	0.0524	0.0524	0.0524		icosahedron Pt ₆ Zn ₆
M9	16e	.3m	0.1850	0.1850	0.1850	0.5	non-coplanar triangle Zn ₃
M10	16e	.3m	0.3006	0.3006	0.3006	0.5	icosahedron Pt ₆ Zn ₆
Pt11	16e	.3m	0.4155	0.4155	0.4155		icosahedron Zn ₁₂
Zn12	16e	.3m	0.5751	0.5751	0.5751		bicapped square prism Zn ₆ Pt ₄
Pt13	16e	.3m	0.6604	0.6604	0.6604		bicapped square prism Zn ₁₀
Zn14	16e	.3m	0.8077	0.8077	0.8077		10-vertex polyhedron Zn ₆ Pt ₄
Pt15	16e	.3m	0.9111	0.9111	0.9111		pseudo Frank-Kasper Zn ₁₀ Pt ₃

M5 = 0.667Pt + 0.333Zn; M6 = 0.667Pt + 0.333Zn; M7 = 0.917Zn + 0.083Pt; M9 = 0.5Pt + 0.5Zn; M10 = 0.917Zn + 0.083Pt

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.093$

Remarks: Preliminary data in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Johansson A., Westman S. (1970), Acta Chem. Scand. 24, 3471-3479. [2] Ekman W. (1931), Z. Phys. Chem., Abt. B 12, 57-78.

216
cF396

$\text{Mg}_{83}(\text{Mg}_{0.51}\text{Pd}_{0.49})_4\text{Pd}_{12}$	cF396	(216) $F-43m - h^5g^2fe^5a$
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Mg₆Pd [1]

Structural features: 29-atom α Mn-, 26-atom γ brass- and 22-atom Ti_2Ni -type nested polyhedra units in the ratio 1:1:2.

Samson S. (1972) [1]

$\text{Mg}_{85.01}\text{Pd}_{13.96}$

$a = 2.0108 \text{ nm}$, $V = 8.1303 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	48h	.m	0.04984	0.04984	0.15720		pseudo Frank-Kasper Mg_{12}Pd
Mg2	48h	.m	0.09903	0.09903	0.77812		pseudo Frank-Kasper Mg_{12}Pd
Mg3	48h	.m	0.10645	0.10645	0.28398		12-vertex polyhedron $\text{Pd}_2\text{Mg}_{10}$
Mg4	48h	.m	0.15605	0.15605	0.52391		14-vertex Frank-Kasper $\text{Pd}_2\text{Mg}_{12}$
Mg5	48h	.m	0.19345	0.19345	0.01760		tricapped pentagonal prism PdMg_{12}
Mg6	24g	2.mm	0.14280	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron $\text{Pd}_2\text{Mg}_{10}$
Mg7	24g	2.mm	0.63134	$\frac{1}{4}$	$\frac{1}{4}$		14-vertex polyhedron $\text{Pd}_2\text{Mg}_{12}$
Mg8	24f	2.mm	0.31482	0	0		14-vertex Frank-Kasper $\text{Mg}_{12}\text{Pd}_2$
Pd9	16e	.3m	0.15038	0.15038	0.15038		icosahedron Mg_{12}
Pd10	16e	.3m	0.41790	0.41790	0.41790		icosahedron Mg_{12}
Mg11	16e	.3m	0.55250	0.55250	0.55250		pseudo Frank-Kasper Pd_4Mg_9
Pd12	16e	.3m	0.65653	0.65653	0.65653		bicapped square prism Mg_{10}
M13	16e	.3m	0.91868	0.91868	0.91868		pseudo Frank-Kasper Mg_{13}
Mg14	4a	-43m	0	0	0	0.97	16-vertex Frank-Kasper Mg_{16}

$\text{M13} = 0.51\text{Mg} + 0.49\text{Pd}$

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

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

Remarks: Homogeneity range $\text{Mg}_{100-x}\text{Pd}_x$, $12.86 < x < 15.09$.

References: [1] Samson S. (1972), Acta Crystallogr. B 28, 936-945.

216
cF396

$\text{Mg}_{29}\text{Ir}_4$	cF396	(216) $F-43m - h^5g^2fe^5a$
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Mg₂₉Ir₄ [1]

Structural features: 29-atom α Mn- (a central Mg atom surrounded by a Mg_4 tetrahedron, a Mg_{12} truncated tetrahedron and a Mg_{12} cuboctahedron), 26-atom γ brass- (an inner Mg_4 tetrahedron surrounded by a Ir_4 outer tetrahedron, a Mg_6 octahedron and a Mg_{12} cuboctahedron) and 22-atom Ti_2Ni -type (a Mg_6 octahedron surrounded by an Ir_4 tetrahedron and a Mg_{12} cuboctahedron) nested polyhedra units in the ratio 1:1:2.

Bonhomme F., Yvon K. (1995) [1]

$\text{Ir}_4\text{Mg}_{29}$

$a = 2.01148 \text{ nm}$, $V = 8.1386 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	48h	..m	0.0516	0.0516	0.1600		pseudo Frank-Kasper IrMg_{12}
Mg2	48h	..m	0.0989	0.0989	0.7725		pseudo Frank-Kasper IrMg_{12}
Mg3	48h	..m	0.1084	0.1084	0.2812		12-vertex polyhedron $\text{Ir}_2\text{Mg}_{10}$
Mg4	48h	..m	0.1548	0.1548	0.5209		12-vertex polyhedron $\text{Ir}_2\text{Mg}_{10}$
Mg5	48h	..m	0.1917	0.1917	0.0187		tricapped pentagonal prism IrMg_{12}
Mg6	24g	2.mm	0.1422	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron $\text{Ir}_2\text{Mg}_{10}$
Mg7	24g	2.mm	0.6171	$\frac{1}{4}$	$\frac{1}{4}$		14-vertex polyhedron $\text{Ir}_2\text{Mg}_{12}$
Mg8	24f	2.mm	0.3211	0	0		14-vertex Frank-Kasper $\text{Mg}_{12}\text{Ir}_2$
Ir9	16e	.3m	0.1510	0.1510	0.1510		icosahedron Mg_{12}
Ir10	16e	.3m	0.4172	0.4172	0.4172		icosahedron Mg_{12}
Mg11	16e	.3m	0.5524	0.5524	0.5524		pseudo Frank-Kasper Ir_4Mg_9
Ir12	16e	.3m	0.6584	0.6584	0.6584		tricapped trigonal prism Mg_9
Mg13	16e	.3m	0.9196	0.9196	0.9196		pseudo Frank-Kasper Mg_{13}
Mg14	4a	-43m	0	0	0		16-vertex Frank-Kasper Mg_{16}

Experimental: powder, diffractometer, X-rays, $R_B = 0.044$, $T = 298 \text{ K}$

References: [1] Bonhomme F., Yvon K. (1995), J. Alloys Compd. 227, L1-L3.

216
cF408

$\text{Mg}_{44}\text{Rh}_7$	cF408	(216) $F-43m - h^5g^2fe^6$
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RhMg₆ [1]; Na_6Ti [2]

Structural features: 26-atom γ brass-, 28-atom α Mn- (central site vacant) and 22-atom Ti_2Ni -type nested polyhedra units in the ratio 2:1:1.

Westin L., Edshammar L.E. (1971) [1]

$\text{Mg}_{44}\text{Rh}_7$

$a = 2.0148 \text{ nm}$, $V = 8.1789 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	48h	..m	0.0525	0.0525	0.6620		12-vertex polyhedron RhMg_{11}
Mg2	48h	..m	0.0961	0.0961	0.2794		14-vertex Frank-Kasper $\text{Mg}_{12}\text{Rh}_2$
Mg3	48h	..m	0.1072	0.1072	0.7859		12-vertex polyhedron $\text{Rh}_2\text{Mg}_{10}$
Mg4	48h	..m	0.1565	0.1565	0.0205		12-vertex polyhedron $\text{Mg}_{10}\text{Rh}_2$
Mg5	48h	..m	0.1949	0.1949	0.5194		12-vertex polyhedron $\text{Rh}_2\text{Mg}_{10}$
Rh6	24g	2.mm	0.0867	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Mg_{12}
Mg7	24g	2.mm	0.6447	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron $\text{Rh}_2\text{Mg}_{10}$
Mg8	24f	2.mm	0.1824	0	0		14-vertex Frank-Kasper $\text{Mg}_{12}\text{Rh}_2$
Mg9	16e	.3m	0.0524	0.0524	0.0524		icosahedron Rh_3Mg_9
Mg10	16e	.3m	0.1662	0.1662	0.1662		icosahedron Rh_3Mg_9
Mg11	16e	.3m	0.3044	0.3044	0.3044		icosahedron Rh_3Mg_9
Mg12	16e	.3m	0.4382	0.4382	0.4382		anticuboctahedron Mg_{12}
Rh13	16e	.3m	0.6512	0.6512	0.6512		icosahedron Mg_{12}
Rh14	16e	.3m	0.9167	0.9167	0.9167		icosahedron Mg_{12}

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.085$

Remarks: For Na₆Tl [2] partial occupation of Wyckoff position 4*b* (position 4*d* in the original description) could not be excluded.

References: [1] Westin L., Edshammar L.E. (1971), Acta Chem. Scand. 25, 1480-1481. [2] Samson S., Hansen D.A. (1972), Acta Crystallogr. B 28, 930-935.

216
cF412

Cu _{18.5} Cr _{17.0} Al _{66.8}	cF412	(216) $F-43m - h^5g^2fe^6b$
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Cr_{18.3}Cu_{14.3}Al_{67.4} [1]

Structural features: 26-atom γ brass-, 29-atom α Mn- (partial vacancies on the central site) and 22-atom Ti₂Ni-type nested polyhedra units in the ratio 2:1:1.

Sugiyama K. et al. (2002) [1]

Al_{66.84}Cr_{16.96}Cu_{18.48}

$a = 1.816$ nm, $V = 5.9889$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	48 <i>h</i>	. <i>m</i>	0.0406	0.0406	0.6711		pseudo Frank-Kasper Cu ₄ Al ₈ Cr
Al2	48 <i>h</i>	. <i>m</i>	0.0932	0.0932	0.2762		14-vertex Frank-Kasper Al ₉ Cr ₃ Cu ₂
M3	48 <i>h</i>	. <i>m</i>	0.1086	0.1086	0.7803		12-vertex polyhedron Cr ₂ CuAl ₉
Al4	48 <i>h</i>	. <i>m</i>	0.1559	0.1559	0.0226		14-vertex Frank-Kasper Cr ₃ Al ₁₁
Al5	48 <i>h</i>	. <i>m</i>	0.1883	0.1883	0.5227		tricapped pentagonal prism Cr ₂ Al ₉ Cu ₂
Cr6	24 <i>g</i>	2. <i>mm</i>	0.0803	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Al ₁₀ Cr ₂
M7	24 <i>g</i>	2. <i>mm</i>	0.6464	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron Cr ₂ Al ₁₀
Al8	24 <i>f</i>	2. <i>mm</i>	0.1838	0	0		14-vertex Frank-Kasper Al ₁₀ Cr ₂ Cu ₂
M9	16 <i>e</i>	.3 <i>m</i>	0.0527	0.0527	0.0527		icosahedron Cr ₃ Al ₉
Cr10	16 <i>e</i>	.3 <i>m</i>	0.1655	0.1655	0.1655		icosahedron Al ₉ Cr ₃
Al11	16 <i>e</i>	.3 <i>m</i>	0.3031	0.3031	0.3031		icosahedron Cr ₆ Al ₆
Al12	16 <i>e</i>	.3 <i>m</i>	0.4223	0.4223	0.4223		10-vertex polyhedron Cu ₇ Al ₃
Cr13	16 <i>e</i>	.3 <i>m</i>	0.6503	0.6503	0.6503		icosahedron Al ₉ Cu ₃
M14	16 <i>e</i>	.3 <i>m</i>	0.9152	0.9152	0.9152		icosahedron Al ₁₂
Cu15	4 <i>b</i>	-43 <i>m</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.28	tetrahedron Al ₄

M3 = 0.85Al + 0.15Cu; M7 = 0.58Al + 0.42Cu; M9 = 0.79Al + 0.21Cu; M14 = 0.74Cr + 0.26Cu

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.059

Remarks: Phase referred to as β -(AlCuCr). A similar structure was proposed for Na₆Tl [2], however, partial occupation of Wyckoff position 4*b* (position 4*d* in the original description) could not be confirmed.

References: [1] Sugiyama K., Saito H., Hiraga K. (2002), J. Alloys Compd. 342, 148-152. [2] Samson S., Hansen D.A. (1972), Acta Crystallogr. B 28, 930-935.

216
cF416

Cu ₄₁ Sn ₁₁	cF416	(216) $F-43m - h^4g^2f^2e^8$
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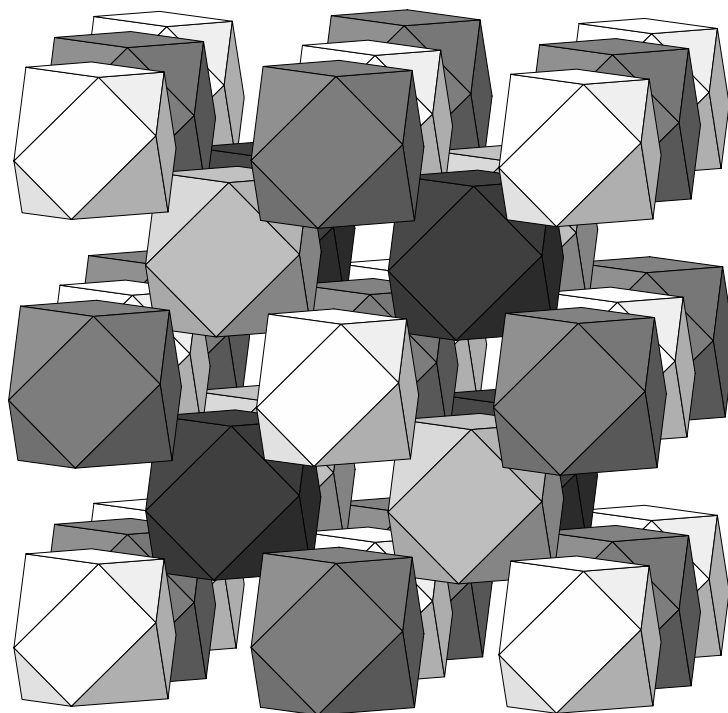
Sn₁₁Cu₄₁ [2], γ -brass

Structural features: Four kinds of 26-atom γ brass-type nested polyhedron unit (an inner tetrahedron surrounded by an outer tetrahedron, an octahedron and a cuboctahedron) where the Sn atoms occupy the following positions: none, cuboctahedron, outer tetrahedron, and octahedron, respectively. See Fig. II.22.

Booth M.H. et al. (1977) [1]

 $\text{Cu}_{40.50}\text{Sn}_{11}$ $a = 1.7980 \text{ nm}$, $V = 5.8126 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	48h	.m	0.0913	0.0913	0.2631		pentacapped trigonal prism Cu_8Sn_3
Sn2	48h	.m	0.0916	0.0916	0.7680		pentacapped trigonal prism Cu_{11}
Cu3	48h	.m	0.1465	0.1465	0.0278		pseudo Frank-Kasper $\text{Cu}_{10}\text{Sn}_3$
Cu4	48h	.m	0.1562	0.1562	0.5186		pentacapped trigonal prism Sn_4Cu_7
Sn5	24g	2.mm	0.0691	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Cu_{13}
Cu6	24g	2.mm	0.5759	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Cu_8Sn_5
Cu7	24f	2.mm	0.1765	0	0		pseudo Frank-Kasper $\text{Sn}_2\text{Cu}_{11}$
Cu8	24f	2.mm	0.3237	0	0		pseudo Frank-Kasper Cu_9Sn_4
Cu9	16e	.3m	0.0504	0.0504	0.0504		icosahedron Cu_{12}
Cu10	16e	.3m	0.1664	0.1664	0.1664		icosahedron Cu_9Sn_3
Cu11	16e	.3m	0.3062	0.3062	0.3062		pseudo Frank-Kasper Cu_9Sn_4
Sn12	16e	.3m	0.4113	0.4113	0.4113		pseudo Frank-Kasper Cu_{13}
Cu13	16e	.3m	0.5573	0.5573	0.5573	0.75	pseudo Frank-Kasper $\text{Cu}_{10}\text{Sn}_3$
Cu14	16e	.3m	0.6657	0.6657	0.6657		pseudo Frank-Kasper $\text{Cu}_{10}\text{Sn}_3$
Cu15	16e	.3m	0.8005	0.8005	0.8005		icosahedron Cu_9Sn_3
Cu16	16e	.3m	0.9166	0.9166	0.9166		icosahedron Cu_9Sn_3

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.070$ Remarks: Phase referred to as δ -(CuSn).Fig. II.22. $\text{Sn}_{11}\text{Cu}_{41}$

Arrangement of Cu_{12} and Sn_{12} cuboctahedra, which represent 26-atom γ brass-type nested polyhedra units (Cu_4 inner tetrahedron + Cu_4 outer tetrahedron + Cu_6 octahedron + Cu_{12} cuboctahedron, light; Cu_4 + Sn_4 + Cu_6 + Cu_{12} , medium dark; Cu_4 + Cu_4 + Sn_6 + Cu_{12} , medium light; Cu_4 + Cu_4 + Cu_6 + Sn_{12} , dark).

References: [1] Booth M.H., Brandon J.K., Brizard R.Y., Chieh C., Pearson W.B. (1977), Acta Crystallogr. B 33, 30-36. [2] Arnberg L., Jonsson A., Westman S. (1976), Acta Chem. Scand. A 30, 187-192.

216
cF416

$\text{Li}_{21}\text{Si}_5$	cF416	(216) $F\bar{4}3m - h^4g^2f^2e^8$
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$\text{Li}_{21}\text{Si}_5$ [1]

Structural features: Two kinds of 26-atom γ brass-type nested polyhedron unit (a Li_4 inner tetrahedron surrounded by a Li_4/Si_4 outer tetrahedron, a Si_6/Li_6 octahedron and a Li_{12} cuboctahedron) in the ratio 1:1 (sequence along $\langle 111 \rangle$: -A-A-B-B-).

Nesper R., Von Schnering H.G. (1987) [1]

$\text{Li}_{21}\text{Si}_5$

$a = 1.8710 \text{ nm}$, $V = 6.5497 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	.m	0.088	0.088	0.261		pseudo Frank-Kasper Li_9Si_4
Li2	48h	.m	0.092	0.092	0.762		pentacapped trigonal prism Si_2Li_9
Li3	48h	.m	0.153	0.153	0.021		15-vertex Frank-Kasper $\text{Li}_{12}\text{Si}_3$
Li4	48h	.m	0.164	0.164	0.500		14-vertex Frank-Kasper $\text{Li}_{11}\text{Si}_3$
Si5	24g	2.mm	0.0691	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Li_{13}
Li6	24g	2.mm	0.573	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Li}_{10}\text{Si}_3$
Si7	24f	2.mm	0.1780	0	0		pseudo Frank-Kasper Li_{13}
Li8	24f	2.mm	0.326	0	0		pseudo Frank-Kasper $\text{Li}_{10}\text{Si}_3$
Li9	16e	.3m	0.059	0.059	0.059		icosahedron Li_9Si_3
Li10	16e	.3m	0.188	0.188	0.188		15-vertex Frank-Kasper $\text{Li}_{12}\text{Si}_3$
Li11	16e	.3m	0.329	0.329	0.329		pseudo Frank-Kasper Li_9Si_4
Si12	16e	.3m	0.4175	0.4175	0.4175		pseudo Frank-Kasper Li_{13}
Li13	16e	.3m	0.571	0.571	0.571		bicapped square prism Li_6Si_4
Si14	16e	.3m	0.6595	0.6595	0.6595		pseudo Frank-Kasper Li_{13}
Li15	16e	.3m	0.804	0.804	0.804		icosahedron Li_9Si_3
Li16	16e	.3m	0.917	0.917	0.917		icosahedron Li_9Si_3

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.052$

Remarks: Supersedes a report on $\text{Li}_{22}\text{Si}_5$ with $\text{Li}_{22}\text{Pb}_5$ -type structure in [2]. In table I of [1] the unit of the cell parameter is misprinted as pm instead of Å.

References: [1] Nesper R., Von Schnering H.G. (1987), J. Solid State Chem. 70, 48-57. [2] Axel H., Schäfer H., Weiss A. (1966), Z. Naturforsch. B 21, 115-117.

216
cF420

$\text{Li}_{17}\text{Pb}_4$	cF420	(216) $F\bar{4}3m - h^4g^2f^2e^8a$
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$\text{Li}_{17}\text{Pb}_4$ [1]; $\text{Li}_{17}\text{Sn}_4$ [4]

Structural features: 26-atom γ brass- (a Li_4 inner tetrahedron surrounded by a $\text{Li}_4/\text{Li}_4/\text{Pb}_4$ outer tetrahedron, a $\text{Pb}_6/\text{Pb}_6/\text{Li}_6$ octahedron and a Li_{12} cuboctahedron) and 27-atom W-type (a central Li atom surrounded by a (Li_4Pb_4) cube, a Li_6 octahedron and a Li_{12} cuboctahedron) nested polyhedra units in the ratio 3:1. Defect derivative of W (b.c.c. arrangement) with vacancies in three of the four 8-fold Wyckoff positions.

Goward G.R. et al. (2001) [1]

 $\text{Li}_{17}\text{Pb}_4$ $a = 1.9842 \text{ nm}$, $V = 7.8119 \text{ nm}^3$, $Z = 20$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	..m	0.0914	0.0914	0.7622		pentacapped trigonal prism Li_7Pb_4
Li2	48h	..m	0.0943	0.0943	0.2678		16-vertex Frank-Kasper $\text{Pb}_2\text{Li}_{14}$
Li3	48h	..m	0.1552	0.1552	0.5204		15-vertex Frank-Kasper $\text{Pb}_3\text{Li}_{12}$
Li4	48h	..m	0.1627	0.1627	0.0075		rhombic dodecahedron $\text{Li}_{11}\text{Pb}_3$
Li5	24g	2.mm	0.0747	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Li}_{10}\text{Pb}_3$
Pb6	24g	2.mm	0.57081	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Li_{13}
Li7	24f	2.mm	0.1732	0	0		rhombic dodecahedron $\text{Li}_{11}\text{Pb}_3$
Pb8	24f	2.mm	0.32006	0	0		pseudo Frank-Kasper Li_{13}
Li9	16e	.3m	0.0738	0.0738	0.0738		pentacapped trigonal prism Li_7Pb_4
Pb10	16e	.3m	0.15897	0.15897	0.15897		pseudo Frank-Kasper Li_{13}
Li11	16e	.3m	0.3034	0.3034	0.3034		icosahedron Li_9Pb_3
Li12	16e	.3m	0.4151	0.4151	0.4151		icosahedron Li_9Pb_3
Li13	16e	.3m	0.5559	0.5559	0.5559		icosahedron Li_9Pb_3
Li14	16e	.3m	0.6831	0.6831	0.6831		15-vertex Frank-Kasper $\text{Pb}_3\text{Li}_{12}$
Li15	16e	.3m	0.8305	0.8305	0.8305		pseudo Frank-Kasper Li_9Pb_4
Pb16	16e	.3m	0.91638	0.91638	0.91638		rhombic dodecahedron Li_{14}
Li17	4a	-43m	0	0	0		rhombic dodecahedron $\text{Li}_{10}\text{Pb}_4$

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.023$, $T = 150.1 \text{ K}$

Remarks: Space group (196) $F23$ was tested and rejected. Supersedes a structure proposal for so-called $\text{Li}_{22}\text{Pb}_5$ with 432 atoms in the unit cell ([5], [6]). Reports on so-called $\text{Li}_{22}\text{Sn}_5$ with $\text{Li}_{22}\text{Pb}_5$ -type structure [2] and $\text{Li}_{21}\text{Sn}_5$ with $\text{Li}_{21}\text{Si}_5$ -type structure [3] are also superseded (see [4]).

References: [1] Goward G.R., Taylor N.J., Souza D.C.S., Nazar L.F. (2001), J. Alloys Compd. 329, 82-91. [2] Gladyshevskii E.I., Oleksiv G.I., Kripyakevich P.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 9, 269-271. [3] Nesper R. (1997), thesis, Stuttgart (Germany). [4] Lupu C., Mao J.G., Rabalais J.W., Guloy A.M., Richardson J.W. Jr. (2003), Inorg. Chem. 42, 3765-3771. [5] Zalkin A., Ramsey W.J. (1958), J. Phys. Chem. 62, 689-693. [6] Zalkin A. (1957), Acta Crystallogr. 10, 791c.

216
cF420

$\text{Zn}_{93}(\text{Zn}_{0.43}\text{Mo}_{0.57})\text{Mo}_4$	<i>cF420</i>	(216) $F-43m - h^5g^2fe^6cba$
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MoZn_{20.44} [1]

Structural features: 26-atom γ brass-, 29-atom α Mn-, and 22-atom Ti_2Ni -type nested polyhedra units in the ratio 2:1:1. Part of the γ brass-type units are centered by an additional atom (27-atom W-type unit, partial disorder).

Nasch T., Jeitschko W. (1999) [1]

 $\text{Mo}_{4.57}\text{Zn}_{93.44}$ $a = 1.8464 \text{ nm}$, $V = 6.2947 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	48h	..m	0.0475	0.0475	0.6528		pseudo Frank-Kasper Zn_{12}Mo
Zn2	48h	..m	0.0760	0.0760	0.2649		14-vertex polyhedron Zn_{14}
Zn3	48h	..m	0.1049	0.1049	0.7786		14-vertex polyhedron Zn_{13}Mo
Zn4	48h	..m	0.1542	0.1542	0.0234		14-vertex Frank-Kasper Zn_{14}

Zn5	48h	.m	0.1910	0.1910	0.5162		14-vertex Frank-Kasper Zn ₁₃ Mo
Zn6	24g	2.mm	0.0935	$\frac{1}{4}$	$\frac{1}{4}$	0.70	pseudo Frank-Kasper Zn ₁₂ Mo
Zn7	24g	2.mm	0.6433	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron Mo ₂ Zn ₁₀
Zn8	24f	2.mm	0.1644	0	0		15-vertex Frank-Kasper Zn ₁₅
Zn9	16e	.3m	0.0543	0.0543	0.0543	0.35	
Zn10	16e	.3m	0.1656	0.1656	0.1656		14-vertex Frank-Kasper Zn ₁₃ Mo
Zn11	16e	.3m	0.3324	0.3324	0.3324	0.44	rhombic dodecahedron Zn ₁₃ Mo
Zn12	16e	.3m	0.4128	0.4128	0.4128		14-vertex Frank-Kasper Zn ₁₄
Mo13	16e	.3m	0.6485	0.6485	0.6485		icosahedron Zn ₁₂
Zn14	16e	.3m	0.9156	0.9156	0.9156		pseudo Frank-Kasper Zn ₁₃
M15	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Zn ₁₄
Zn16	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper Zn ₁₆
Zn17	4a	-43m	0	0	0	0.65	

M15 = 0.57Mo + 0.43Zn

Experimental: single crystal, diffractometer, X-rays, R = 0.059

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

References: [1] Nasch T., Jeitschko W. (1999), J. Solid State Chem. 143, 95-103.

216
cF432

Li ₂₂ Pb ₅	cF432	(216) $F\bar{4}3m - h^4g^2f^2e^8dcba$
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Li₂₂Pb₅ [1]

Structural features: Ordering variant of W. Two kinds of 27-atom W-type nested polyhedra unit (a central Li atom surrounded by a Li₈/(Li₄Pb₄) cube, a Pb₆/Li₆ octahedron and a Li₁₂ cuboctahedron) in the ratio 1:1 (sequence along <111>: -A-A-B-B-).

Zalkin A., Ramsey W.J. (1958) [1]

Li₂₂Pb₅

$a = 2.008$ nm, $V = 8.0964$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	.m	0.08333	0.08333	0.25		rhombic dodecahedron Pb ₂ Li ₁₂
Li2	48h	.m	0.08333	0.08333	0.75		rhombic dodecahedron Pb ₄ Li ₁₀
Li3	48h	.m	0.16667	0.16667	0.0		rhombic dodecahedron Pb ₃ Li ₁₁
Li4	48h	.m	0.16667	0.16667	0.5		rhombic dodecahedron Pb ₃ Li ₁₁
Li5	24g	2.mm	0.08333	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Li ₁₁ Pb ₃
Pb6	24g	2.mm	0.5711	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Li ₁₄
Li7	24f	2.mm	0.16667	0	0		rhombic dodecahedron Li ₁₁ Pb ₃
Pb8	24f	2.mm	0.3211	0	0		rhombic dodecahedron Li ₁₄
Li9	16e	.3m	0.08333	0.08333	0.08333		rhombic dodecahedron Pb ₄ Li ₁₀
Pb10	16e	.3m	0.1641	0.1641	0.1641		rhombic dodecahedron Li ₁₄
Li11	16e	.3m	0.33333	0.33333	0.33333		rhombic dodecahedron Li ₁₁ Pb ₃
Li12	16e	.3m	0.41667	0.41667	0.41667		rhombic dodecahedron Li ₁₁ Pb ₃
Li13	16e	.3m	0.58333	0.58333	0.58333		rhombic dodecahedron Li ₁₁ Pb ₃
Li14	16e	.3m	0.66667	0.66667	0.66667		rhombic dodecahedron Li ₁₁ Pb ₃
Li15	16e	.3m	0.83333	0.83333	0.83333		rhombic dodecahedron Pb ₄ Li ₁₀
Pb16	16e	.3m	0.9141	0.9141	0.9141		rhombic dodecahedron Li ₁₄
Li17	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		rhombic dodecahedron Li ₈ Pb ₆
Li18	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Li ₁₀ Pb ₄
Li19	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron Li ₈ Pb ₆

Li20 4a -43m 0 0 0 rhombic dodecahedron Li₁₀Pb₄

Transformation from published data (*F*23): origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Idealized coordinates for the Li sites. Identical to so-called Li₄Pb in [2]. The description in space group (196) *F*23 in [1] does not take into consideration all symmetry elements of the proposed model. A report on so-called Li₂₂Si₅ with this structure type in [3] is superseded (Li₂₁Si₅; see [5]). In [4] the *z*-coordinate of the penultimate Li site is misprinted as $\frac{1}{2}$ instead of $\frac{1}{12}$.

References: [1] Zalkin A., Ramsey W.J. (1958), J. Phys. Chem. 62, 689-693. [2] Grube G., Klaiber H. (1934), Z. Elektrochem. Angew. Phys. Chem. 40, 745-754. [3] Axel H., Schäfer H., Weiss A. (1966), Z. Naturforsch. B 21, 115-117. [4] (1968), Structure Reports 22, 158. [5] Nesper R., Von Schnering H.G. (1987), J. Solid State Chem. 70, 48-57.

216
cF432

Zn₈₉(Fe_{0.5}Ni_{0.5})_{13.8}

cF432

(216) *F*-43m – h⁵gf²e⁷ca

Zn_{6.5}Fe_{0.5}Ni_{0.5} [1]

Structural features: 26-atom γ brass-, 29-atom α Mn- and 22-atom Ti₂Ni-type nested polyhedra units in the ratio 2:1:1. Part of the γ brass-type units are centered by an additional atom (27-atom W-type unit) causing splitting of the surrounding tetrahedron.

Lidin S. et al. (1994) [1]

Fe_{6.90}Ni_{6.90}Zn₈₉

a = 1.80838 nm, *V* = 5.9138 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	48h	..m	0.059	0.059	0.2679		12-vertex polyhedron Fe ₂ Zn ₁₀
Zn2	48h	..m	0.0941	0.0941	0.7695		12-vertex polyhedron Zn ₁₁ Fe
Zn3	48h	..m	0.1437	0.1437	0.5302		12-vertex polyhedron Zn ₁₁ Fe
Zn4	48h	..m	0.1617	0.1617	0.0217		
Zn5	48h	..m	0.201	0.201	0.4064		tricapped pentagonal prism Zn ₁₂ Fe
Zn6	24g	2.mm	0.5722	$\frac{1}{4}$	$\frac{1}{4}$		14-vertex Frank-Kasper Zn ₁₄
M7	24f	2.mm	0.1586	0	0		
Zn8	24f	2.mm	0.3916	0	0		12-vertex polyhedron Fe ₂ Zn ₁₀
M9	16e	.3m	0.055	0.055	0.055	0.53	
M10	16e	.3m	0.074	0.074	0.074	0.25	
Zn11	16e	.3m	0.1661	0.1661	0.1661		icosahedron Zn ₁₂
M12	16e	.3m	0.4002	0.4002	0.4002		icosahedron Zn ₁₂
Zn13	16e	.3m	0.6648	0.6648	0.6648		icosahedron Zn ₁₂
Zn14	16e	.3m	0.8022	0.8022	0.8022		icosahedron Zn ₁₂
Zn15	16e	.3m	0.915	0.915	0.915		
Zn16	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper Zn ₁₆
M17	4a	-43m	0	0	0	0.68	tetrahedron Fe ₄

M7 = 0.5Fe + 0.5Ni; M9 = 0.5Fe + 0.5Ni; M10 = 0.5Fe + 0.5Ni; M12 = 0.5Fe + 0.5Ni; M17 = 0.5Fe + 0.5Ni

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.041, *T* = 298 K

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

References: [1] Lidin S., Jacob M., Larsson A.K. (1994), Acta Crystallogr. C 50, 340-342.

216
cF436

Li ₁₇ Ge ₄	cF436	(216) $F-43m - h^4g^2f^2e^9a$
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Li₁₇Ge₄ [1]

Structural features: 26-atom γ brass- (a Li₄ inner tetrahedron surrounded by a Li₄/Li₄/Ge₄ outer tetrahedron, a Ge₆/Ge₆/Li₆ octahedron and a Li₁₂ cuboctahedron) and 27-atom W-type (a central Li atom surrounded by a (Li₄Ge₄) cube, a Li₆ octahedron and a Li₁₂ cuboctahedron) nested polyhedra units; partial vacancies on the central site of the latter cause splitting of the surrounding Li₄ tetrahedron.

Goward G.R. et al. (2001) [1]

Ge₄Li_{16.95} $a = 1.8756$ nm, $V = 6.5981$ nm³, $Z = 20$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	..m	0.0907	0.0907	0.266		pentacapped trigonal prism Ge ₂ Li ₉
Li2	48h	..m	0.0914	0.0914	0.7597		pentacapped trigonal prism Li ₇ Ge ₄
Li3	48h	..m	0.154	0.154	0.5216		15-vertex Frank-Kasper Li ₁₂ Ge ₃
Li4	48h	..m	0.1625	0.1625	0.0051		
Li5	24g	2.mm	0.0752	¹ / ₄	¹ / ₄		pseudo Frank-Kasper Li ₁₀ Ge ₃
Ge6	24g	2.mm	0.56965	¹ / ₄	¹ / ₄		pseudo Frank-Kasper Li ₁₃
Li7	24f	2.mm	0.1697	0	0		
Ge8	24f	2.mm	0.32112	0	0		pseudo Frank-Kasper Li ₁₃
Li9	16e	.3m	0.0587	0.0587	0.0587	0.25	
Li10	16e	.3m	0.0775	0.0775	0.0775	0.75	
Ge11	16e	.3m	0.15952	0.15952	0.15952		
Li12	16e	.3m	0.3032	0.3032	0.3032		icosahedron Li ₉ Ge ₃
Li13	16e	.3m	0.4169	0.4169	0.4169		icosahedron Li ₉ Ge ₃
Li14	16e	.3m	0.5579	0.5579	0.5579		icosahedron Li ₉ Ge ₃
Li15	16e	.3m	0.6876	0.6876	0.6876		15-vertex Frank-Kasper Ge ₃ Li ₁₂
Li16	16e	.3m	0.8329	0.8329	0.8329		pseudo Frank-Kasper Li ₉ Ge ₄
Ge17	16e	.3m	0.91684	0.91684	0.91684		
Li18	4a	-43m	0	0	0	0.75	

Transformation from published data: origin shift ³/₄ ³/₄ ³/₄

Experimental: single crystal, diffractometer, X-rays, R = 0.019, T = 160 K

Remarks: Short interatomic distances for partly occupied site(s). Supersedes a report on so-called Li₂₂Ge₅ with Li₂₂Pb₅-type structure in [2].

References: [1] Goward G.R., Taylor N.J., Souza D.C.S., Nazar L.F. (2001), J. Alloys Compd. 329, 82-91. [2] Gladyshevskii E.I., Oleksiv G.I., Kripyakevich P.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 9, 269-271.

216
cF440

Li ₁₇ Sn ₄	cF440	(216) $F-43m - h^4g^2f^2e^9ba$
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Li₁₇Sn₄ [1]

Structural features: 26-atom γ brass- (an inner tetrahedron surrounded by an outer tetrahedron, an octahedron and a cuboctahedron) and 27-atom W-type (a central atom surrounded by a cube, an octahedron and a cuboctahedron) nested polyhedra units. Defect derivative of W with partly ordered vacancies on the 8-fold Wyckoff positions.

Goward G.R. et al. (2001) [1]

 $\text{Li}_{17.05}\text{Sn}_4$ $a = 1.969 \text{ nm}$, $V = 7.6337 \text{ nm}^3$, $Z = 20$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	48h	..m	0.0899	0.0899	0.2616		pentacapped trigonal prism Li_7Sn_4
Li2	48h	..m	0.0946	0.0946	0.7658		16-vertex Frank-Kasper $\text{Sn}_2\text{Li}_{14}$
Li3	48h	..m	0.1518	0.1518	0.021		
Li4	48h	..m	0.1632	0.1632	0.505		rhombic dodecahedron $\text{Li}_{11}\text{Sn}_3$
Sn5	24g	2.mm	0.06981	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Li_{13}
Li6	24g	2.mm	0.5747	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Li}_{10}\text{Sn}_3$
Sn7	24f	2.mm	0.17928	0	0		
Li8	24f	2.mm	0.3295	0	0		rhombic dodecahedron $\text{Li}_{11}\text{Sn}_3$
Li9	16e	.3m	0.0522	0.0522	0.0522	0.75	
Li10	16e	.3m	0.0735	0.0735	0.0735	0.25	
Li11	16e	.3m	0.1882	0.1882	0.1882		16-vertex Frank-Kasper $\text{Li}_{13}\text{Sn}_3$
Li12	16e	.3m	0.3308	0.3308	0.3308		pseudo Frank-Kasper Li_9Sn_4
Sn13	16e	.3m	0.41663	0.41663	0.41663		rhombic dodecahedron Li_{14}
Li14	16e	.3m	0.5731	0.5731	0.5731		pentacapped trigonal prism Li_7Sn_4
Sn15	16e	.3m	0.65972	0.65972	0.65972		pseudo Frank-Kasper Li_{13}
Li16	16e	.3m	0.8022	0.8022	0.8022		icosahedron Li_9Sn_3
Li17	16e	.3m	0.9186	0.9186	0.9186		
Li18	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron $\text{Li}_{10}\text{Sn}_4$
Li19	4a	-43m	0	0	0	0.25	

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.019$, $T = 160 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). Supersedes a report on so-called $\text{Li}_{22}\text{Sn}_5$ with $\text{Li}_{22}\text{Pb}_5$ -type structure in [3]. A fully ordered structure was found by neutron diffraction at 223 K in [2].

References: [1] Goward G.R., Taylor N.J., Souza D.C.S., Nazar L.F. (2001), J. Alloys Compd. 329, 82-91. [2] Lupu C., Mao J.G., Rabalais J.W., Guloy A.M., Richardson J.W. Jr. (2003), Inorg. Chem. 42, 3765-3771. [3] Gladyshevskii E.I., Oleksiv G.I., Kripyakevich P.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 9, 269-271.

216
cF444

$\text{Ta}_{39}\text{Al}_{69}$	cF444	(216) $F-43m - h^6gfe^6cba$
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Ta₃₉Al₆₉ [1]

Structural features: 27-atom W-, 26-atom γ brass- and 29-atom α Mn-type nested polyhedra units in the ratio 1:1:2. Partial vacancies in the octahedron of the W-type units.

Mahne S., Harbrecht B. (1994) [1]

 $\text{Al}_{69}\text{Ta}_{39}$ $a = 1.9153 \text{ nm}$, $V = 7.0260 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	48h	..m	0.0463	0.0463	0.6474		icosahedron Al_5Ta_7
Ta2	48h	..m	0.06506	0.06506	0.2564		15-vertex Frank-Kasper $\text{Al}_{10}\text{Ta}_5$
Ta3	48h	..m	0.09397	0.09397	0.7774		15-vertex Frank-Kasper $\text{Al}_{10}\text{Ta}_5$
Al4	48h	..m	0.173	0.173	0.017		14-vertex Frank-Kasper Ta_5Al_9

Al5	48h	.m	0.1744	0.1744	0.5097		icosahedron Al ₆ Ta ₆
Al6	48h	.m	0.2028	0.2028	0.3911		icosahedron Al ₆ Ta ₆
Al7	24g	2.mm	0.5859	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Al ₆ Ta ₆
Al8	24f	2.mm	0.149	0	0	0.5	pseudo Frank-Kasper Al ₈ Ta ₅
Al9	16e	.3m	0.075	0.075	0.075		rhombic dodecahedron Al ₉ Ta ₅
Ta10	16e	.3m	0.1619	0.1619	0.1619		14-vertex Frank-Kasper Al ₁₀ Ta ₄
Ta11	16e	.3m	0.4064	0.4064	0.4064		16-vertex Frank-Kasper Al ₁₂ Ta ₄
Ta12	16e	.3m	0.6566	0.6566	0.6566		15-vertex Frank-Kasper Al ₁₂ Ta ₃
Al13	16e	.3m	0.805	0.805	0.805		icosahedron Al ₆ Ta ₆
Al14	16e	.3m	0.917	0.917	0.917		14-vertex Frank-Kasper Al ₁₀ Ta ₄
Ta15	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper Ta ₄ Al ₁₂
Ta16	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper Al ₁₂ Ta ₄
Ta17	4a	-43m	0	0	0		rhombic dodecahedron Al ₁₄

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.025

Remarks: Different models in space group (196) *F*23 were tested and rejected.

References: [1] Mahne S., Harbrecht B. (1994), J. Alloys Compd. 203, 271-279.

216
cF448

Cd ₄₅ Sm ₁₁	cF448	(216) <i>F</i> -43m – h ⁶ gfe ⁶ dcb
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Sm₁₁Cd₄₅ [1]; GdMg₅ [2]

Structural features: 27-atom W- and 29-atom α Mn-type nested polyhedra units in the ratio 1:1 (sequence along <111>: -W-W-Mn-Mn-).

Fornasini M.L. et al. (1978) [1]

Cd₄₅Sm₁₁

a = 2.1699 nm, *V* = 10.2169 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cd1	48h	.m	0.0458	0.0458	0.6404		icosahedron Cd ₈ Sm ₄
Sm2	48h	.m	0.0765	0.0765	0.2642		15-vertex polyhedron Cd ₁₅
Cd3	48h	.m	0.0772	0.0772	0.7623		icosahedron Cd ₈ Sm ₄
Cd4	48h	.m	0.1661	0.1661	0.0137		pseudo Frank-Kasper Cd ₁₀ Sm ₃
Cd5	48h	.m	0.1877	0.1877	0.5127		15-vertex Frank-Kasper Cd ₁₂ Sm ₃
Cd6	48h	.m	0.2045	0.2045	0.8903		icosahedron Cd ₉ Sm ₃
Cd7	24g	2.mm	0.0927	$\frac{1}{4}$	$\frac{1}{4}$		pseudo Frank-Kasper Cd ₈ Sm ₅
Cd8	24f	2.mm	0.1605	0	0		pseudo Frank-Kasper Cd ₉ Sm ₄
Cd9	16e	.3m	0.0797	0.0797	0.0797		rhombic dodecahedron Cd ₈ Sm ₆
Cd10	16e	.3m	0.1626	0.1626	0.1626		rhombic dodecahedron Cd ₁₀ Sm ₄
Cd11	16e	.3m	0.3334	0.3334	0.3334		rhombic dodecahedron Cd ₁₀ Sm ₄
Cd12	16e	.3m	0.4136	0.4136	0.4136		14-vertex Frank-Kasper Cd ₁₀ Sm ₄
Sm13	16e	.3m	0.6559	0.6559	0.6559		16-vertex Frank-Kasper Cd ₁₆
Sm14	16e	.3m	0.9118	0.9118	0.9118		16-vertex Frank-Kasper Cd ₁₆
Cd15	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		16-vertex Frank-Kasper Cd ₁₂ Sm ₄
Sm16	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron Cd ₁₄
Sm17	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper Cd ₁₆
Cd18	4a	-43m	0	0	0		rhombic dodecahedron Cd ₁₀ Sm ₄

Transformation from published data: origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.050

Remarks: Site occupancy $\text{Gd}_5(\text{Gd}_{0.68}\text{Mg}_{0.32})_6\text{Mg}_{43}$ reported for GdMg_5 .

References: [1] Fornasini M.L., Chabot B., Parthé E. (1978), Acta Crystallogr. B 34, 2093-2099. [2] Fornasini M.L., Manfrinetti P., Gschneidner K.A. Jr. (1986), Acta Crystallogr. C 42, 138-141.

216
cF456

$\text{Na}_{28}\text{In}_{14}\text{Sn}_{15}$ *cF456* (216) *F-43m* – h^7fe^5dcba

$\text{Na}_{28}\text{In}_{14}\text{Sn}_{15}$ [1]

Structural features: 27-atom W- and 29-atom α Mn-type nested polyhedra units in the ratio 1:3.

Blase W. et al. (1991) [1]

$\text{In}_{13.98}\text{Na}_{28}\text{Sn}_{15.02}$

$a = 2.2993 \text{ nm}$, $V = 12.1559 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	..m	0.0463	0.0463	0.6402		icosahedron In_3SnNa_8
Na2	48h	..m	0.0657	0.0657	0.2649		15-vertex Frank-Kasper $\text{In}_3\text{Sn}_5\text{Na}_7$
Sn3	48h	..m	0.0761	0.0761	0.7653		icosahedron In_4Na_8
Na4	48h	..m	0.1691	0.1691	0.017		14-vertex Frank-Kasper $\text{In}_3\text{Sn}_5\text{Na}_6$
Na5	48h	..m	0.1842	0.1842	0.5213		15-vertex Frank-Kasper $\text{Sn}_4\text{Na}_7\text{In}_4$
Sn6	48h	..m	0.2047	0.2047	0.3888		icosahedron Sn_3Na_9
In7	48h	..m	0.2052	0.2052	0.8893		icosahedron $\text{In}_3\text{Sn}_2\text{Na}_7$
In8	24f	2.mm	0.1534	0	0		pseudo Frank-Kasper Sn_4Na_9
Sn9	16e	.3m	0.0793	0.0793	0.0793		rhombic dodecahedron $\text{In}_3\text{Na}_{11}$
Na10	16e	.3m	0.1653	0.1653	0.1653		14-vertex Frank-Kasper Sn_7Na_7
Na11	16e	.3m	0.4092	0.4092	0.4092		16-vertex Frank-Kasper $\text{Na}_7\text{In}_6\text{Sn}_3$
Na12	16e	.3m	0.6596	0.6596	0.6596		16-vertex Frank-Kasper $\text{Na}_4\text{In}_9\text{Sn}_3$
Na13	16e	.3m	0.9095	0.9095	0.9095		16-vertex Frank-Kasper $\text{In}_6\text{Sn}_6\text{Na}_4$
Na14	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		16-vertex Frank-Kasper $\text{In}_{12}\text{Na}_4$
Na15	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper $\text{Na}_4\text{Sn}_{12}$
Na16	4b	-43m	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		16-vertex Frank-Kasper $\text{In}_{12}\text{Na}_4$
Na17	4a	-43m	0	0	0		14-vertex Frank-Kasper $\text{Sn}_4\text{In}_6\text{Na}_4$

$\text{M1} = 0.83\text{In} + 0.17\text{Sn}$

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.070$

References: [1] Blase W., Cordier G., Vogt T. (1991), Z. Anorg. Allg. Chem. 606, 79-90.

216
cF620

$\text{Y}_{15}\text{Ni}_{32}\text{H}_{41.6}$ *cF620* (216) *F-43m* – $i^3h^5fe^4c$

$\text{Y}_{0.95}\text{Ni}_2\text{H}_{2.6}$ [1]

Structural features: Filled-up derivative of defect MgCu_2 (part of the minority atom positions vacant) with H in tetrahedral (Y_2Ni_2 and Ni_4) voids.

Percheron Guégan A. et al. (1991) [1]

$\text{D}_{45.36}\text{Ni}_{32}\text{Y}_{15}$

$a = 1.5113 \text{ nm}$, $V = 3.4519 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	96i	1	0.012	0.123	0.263	0.38	single atom D

D2	96i	1	0.095	0.155	0.515	0.19	non-collinear D ₂
D3	96i	1	0.126	0.373	0.502	0.38	
D4	48h	..m	0.005	0.005	0.38	0.65	non-coplanar square Ni ₂ D ₂
D5	48h	..m	0.122	0.122	0.247	0.79	
Ni6	48h	..m	0.1814	0.1814	0.5573		
Ni7	48h	..m	0.1912	0.1912	0.0556		non-coplanar square D ₄
D8	48h	..m	0.241	0.241	0.961	0.44	
Y9	24f	2.mm	0.2292	0	0		9-vertex polyhedron D ₉
Ni10	16e	.3m	0.0595	0.0595	0.0595		
Y11	16e	.3m	0.3846	0.3846	0.3846		cuboctahedron D ₁₂
Ni12	16e	.3m	0.5612	0.5612	0.5612		
Y13	16e	.3m	0.8453	0.8453	0.8453		
Y14	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		

Transformation from published data: origin shift $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

Experimental: powder, diffractometer, neutrons, R_p = 0.057, T = 293 K

Remarks: Refinement of the occupancy of Wyckoff position 4a showed no significant deviation from zero. Short interatomic distances for partly occupied site(s); impossibly short distances occur for the refined occupation factor of site D4.

References: [1] Percheron Guégan A., Paul Boncour V., Latroche M., Achard J.C., Bourée Vigneron F. (1991), J. Less-Common Met. 172, 198-205.

216
cF700

Ag ₈ TiS ₆	cF700	(216) <i>F</i> -43 <i>m</i> – i ⁷ edca
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Ag₈TiS₆ [1], argyrodite family

Structural features: S forms a tetrahedrally close-packed (MgCu₂-type) framework; Ti in tetrahedral voids, Ag distributed over several voids of low coordination (high degree of disorder). Single TiS₄ tetrahedra.

Wada H. et al. (1996) [1]

Ag_{8.02}S₆Ti

a = 1.0628 nm, *V* = 1.2005 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	96i	1	0.0008	0.0388	0.2211	0.079	
Ag2	96i	1	0.0356	0.2125	0.2506	0.042	
Ag3	96i	1	0.0369	0.1727	0.2841	0.028	
Ag4	96i	1	0.0413	0.0716	0.2344	0.043	
Ag5	96i	1	0.0455	0.1307	0.1981	0.088	
Ag6	96i	1	0.0624	0.0944	0.2213	0.037	
Ag7	96i	1	0.083	0.103	0.311	0.017	
S8	16e	.3m	0.6231	0.6231	0.6231		
Ti9	4d	-43m	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		tetrahedron S ₄
S10	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
S11	4a	-43m	0	0	0		

Transformation from published data: -*x*, -*y*, -*z*; origin shift $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays, R = 0.110, T = 297 K

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

References: [1] Wada H., Ishii M., Onoda M., Tansho M., Sato A. (1996), Solid State Ionics 86/88, 159-163.

216
cF1064

Sc_{19.3}Si_{1.4}B_{231.2}C_{12.84}

cF1064

(216) *F*-43*m* – i²h¹⁶e⁶ca

ScB₁₂C_{0.65}Si_{0.07} [1]

Structural features: B and C form a 3D-framework with icosahedra and 10-vertex polyhedra arranged in so-called super-tetrahedra (four icosahedra interconnected via exo-bonds or via a central Si(B,C)₄ tetrahedron) and octahedra (six 10-vertex polyhedra interconnected via a central SiC₄ tetrahedron and additional (B,C) atoms).

Tanaka T., Sato A. (2002) [1]

B_{231.32}C_{12.68}Sc_{19.36}Si_{1.38}

a = 2.03085 nm, *V* = 8.3759 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
B1	96i	1	0.0238	0.0845	0.2875		square pyramid B ₅
B2	96i	1	0.048	0.1663	0.2693		pentagonal pyramid B ₆
B3	48h	..m	0.0326	0.0326	0.7616		square pyramid B ₅
B4	48h	..m	0.034	0.034	0.3597		pentagonal pyramid B ₆
B5	48h	..m	0.0485	0.0485	0.6788		pentagonal pyramid B ₆
B6	48h	..m	0.0613	0.0613	0.8362		pentagonal pyramid B ₆
Sc7	48h	..m	0.0689	0.0689	0.1784	0.95	20-vertex polyhedron B ₁₈ Sc ₂
B8	48h	..m	0.0864	0.0864	0.9794		pentagonal pyramid B ₆
B9	48h	..m	0.1068	0.1068	0.668		pentagonal pyramid B ₆
B10	48h	..m	0.1209	0.1209	0.8168		pentagonal pyramid B ₆
B11	48h	..m	0.141	0.141	0.7404		pentagonal pyramid B ₆
B12	48h	..m	0.1478	0.1478	0.9562		pentagonal pyramid B ₆
B13	48h	..m	0.1899	0.1899	0.5902		pentagonal pyramid B ₆
B14	48h	..m	0.1981	0.1981	0.0073		pentagonal pyramid B ₆
B15	48h	..m	0.1982	0.1982	0.097		pentagonal pyramid B ₆
B16	48h	..m	0.2184	0.2184	0.3783		pentagonal pyramid CB ₅
B17	48h	..m	0.2191	0.2191	0.5204		pentagonal pyramid B ₆
M18	48h	..m	0.2219	0.2219	0.6622		pentagonal pyramid B ₆
M19	16e	.3m	0.0553	0.0553	0.0553		4-vertex polyhedron B ₃ Si
M20	16e	.3m	0.1506	0.1506	0.1506		non-coplanar triangle B ₃
C21	16e	.3m	0.3053	0.3053	0.3053		tetrahedron B ₃ Si
Sc22	16e	.3m	0.373	0.373	0.373	0.99	pseudo Frank-Kasper B ₁₉ C
M23	16e	.3m	0.4377	0.4377	0.4377		non-coplanar triangle B ₃
Sc24	16e	.3m	0.5591	0.5591	0.5591		octahedron B ₆
Si25	4c	-43m	¹ / ₄	¹ / ₄	¹ / ₄		tetrahedron C ₄
Si26	4a	-43m	0	0	0	0.38	tetrahedron B ₄

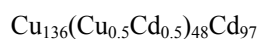
M18 = 0.58B + 0.42C; M19 = 0.73B + 0.27C; M20 = 0.51B + 0.49C; M23 = 0.85B + 0.15C

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.048

Remarks: In table 3 of [1] the Wyckoff positions of former Si(1) and Si(2) are misprinted as 4*a* instead of 4*c* and 4*b*, respectively.

References: [1] Tanaka T., Sato A. (2002), J. Solid State Chem. 165, 148-158.



cF1124

 $(216) F-43m - i^2h^{15}g^2f^2e^7c$ **Cu₄Cd₃ [1]**

Structural features: 568 icosahedra and 124 Friauf polyhedra in the unit cell.

Samson S. (1967) [1]

 $\text{Cd}_{121}\text{Cu}_{160}$ $a = 2.5871 \text{ nm}$, $V = 17.3157 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	96i	1	0.0036	0.1362	0.2256		15-vertex Frank-Kasper Cu ₈ Cd ₇
Cu2	96i	1	0.0338	0.1018	0.3286		icosahedron Cu ₅ Cd ₇
Cu3	48h	..m	0.0339	0.0339	0.2604		icosahedron Cu ₆ Cd ₆
M4	48h	..m	0.0354	0.0354	0.8091		icosahedron Cu ₅ Cd ₇
Cu5	48h	..m	0.0560	0.0560	0.1683		icosahedron Cu ₆ Cd ₆
Cd6	48h	..m	0.0663	0.0663	0.7043		15-vertex Frank-Kasper Cu ₈ Cd ₇
Cu7	48h	..m	0.1026	0.1026	0.5335		icosahedron Cu ₆ Cd ₆
M8	48h	..m	0.1060	0.1060	0.8117		12-vertex polyhedron Cu ₂ Cd ₁₀
Cd9	48h	..m	0.1119	0.1119	0.9796		14-vertex polyhedron Cu ₆ Cd ₈
Cd10	48h	..m	0.1138	0.1138	0.2499		16-vertex Frank-Kasper Cu ₁₂ Cd ₄
Cu11	48h	..m	0.1476	0.1476	0.0784		icosahedron Cu ₆ Cd ₆
M12	48h	..m	0.1498	0.1498	0.7244		12-vertex polyhedron Cu ₄ Cd ₈
Cd13	48h	..m	0.1793	0.1793	0.5474		14-vertex polyhedron Cu ₆ Cd ₈
Cu14	48h	..m	0.1931	0.1931	0.4424		icosahedron Cu ₆ Cd ₆
M15	48h	..m	0.2130	0.2130	0.9138		12-vertex polyhedron Cu ₃ Cd ₉
Cu16	48h	..m	0.2142	0.2142	0.0813		icosahedron Cu ₇ Cd ₅
Cu17	48h	..m	0.2157	0.2157	0.3517		icosahedron Cu ₆ Cd ₆
Cu18	24g	2.mm	0.5006	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Cu ₄ Cd ₈
Cu19	24g	2.mm	0.6793	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron Cu ₆ Cd ₆
Cd20	24f	2.mm	0.0876	0	0		14-vertex polyhedron Cu ₆ Cd ₈
Cd21	24f	2.mm	0.3635	0	0		16-vertex Frank-Kasper Cu ₁₂ Cd ₄
Cu22	16e	.3m	0.0744	0.0744	0.0744		icosahedron Cu ₆ Cd ₆
Cd23	16e	.3m	0.1815	0.1815	0.1815		16-vertex Frank-Kasper Cu ₁₂ Cd ₄
Cd24	16e	.3m	0.3632	0.3632	0.3632		16-vertex Frank-Kasper Cu ₁₂ Cd ₄
Cd25	16e	.3m	0.4315	0.4315	0.4315		16-vertex Frank-Kasper Cu ₁₂ Cd ₄
Cu26	16e	.3m	0.5346	0.5346	0.5346		icosahedron Cu ₆ Cd ₆
Cu27	16e	.3m	0.6262	0.6262	0.6262		icosahedron Cu ₃ Cd ₉
Cu28	16e	.3m	0.8203	0.8203	0.8203		icosahedron Cu ₃ Cd ₉
Cd29	4c	-43m	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		16-vertex Frank-Kasper Cu ₁₂ Cd ₄

M4 = 0.67Cu + 0.33Cd; M8 = 0.67Cd + 0.33Cu; M12 = 0.5Cd + 0.5Cu; M15 = 0.5Cd + 0.5Cu

Experimental: single crystal, diffractometer, X-rays, R = 0.128

References: [1] Samson S. (1967), Acta Crystallogr. 23, 586-600.