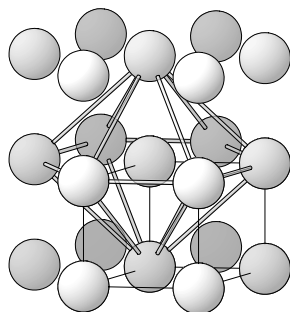


Space group (191) $P6/mmm$ 191
 $hP1$

$(\text{Hg}_{0.1}\text{Sn}_{0.9})$	$hP1$	(191) $P6/mmm - a$
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HgSn₉ [2], s.h. (simple hexagonal), Strukturbericht notation A₆; (BiIn) γ [4]; Si form V [3]; "Sn γ " [2]
Structural features: Directly superposed close-packed (Sn,Hg) layers (the atoms form a triangle mesh). See Fig. III.66.

Fig. III.66. **HgSn₉**

Arrangement of (Sn,Hg) atoms emphasizing a hexagonal bipyramid.

Grigorjeva T.F. et al. (1989) [1]

$\text{Hg}_{0.14}\text{Sn}_{0.86}$

$a = 0.3205$, $c = 0.2984$ nm, $c/a = 0.931$, $V = 0.0266$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	1a	6/mmm	0	0	0		hexagonal bipyramid Sn ₈

$\text{M1} = 0.86\text{Sn} + 0.14\text{Hg}$

Experimental: powder, diffractometer, X-rays

Remarks: We assigned an approximate value to the Hg/Sn ratio of site M1 based on the nominal composition. Also referred to as HgSn_{12} and HgSn_6 ; homogeneity range $\text{Hg}_{100-x}\text{Sn}_x$, $88 < x < 92$ according to [5].

References: [1] Grigorjeva T.F., Ivanov E.Y., Boldyrev V.V., Petrachekov E.I., Samsonova T.I. (1989), Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk 1989(4), 46-49. [2] (1931), Strukturberichte 1, 570. [3] Olijnyk H., Sikka S.K., Holzapfel W.B. (1984), Phys. Lett. A 103, 137-140. [4] Giessen B.C., Morris M., Grant N.J. (1967), Trans. Metall. Soc. AIME 239, 883-889. [5] Che G.C., Ellner M., Schubert K. (1991), J. Mater. Sci. 26, 2417-2420.

191
 $hP3$

Ti	$hP3$	(191) $P6/mmm - da$
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Ti ω [1], ω phase; Hg_{99}As [3]; (TiBi) γ [2]

Structural features: Triangle-mesh Ti layers and hexagon-mesh Ti₂ layers alternate along [001]. See Fig. III.67.

Jamieson J.C. (1963) [1]

Ti

$a = 0.4625$, $c = 0.2813$ nm, $c/a = 0.608$, $V = 0.0521$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pentacapped trigonal prism Ti ₁₁
Ti2	1a	6/mmm	0	0	0		bicapped hexagonal prism Ti ₁₄

Experimental: powder, film, X-rays

Remarks: High-pressure phase. According to [4] true symmetry is space group (164) $P-3m1$. The description of Hg₉₉As in space group (187) $P-6m2$ with double cell volume in [3] does not take into consideration all symmetry elements of the proposed model (new axes a,b,c/2; origin shift $\frac{2}{3} \frac{1}{3} 0$).

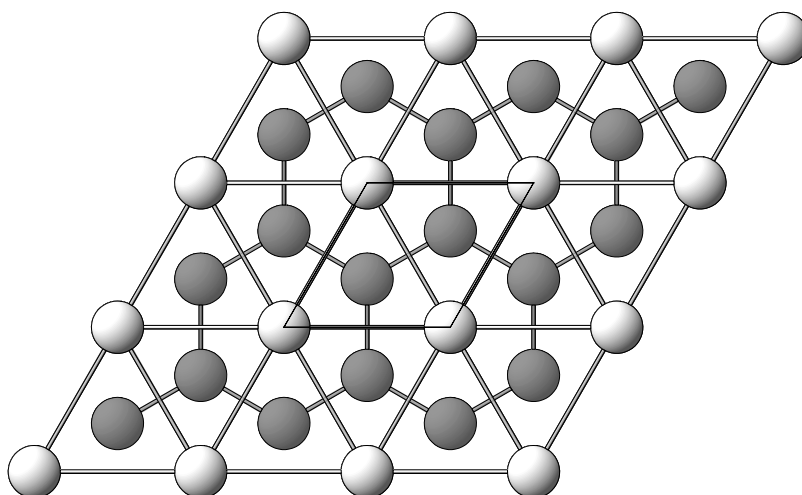


Fig. III.67. Ti ω

Arrangement of Ti atoms viewed along [001]. Light and dark atoms are shifted by $c/2$.

References: [1] Jamieson J.C. (1963), Science (Washington D.C.) 140, 72-73. [2] Makarov E.S. (1950), Dokl. Akad. Nauk SSSR 74, 935-938. [3] Puselj M., Ban Z. (1974), J. Less-Common Met. 37, 213-216. [4] Bagazyatskii Y.A., Nosova G.I., Tagunova T.V. (1955), Dokl. Akad. Nauk SSSR 105, 1225-1228.

191
hP3

AlB ₂	hP3	(191) $P6/mmm$ – da
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AlB₂ [2], Strukturbericht notation C32

Structural features: Directly superposed close-packed Al layers; B occupies all trigonal prismatic voids. 3D-framework of fused BA₁₆ trigonal prisms. B forms planar hexagon-mesh layers. See Fig. III.68.

Burkhardt U. et al. (2004) [1]

Al_{0.91}B₂

$a = 0.3005$, $c = 0.32537$ nm, $c/a = 1.083$, $V = 0.0254$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		coplanar triangle B ₃
Al2	1a	6/mmm	0	0	0	0.91	pseudo Frank-Kasper B ₁₂ Al ₈

Experimental: single crystal, diffractometer, X-rays, R = 0.023

Remarks: Defect model confirmed by density measurements and ^{11}B NMR spectroscopy.

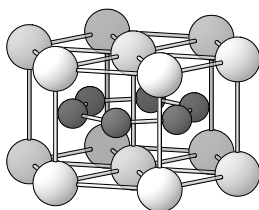


Fig. III.68. AlB_2

Arrangement of Al_6 trigonal prisms (Al atoms large) centered by B atoms (small).

References: [1] Burkhardt U., Gurin V., Haarmann F., Borrmann H., Schnelle W., Yaresko A., Grin Y. (2004), J. Solid State Chem. 177, 389-394. [2] Hofmann W., Jäniche W. (1935), Naturwissenschaften 23, 851.

191
hP3

Hg_2U	<i>hP3</i>	(191) <i>P6/mmm</i> – da
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UHg₂ [2]; **NaHg₂** [3]

Structural features: 3D-framework of fused compressed HgU_6 trigonal prisms; infinite linear -U- chains parallel to [001]. Branch of AlB_2 with $c/a = 0.65$ instead of 1.08 for AlB_2 ; ordering variant of ω -Ti.

Frost B.R.T. (1953/54) [1]

Hg_2U

$a = 0.4976$, $c = 0.3218$ nm, $c/a = 0.647$, $V = 0.0690$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Hg1	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pentacapped trigonal prism Hg_5U_6
U2	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		rhombic dodecahedron U_2Hg_{12}

Experimental: powder, film, X-rays, T = 293 K

Remarks: The data from [3] are also reported in [4].

References: [1] Frost B.R.T. (1953/54), J. Inst. Met. 82, 456-462. [2] Rundle R.E., Wilson A.S. (1949), Acta Crystallogr. 2, 148-150. [3] Nielsen J.W., Baenziger N.C. (1953), U.S. At. Energy Comm., Publ. AECU-2727. [4] Nielsen J.W., Baenziger N.C. (1954), Acta Crystallogr. 7, 277-282.

191
hP3

$\text{Au}[\text{CN}]$	<i>hP3</i>	(191) <i>P6/mmm</i> – ea
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AuCN [1]

Structural features: Infinite linear -Au-(C,N)-(N,C)- chains parallel to [001] (2-fold orientational disorder for the CN units).

Zhdanov G.S., Shugam E.A. (1945) [1]

AuCN

$a = 0.34$, $c = 0.509$ nm, $c/a = 1.497$, $V = 0.0510$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	2 <i>e</i>	6 <i>mm</i>	0	0	0.4		single atom C
Au2	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		colinear C ₂

$\text{M1} = 0.5\text{C} + 0.5\text{N}$

Experimental: powder, film, X-rays

Remarks: A model in space group (187) $P-6m2$ with CN inside trigonal prisms was tested and rejected. The structure was later redetermined with an ordered arrangement of C and N in space group (183) $P6mm$ [2].

References: [1] Zhdanov G.S., Shugam E.A. (1945), Zh. Fiz. Khim. 19, 519-522. [2] Bowmaker G.A., Kennedy B.J., Reid J.C. (1998), Inorg. Chem. 37, 3968-3974.

191
hP4

Li_3N	hP4	(191) $P6/mmm - cba$
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Li_3N [2]

Structural features: Planar Li_2N layers (edge-linked LiN_3 trigonal units) and triangle-mesh Li layers alternate along [001]. NLi_8 hexagonal bipyramids share edges to form infinite layers, which are interconnected via common vertices to form a 3D-framework. See Fig. III.69.

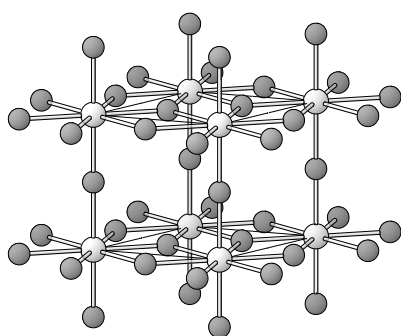


Fig. III.69. Li_3N

Arrangement of NLi_8 hexagonal bipyramids (Li atoms dark, N atoms light).

Gregory D.H. et al. (2002) [1]

$\text{Li}_{2.92}\text{N}$

$a = 0.36576$, $c = 0.38735$ nm, $c/a = 1.059$, $V = 0.0449$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.96	coplanar hexagon N_3Li_3
Li2	1b	6/mmm	0	0	$\frac{1}{2}$		colinear N_2
N3	1a	6/mmm	0	0	0		8-vertex polyhedron Li_8

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_p = 0.026$, $T = 298$ K

Remarks: Electron density study in [3].

References: [1] Gregory D.H., O'Meara P.M., Gordon A.G., Hodges J.P., Short S., Jorgensen J.D. (2002), Chem. Mater. 14, 2063-2070. [2] Zintl E., Brauer G. (1935), Z. Elektrochem. Angew. Phys. Chem. 41, 102-107. [3] Schulz H., Schwarz K. (1978), Acta Crystallogr. A 34, 999-1005.

191
hP4

$\text{Li}_2(\text{Li}_{0.27}\text{Mn}_{0.73})\text{N}$	hP4	(191) $P6/mmm - cba$
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$\text{Li}_{2.27}\text{Mn}_{0.73}\text{N}$ [2]

Structural features: Planar Li_2N layers (edge-linked LiN_3 trigonal units) and triangle-mesh (Mn,Li) layers alternate along [001]. $\text{N}[\text{Li}_6(\text{Mn,Li})_2]$ hexagonal bipyramids share Li-Li edges to form infinite layers,

which are interconnected via common (Mn,Li) vertices to form a 3D-framework. Ordering variant of Li_3N .

Niewa R. et al. (2001) [1]

$\text{Li}_{2.33}\text{Mn}_{0.67}\text{N}$

$a = 0.37125$, $c = 0.38212$ nm, $c/a = 1.029$, $V = 0.0456$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar hexagon N_3Li_3
M2	1b	6/mmm	0	0	$\frac{1}{2}$		colinear N_2
N3	1a	6/mmm	0	0	0		8-vertex polyhedron Mn_2Li_6

$\text{M2} = 0.67\text{Mn} + 0.33\text{Li}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.021$, $T = 293$ K

References: [1] Niewa R., Wagner F.R., Schnelle W., Hochrein O., Kniep R. (2001), Inorg. Chem. 40, 5215-5222. [2] Klatyk J., Kniep R. (1999), Z. Kristallogr. New Cryst. Struct. 214, 445-446.

191
hP5

$\text{Be}_2\text{ZrH}_{1.5}$	<i>hP5</i>	(191) <i>P6/mmm</i> – dca
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$\text{Be}_2\text{ZrH}_{1.5}$ [1]

Structural features: Filled-up derivative of AlB_2 with H in trigonal bipyramidal (Be_2Zr_3) voids.

Andresen A.F. et al. (1983) [1]

$\text{Be}_2\text{D}_{1.49}\text{Zr}$

$a = 0.37139$, $c = 0.34704$ nm, $c/a = 0.934$, $V = 0.0415$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Be1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal bipyramid D_2Be_3
D2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.745	colinear Be_2
Zr3	1a	6/mmm	0	0	0		coplanar hexagon D_6

Experimental: powder, diffractometer, neutrons, $R = 0.040$

References: [1] Andresen A.F., Otnes K., Maeland A.J. (1983), J. Less-Common Met. 89, 201-204.

191
hP6

CoSn	<i>hP6</i>	(191) <i>P6/mmm</i> – fda
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CoSn [2], Strukturbericht notation B35; PtTi [3]

Structural features: Directly superposed Kagomé-mesh Co layers; Sn in trigonal prismatic voids between the layers and at the centers of the hexagons of the Kagomé mesh. See Fig. III.70.

Larsson A.K. et al. (1996) [1]

CoSn

$a = 0.5279$, $c = 0.42597$ nm, $c/a = 0.807$, $V = 0.1028$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	3f	mmm	$\frac{1}{2}$	0	0		bicapped square antiprism Sn_6Co_4
Sn2	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism Co_6
Sn3	1a	6/mmm	0	0	0		coplanar hexagon Co_6

Experimental: single crystal, diffractometer, X-rays, $R = 0.018$

Remarks: Space group (191) $P6/mmm$ was confirmed by convergent beam electron diffraction. The atom distribution could not be determined in [3] (PtI).

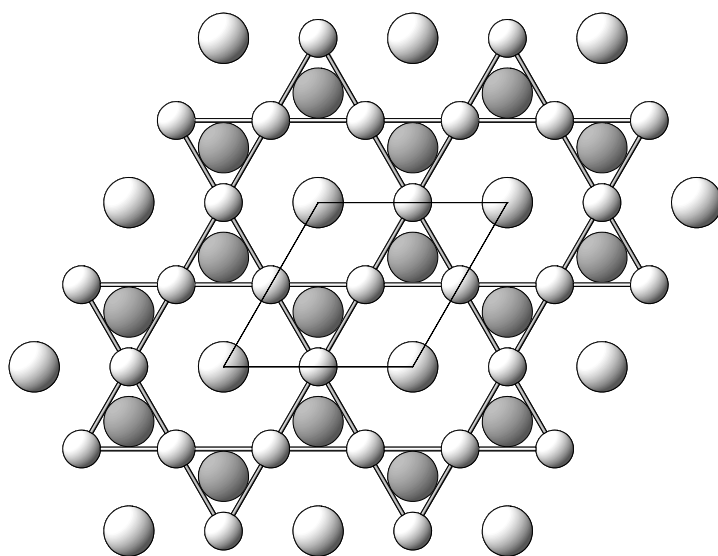


Fig. III.70. CoSn

Arrangement of Co (small) and Sn (large) atoms viewed along [001]. Light and dark atoms are shifted by $c/2$.

References: [1] Larsson A.K., Haeberlein M., Lidin S., Schwarz U. (1996), J. Alloys Compd. 240, 79-84. [2] Nial O. (1938), Z. Anorg. Allg. Chem. 238, 287-296. [3] Zintl E., Harder A. (1935), Z. Elektrochem. Angew. Phys. Chem. 41, 767-771.

191
hP6

TiO _{0.5}	hP6	(191) $P6/mmm$ – fda
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TiO_x δ [1]; TaN (see remark)

Structural features: Filled-up derivative of ω -Ti with O in octahedral voids (elongated).

Andersson S. (1959) [1]

O_{0.50}Ti

$a = 0.49915$, $c = 0.28794$ nm, $c/a = 0.577$, $V = 0.0621$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	3f	mmm	$\frac{1}{2}$	0	0	0.5	coplanar square Ti ₄
Ti2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism O ₆
Ti3	1a	$6/mmm$	0	0	0		8-vertex polyhedron O ₆ Ti ₂

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

Remarks: Exact oxygen content unknown, probably underestimated. The tetragonal cells reported in [5] and [6] are stated to be doubtful. A similar structure proposal for TaN ([2]; [3]; [4]) was superseded in [7].

References: [1] Andersson S. (1959), Acta Chem. Scand. 13, 415-419. [2] Brauer G., Zapp K.H. (1953), Naturwissenschaften 40, 604. [3] Schönberg N. (1954), Acta Chem. Scand. 8, 199-203. [4] Brauer G., Zapp K.H. (1954), Z. Anorg. Allg. Chem. 277, 129-139. [5] Bumps E.S., Kessler H.D., Hansen M. (1953), Trans. Am. Soc. Met. 45, 1008-1028. [6] Schofield T.H., Bacon A.E. (1955/56), J. Inst. Met. 84, 47-53. [7] Christensen A.N., Lebech B. (1978), Acta Crystallogr. B 34, 261-263.

191
hP6

CaCu ₅	hP6	(191) P6/mmm – gca
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CaCu₅ [2], Strukturbericht notation D2_d; CaZn₅ [2]; ErCo₅ [3]

Structural features: Kagomé-mesh Cu₃ layers and CaCu₂ layers (a Cu hexagon mesh, the hexagons of which are centered by a Ca atom) alternate along [001]. CaCu₁₂Cu₆ hexacapped hexagonal prisms share faces and edges to form a dense 3D-framework. Cu₄ tetrahedra share vertices to form a 3D-framework; Ca in channels parallel to [001]. See Fig. III.71.

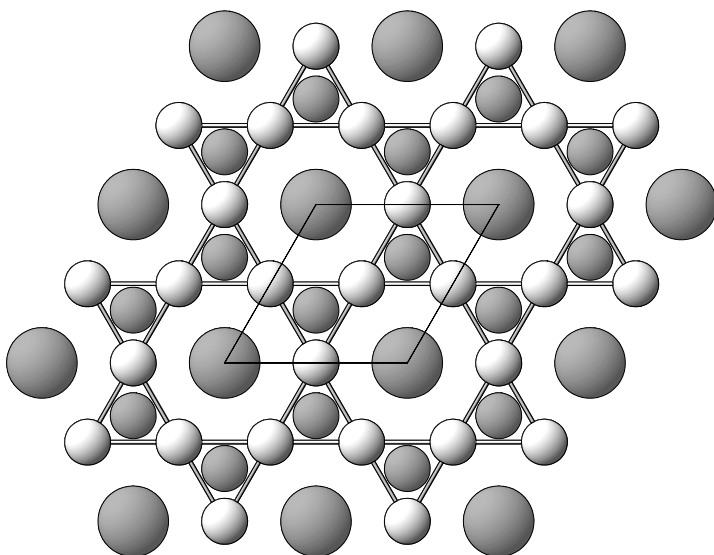


Fig. III.71. **CaCu₅**

Arrangement of Ca (large) and Cu (small) atoms viewed along [001]. Light and dark atoms are shifted by $c/2$.

Nowotny H. (1942) [1]

CaCu₅

$a = 0.5097$, $c = 0.4065$ nm, $c/a = 0.798$, $V = 0.0915$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		cuboctahedron Cu ₈ Ca ₄
Cu2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		anticuboctahedron Cu ₉ Ca ₃
Ca3	1a	6/mmm	0	0	0		pseudo Frank-Kasper Cu ₁₈ Ca ₂

Experimental: powder, film, X-rays

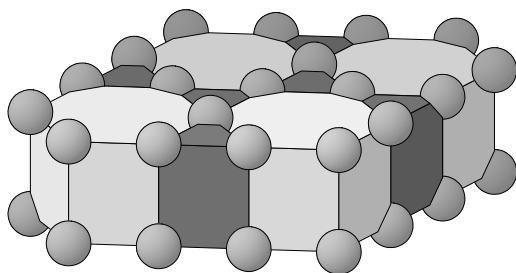
References: [1] Nowotny H. (1942), Z. Metallkd. 34, 247-253. [2] Haucke W. (1940), Z. Anorg. Allg. Chem. 244, 17-22. [3] Wernick J.H., Geller S. (1959), Acta Crystallogr. 12, 662-665.

191
hP6

CeCo ₃ B ₂	hP6	(191) P6/mmm – gca
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CeCo₃B₂ [1]

Structural features: Kagomé-mesh Co₃ layers and CeB₂ layers (a B hexagon mesh, the hexagons of which are centered by a Ce atom) alternate along [001]. Infinite columns of base-linked BCo₆ trigonal prisms share edges to form a 3D-framework; no B-B contact. Ordering variant of CaCu₅ (however, lower c/a ratio). See Fig. III.72.

Fig. III.72. **CeCo₃B₂**

Arrangement of CeCo₁₂ hexagonal (light) and BCo₆ trigonal (dark) prisms.

Kuz'ma Y.B. et al. (1969) [1]

B₂CeCo₃

$a = 0.5057$, $c = 0.3036$ nm, $c/a = 0.600$, $V = 0.0672$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		rhombic dodecahedron B ₄ Co ₆ Ce ₄
B2	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Co ₆
Ce3	1a	$6/mmm$	0	0	0		pseudo Frank-Kasper B ₆ Co ₁₂ Ce ₂

Experimental: single crystal, photographs, X-rays

Remarks: A slightly larger a -parameter is reported in [2] ($a = 0.5067(3)$, $c = 0.3036(2)$ nm).

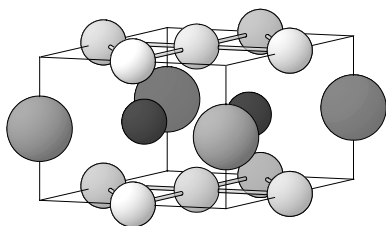
References: [1] Kuz'ma Y.B., Kropyakevich P.I., Bilonizhko N.S. (1969), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1969, 939-941. [2] Bilonizhko N.S., Kuz'ma Y.B. (1974), Inorg. Mater. 10, 227-230 (Izv. Akad. Nauk SSSR, Neorg. Mater. 10, 265-269).

191
hP6

PrNi ₂ Al ₃	<i>hP6</i>	(191) $P6/mmm - gca$
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PrNi₂Al₃ [1]

Structural features: Kagomé-mesh Al₃ layers and PrNi₂ layers (a Ni hexagon mesh, the hexagons of which are centered by a Pr atom) alternate along [001]. PrAl₁₂Ni₆ hexacapped hexagonal prisms share faces and edges to form a dense 3D-framework. Ordering variant of CaCu₅ (branch of CeCo₃B₂ with higher c/a ratio). See Fig. III.73.

Fig. III.73. **PrNi₂Al₃**

Arrangement of Pr (large), Ni (dark) and Al (light) atoms.

Rykhal' R.M. et al. (1978) [1]

Al₃Ni₂Pr

$a = 0.5293$, $c = 0.4064$ nm, $c/a = 0.768$, $V = 0.0986$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		cuboctahedron Ni ₄ Al ₄ Pr ₄
Ni2	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron Al ₆ Pr ₃ Ni ₃
Pr3	1a	$6/mmm$	0	0	0		pseudo Frank-Kasper Ni ₆ Al ₁₂ Pr ₂

Experimental: powder, diffractometer, X-rays

Remarks: In [1] the y -coordinate of the Ni site is misprinted as $1/3$ instead of $2/3$ (agreement with Wyckoff position $2c$).

References: [1] Rykhal' R.M., Zarechnyuk O.S., Kuten' Y.I. (1978), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1978, 1136-1138.

191
hP6

BaSn ₅	<i>hP6</i>	(191) <i>P6/mmm</i> – hba
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BaSn₅ [1]

Structural features: Hexagon-mesh Sn₂ layers alternate with triangle-mesh Sn and Ba layers along [001]. SnSn₁₂ hexagonal prisms share rectangular faces to form infinite slabs. Substitution derivative of ω -Ti.

Fässler T.F. et al. (2001) [1]

BaSn₅

$a = 0.53734$, $c = 0.7097$ nm, $c/a = 1.321$, $V = 0.1775$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	$4h$	$3m.$	$1/3$	$2/3$	0.2085		10-vertex polyhedron Sn ₇ Ba ₃
Ba2	$1b$	$6/mmm$	0	0	$1/2$		bicapped hexagonal prism Sn ₁₄
Sn3	$1a$	$6/mmm$	0	0	0		bicapped hexagonal prism Sn ₁₂ Ba ₂

Experimental: single crystal, diffractometer, X-rays, $R = 0.022$, $T = 293$ K

References: [1] Fässler T.F., Hoffmann S., Kronseder C. (2001), Z. Anorg. Allg. Chem. 627, 2486-2492.

191
hP6

MgAlB ₄	<i>hP6</i>	(191) <i>P6/mmm</i> – hba
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Mg_{0.5}Al_{0.5}B₂ [1]

Structural features: Hexagon-mesh B₂ layers alternate with triangle-mesh Mg and Al layers along [001]. 3D-framework of fused B(Mg₃Al₃) trigonal prisms. Substitution derivative of AlB₂.

Margadonna S. et al. (2002) [1]

AlB₄Mg

$a = 0.30444$, $c = 0.67125$ nm, $c/a = 2.205$, $V = 0.0539$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	$4h$	$3m.$	$1/3$	$2/3$	0.2413		coplanar triangle B ₃
Mg2	$1b$	$6/mmm$	0	0	$1/2$		hexagonal prism B ₁₂
Al3	$1a$	$6/mmm$	0	0	0		hexagonal prism B ₁₂

Experimental: powder, diffractometer, X-rays, synchrotron, $wR_p = 0.054$, $T = 16$ K

Remarks: Homogeneity range Mg_{1-x}Al_xB₂, $0.45 < x < 0.55$. Refinement of the site occupancies showed no significant deviation from unity. In table I of [1] the Wyckoff positions of sites Mg and Al are misprinted as $1a$ and $1b$ instead of $1b$ and $1a$.

References: [1] Margadonna S., Prassides K., Arvanitidis I., Pissas M., Papavassiliou G., Fitch A.N. (2002), Phys. Rev. B: Condens. Matter 66, 014518: 1-5.

Cu_2Te	<i>hP6</i>	(191) <i>P6/mmm</i> – he
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Cu_2Te rt [1], Strukturbericht notation C_h

Structural features: $\text{Te}_3\text{Cu-CuTe}_3$ units ($\text{Cu}(\text{CuTe}_3)$ tetrahedra) share edges to form infinite slabs.

Nowotny H. (1946) [1]

Cu_2Te

$a = 0.4237$, $c = 0.7274$ nm, $c/a = 1.717$, $V = 0.1131$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.340		7-vertex polyhedron Cu_4Te_3
Te2	2 <i>e</i>	6 <i>mm</i>	0	0	0.194		7-vertex polyhedron Cu_6Te

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, film, X-rays

Remarks: On page 41 of [1] the Wyckoff position of the Te site is misprinted as 2*l* instead of 2*e*; the z -coordinate of this site is given as 0.306 on the same page but as 0.308 in the summary. The structure proposal is criticized in [2].

References: [1] Nowotny H. (1946), Z. Metallkd. 37, 40-42. [2] Baranova R.V. (1967), Sov. Phys. Crystallogr. 12, 221-227 (Kristallografiya 12, 266-273).

Zr_4Al_3	<i>hP7</i>	(191) <i>P6/mmm</i> – fed
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Zr_4Al_3 [1], Z phase

Structural features: Kagomé-mesh Al_3 layers and $(\text{Zr}_2)\text{Zr}_2$ layers (a Zr hexagon mesh, the hexagons of which are centered by a Zr_2 dumbbell perpendicular to the layer) alternate along [001]. Tetrahedrally close-packed structure (Frank-Kasper phase). See Fig. III.74.

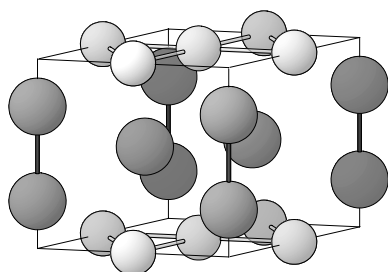


Fig. III.74. **Zr_4Al_3**

Arrangement of Zr (dark) and Al (light) atoms.

Wilson C.G. et al. (1960) [1]

Al_3Zr_4

$a = 0.5433$, $c = 0.539$ nm, $c/a = 0.992$, $V = 0.1378$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	3 <i>f</i>	6 <i>mm</i>	$\frac{1}{2}$	0	0		icosahedron Al_4Zr_8
Zr2	2 <i>e</i>	6 <i>mm</i>	0	0	0.25		14-vertex Frank-Kasper Zr_8Al_6
Zr3	2 <i>d</i>	6 <i>mm</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		15-vertex Frank-Kasper Al_6Zr_9

Transformation from published data (*P*-6): origin shift $\frac{1}{3}$ $\frac{2}{3}$ 0

Experimental: powder, film, X-rays

Remarks: The description in space group (174) $P\bar{6}$ in [1] does not take into consideration all symmetry elements of the proposed structure (see [2]). Short interatomic distances: $d(\text{Zr-Zr}) = 0.270 \text{ nm}$.

References: [1] Wilson C.G., Thomas D.K., Spooner F.J. (1960), Acta Crystallogr. 13, 56-57. [2] Cenxual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439.

191
hP7

LiC_6	<i>hP7</i>	(191) $P6/mmm - ka$
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LiC₆ [1], GIC (graphite intercalation compound)

Structural features: Directly superposed graphite (hexagon-mesh) C layers; Li between hexagons in every interlayer (stage 1). See Fig. III.75.

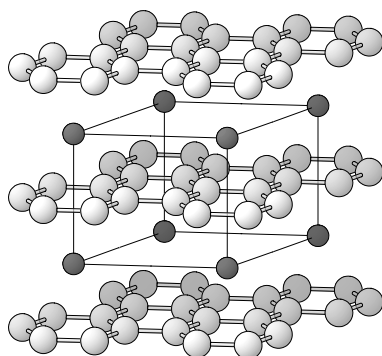


Fig. III.75. **LiC₆**

Arrangement of Li (dark) and C (light) atoms.

Juza R., Wehle V. (1965) [1]

C_6Li

$a = 0.429$, $c = 0.3737 \text{ nm}$, $c/a = 0.871$, $V = 0.0596 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	$6k$	$m\bar{2}m$	0.33333	0	$\frac{1}{2}$		coplanar triangle C_3
Li2	$1a$	$6/mmm$	0	0	0		hexagonal prism C_{12}

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

Remarks: We derived the x -coordinate of the C site from ideal graphite.

References: [1] Juza R., Wehle V. (1965), Naturwissenschaften 52, 560.

191
hP8

$\text{Cu}_{5.44}\text{Tb}_{0.78}$	<i>hP8</i>	(191) $P6/mmm - geca$
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TbCu₇ [1]

Structural features: Kagomé-mesh Cu_3 layers and $(\text{Tb}, \text{Cu}_2)\text{Cu}_2$ layers (a Cu hexagon mesh, the hexagons of which are centered by a Tb atom or a Cu_2 dumbbell perpendicular to the layer) alternate along $[001]$. Intergrowth of CaCu_5 - and Zr_4Al_3 -type blocks (complete substitutional disorder). See Fig. III.76.

Buschow K.H.J., Van Der Goot A.S. (1971) [1]

$\text{Cu}_{5.44}\text{Tb}_{0.78}$

$a = 0.4942$, $c = 0.4164 \text{ nm}$, $c/a = 0.843$, $V = 0.0881 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		
Cu2	2e	<i>6mm</i>	0	0	0.306	0.22	
Cu3	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		
Tb4	1a	<i>6/mmm</i>	0	0	0	0.78	

Experimental: powder, diffractometer, X-rays, R = 0.070

Remarks: Phase stable at high temperature. Short interatomic distances for partly occupied site(s). Probably identical to the phase called TbCu₅ in [2]. Models with simple vacancies on the Tb site or partial substitution by single Cu atoms for Tb were tested and rejected.

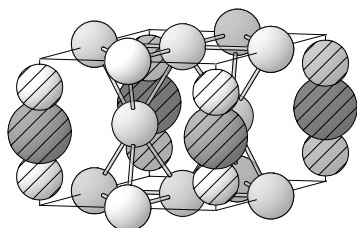


Fig. III.76. **TbCu₇**

Arrangement of Tb (large) and Cu (small) atoms (atoms in partly occupied sites are hatched).

References: [1] Buschow K.H.J., Van Der Goot A.S. (1971), Acta Crystallogr. B 27, 1085-1088. [2] Haszko S.E. (1960), Trans. Am. Inst. Min. Metall. Pet. Eng. 218, 763.

191
hP8

$\text{Y}_{0.5}\text{Co}_3\text{Ge}_3$	<i>hP8</i>	(191) <i>P6/mmm</i> – geca
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YCo₆Ge₆ [1]

Structural features: Kagomé-mesh Co₃ layers and (Y,Ge₂)Ge₂ layers (a Ge hexagon mesh, the hexagons of which are centered by an Y atom or a Ge₂ dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of ternary CaCu₅- and Zr₄Al₃-type blocks (complete substitutional disorder).

Buchholz W., Schuster H.U. (1981) [1]

Co₃Ge₃Y_{0.45}

$a = 0.5074$, $c = 0.3908$ nm, $c/a = 0.770$, $V = 0.0871$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		icosahedron Ge ₈ Co ₄
Ge2	2e	<i>6mm</i>	0	0	0.307	0.5	
Ge3	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		
Y4	1a	<i>6/mmm</i>	0	0	0	0.45	

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

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

References: [1] Buchholz W., Schuster H.U. (1981), Z. Anorg. Allg. Chem. 482, 40-48.

191
hP9

TaNO	<i>hP9</i>	(191) <i>P6/mmm</i> – fdcb
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"TaON α" [1]

Structural features: $\text{Ta}_3(\text{N},\text{O})_3$ layers ((N,O) forms a Kagomé mesh, Ta centers hexagons and triangles) alternate with triangle-mesh $(\text{N},\text{O})_3$ layers along [001]. $\text{Ta}(\text{N},\text{O})_5$ trigonal bipyramids share vertices to form a 3D-framework; infinite linear $-\text{Ta}(\text{N},\text{O})-$ chains in channels.

Buslaev Y.A. et al. (1969) [1]

NOTa

$a = 0.731$, $c = 0.404$ nm, $c/a = 0.553$, $V = 0.1870$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	$3f$	mmm	$\frac{1}{2}$	0	0		colinear Ta_2
M2	$2d$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		colinear Ta_2
Ta3	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal bipyramid N_5
M4	$1b$	$6/mmm$	0	0	$\frac{1}{2}$		colinear Ta_2
Ta5	$1a$	$6/mmm$	0	0	0		colinear N_2

$\text{M1} = 0.5\text{N} + 0.5\text{O}$; $\text{M2} = 0.5\text{N} + 0.5\text{O}$; $\text{M4} = 0.5\text{N} + 0.5\text{O}$

Experimental: single crystal, photographs, X-rays

Remarks: N and O could not be distinguished. The structure is stated to be wrong in [2] (contradictions observed for molar volume, total energy, transport properties, etc.). So-called β -TaON crystallizes in space group (14) $P2_1/c$ and was found to be stable up to the decomposition temperature [3].

References: [1] Buslaev Y.A., Safronov G.M., Pakhomov V.I., Glushkova M.A., Repko V.P., Ershova M.M., Zhukov A.N., Zhdanova T.A. (1969), Inorg. Mater. 5, 37-39 (Izv. Akad. Nauk SSSR, Neorg. Mater. 5, 45-48). [2] Lumey M.W., Dronskowski R. (2003), Z. Anorg. Allg. Chem. 629, 2173-2179. [3] Armytage D., Fender B.E.F. (1974), Acta Crystallogr. B 30, 809-812.

191
hP9

$\text{LaNi}_5\text{H}_{0.2}$	<i>hP9</i>	(191) $P6/mmm - \text{gfca}$
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$\text{LaNi}_5\text{H}_{0.2}$ [1]

Structural features: Filled-up derivative of CaCu_5 with H in octahedral (La_2Ni_4) voids.

Fischer P. et al. (1977) [1]

$\text{D}_{0.26}\text{LaNi}_5$

$a = 0.5025$, $c = 0.3988$ nm, $c/a = 0.794$, $V = 0.0872$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	$3g$	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear D_2
D2	$3f$	mmm	$\frac{1}{2}$	0	0	0.087	colinear Ni_2
Ni3	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle D_3
La4	$1a$	$6/mmm$	0	0	0		coplanar hexagon D_6

Experimental: powder, diffractometer, neutrons, $R_B = 0.037$

References: [1] Fischer P., Furrer A., Busch G., Schlappbach L. (1977), Helv. Phys. Acta 50, 421-430.

191
hP9

$\text{La}_{0.89}\text{Ga}_{2.22}$	<i>hP9</i>	(191) $P6/mmm - \text{jda}$
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$\text{La}_{0.89}\text{Ga}_{2.22}$ [1]

Structural features: Derivative of AlB_2 with part of the La atoms replaced by Ga_2 dumbbells parallel to [100] (3-fold orientational disorder).

Lu X.S. et al. (1982) [1]

$\text{Ga}_{2.22}\text{La}_{0.89}$

$a = 0.4357$, $c = 0.4421$ nm, $c/a = 1.015$, $V = 0.0727$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	6j	$m2m$	0.32	0	0	0.037	
Ga2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		
La3	1a	$6/mmm$	0	0	0	0.89	

Experimental: powder, diffractometer, X-rays, $R_B = 0.100$

Remarks: Homogeneity range $\text{Ga}_{100-x}\text{La}_x$, $28.4 < x < 33.3$. Short interatomic distances for partly occupied site(s).

References: [1] Lu X.S., Xie S.S., Liang J.K. (1982), Wuli Xuebao (Acta Phys. Sin.) 31, 1635-1641.

191
hP9

$\text{Ca}_{0.96}\text{Ga}_{2.24}$	<i>hP9</i>	(191) $P6/mmm - 1a$
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CaGa_{2+x} [1]

Structural features: Derivative of AlB_2 with part of the Ca atoms replaced by Ga_6 hexagons perpendicular to [001] (disorder).

Bruzzzone G. et al. (1989) [1]

$\text{Ca}_{0.96}\text{Ga}_{2.26}$

$a = 0.4319$, $c = 0.4329$ nm, $c/a = 1.002$, $V = 0.0699$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	6l	$mm2$	0.197	0.394	0	0.044	
Ga2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Ga_9
Ca3	1a	$6/mmm$	0	0	0	0.956	

Experimental: single crystal, diffractometer, X-rays, $R = 0.025$

Remarks: Homogeneity range CaGa_{2+x} , $0.1 < x < 0.4$. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies (fixed).

References: [1] Bruzzzone G., Fornasini M.L., Merlo F. (1989), J. Less-Common Met. 154, 67-77.

191
hP10

NaPt_3B	<i>hP10</i>	(191) $P6/mmm - icb_a$
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NaPt_3B [1]

Structural features: BPt_6 trigonal prisms share edges to form infinite slabs. Vacancy derivative of CeCo_3B_2 with every second B layer vacant.

Mirgel R., Jung W. (1988) [1]

BNaPt_3

$a = 0.5547$, $c = 0.5504$ nm, $c/a = 0.992$, $V = 0.1467$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pt1	6i	$2mm$	$\frac{1}{2}$	0	0.2578		icosahedron $\text{B}_2\text{Pt}_6\text{Na}_4$
B2	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Pt_6

Na3	1b	6/mmm	0	0	$\frac{1}{2}$	rhombic dodecahedron Na ₂ Pt ₁₂
Na4	1a	6/mmm	0	0	0	pseudo Frank-Kasper Na ₂ Pt ₁₂ B ₆

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.059

References: [1] Mirgel R., Jung W. (1988), J. Less-Common Met. 144, 87-99.

191
hP11

Hg[NO ₃][CN]	hP11	(191) P6/mmm – leca
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Hg(CN)(NO₃) [1]

Structural features: Infinite linear -Hg-(C,N)-(N,C)- chains (CN units in 2-fold orientational disorder) parallel to [001]; NO₃ trigonal units in trigonal voids of triangle-mesh Hg layers (positional disorder).

Mahon C., Britton D. (1971) [1]

CHgN₂O₃

$a = 0.5422$, $c = 0.5252$ nm, $c/a = 0.969$, $V = 0.1337$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6l	mm2	0.533	0.066	0	0.5	
M2	2e	6mm	0	0	0.393		single atom C
N3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.5	coplanar triangle O ₃
Hg4	1a	6/mmm	0	0	0		colinear C ₂

M2 = 0.5C + 0.5N

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Space group (189) P-62m was tested and rejected (R = 0.038).

References: [1] Mahon C., Britton D. (1971), Inorg. Chem. 10, 2331-2333.

191
hP12

CeCo ₄ B	hP12	(191) P6/mmm – idcba
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CeCo₄B [1]; Eu₃Ni₇B₂ [3]

Structural features: Kagomé-mesh Co₃ layers alternate with CeB₂ and CeCo₂ layers (a B or Co hexagon mesh, the hexagons of which are centered by a Ce atom) along [001]. BCo₆ trigonal prisms share edges to form infinite slabs; no B-B contact. Substitution derivative of CaCu₅ (intergrowth of CaCu₅- and CeCo₃B₂-type layers in the ratio 1:1). See Fig. III.77.

Kuz'ma Y.B., Bilonizhko N.S. (1974) [1]

BCeCo₄

$a = 0.5005$, $c = 0.6932$ nm, $c/a = 1.385$, $V = 0.1504$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6i	2mm	$\frac{1}{2}$	0	0.213		13-vertex polyhedron B ₂ Co ₇ Ce ₄
Co2	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		14-vertex polyhedron Co ₉ Ce ₃ B ₂
B3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Co ₆
Ce4	1b	6/mmm	0	0	$\frac{1}{2}$		pseudo Frank-Kasper Co ₁₈ Ce ₂
Ce5	1a	6/mmm	0	0	0		pseudo Frank-Kasper B ₆ Co ₁₂ Ce ₂

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

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

Remarks: The same data are also reported in [2]. A partly ordered structure is proposed for $\text{Eu}_3\text{Ni}_7\text{B}_2$ [3], $\text{Eu}[(\text{Eu},\text{Ni})\text{Ni}_3]\text{B}$.

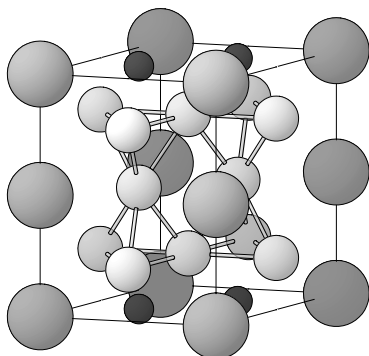


Fig. III.77. **CeCo₄B**

Arrangement of Ce (large), Co (light) and B (dark) atoms.

References: [1] Kuz'ma Y.B., Bilonizhko N.S. (1974), Sov. Phys. Crystallogr. 18, 447-449 (Kristallografiya 18, 710-714). [2] Bilonizhko N.S., Kuz'ma Y.B. (1974), Inorg. Mater. 10, 227-230 (Izv. Akad. Nauk SSSR, Neorg. Mater. 10, 265-269). [3] Felner I. (1983), J. Phys. Chem. Solids 44, 43-48.

191
hP12

KAs₄O₆I

hP12

(191) *P6/mmm* – ihba

KAs₄O₆I [2]

Structural features: $:\text{AsO}_3$ ψ -tetrahedra share vertices to form infinite layers with 6-rings. See Fig. III.78.

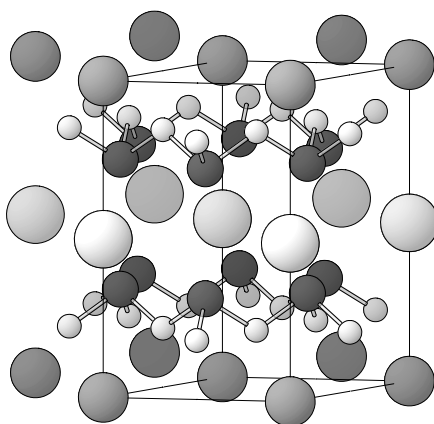


Fig. III.78. **KAs₄O₆I**

Arrangement of $:\text{AsO}_3$ ψ -tetrahedra (As atoms dark, O atoms small), K (medium) and I (large) atoms.

Pertlik F. (1988) [1]

As₄IKO₆

$a = 0.5281$, $c = 0.9169$ nm, $c/a = 1.736$, $V = 0.2215$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6i	2mm	$\frac{1}{2}$	0	0.1791		non-collinear As ₂
As2	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.28497		non-coplanar triangle O ₃
I3	1b	6/mmm	0	0	$\frac{1}{2}$		hexagonal prism As ₁₂

K4 1a 6/*mmm* 0 0 0 hexagonal prism O₁₂

Transformation from published data (*P*622): origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, wR = 0.042

Remarks: The description in space group (177) *P*622 in [1] does not take into consideration all symmetry elements of the proposed structure. The correct space group was used in [2].

References: [1] Pertlik F. (1988), Monatsh. Chem. 119, 451-456. [2] Galdecki Z. (1956), Roczn. Chem. 30, 355-357.

191
hP12

Sm_{0.65}Fe_{5.7}

hP12

(191) *P*6/*mmm* – lgea

SmFe_{8.9} [1]

Structural features: Kagomé-mesh Fe₃ layers and (Sm,Fe₂)Fe₂ layers (a Fe hexagon mesh, the hexagons of which are centered by a Sm atom or a Fe₂ dumbbell perpendicular to the layer) alternate along [001] (splitting of the Fe site forming the hexagon mesh). Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (complete substitutional disorder). Variant of TbCu₇ with split site in the hexagon mesh.

Teresiak A. et al. (1998) [1]

Fe_{5.70}Sm_{0.65}

a = 0.4923, *c* = 0.4163 nm, *c/a* = 0.846, *V* = 0.0874 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	6 <i>l</i>	<i>mm</i> 2	0.292	0.584	0	0.333	
Fe2	3 <i>g</i>	<i>mmm</i>	1/2	0	1/2		
Fe3	2 <i>e</i>	6 <i>mm</i>	0	0	0.283	0.35	
Sm4	1 <i>a</i>	6/ <i>mmm</i>	0	0	0	0.65	

Experimental: powder, diffractometer, X-rays, R_p = 0.027

Remarks: Homogeneity range SmFe_x, 8.8 < *x* < 9.0. Site occupancies given as occ(Fe3) = 0.350-0.363, occ(Sm4) = 0.637-0.650. Short interatomic distances for partly occupied site(s).

References: [1] Teresiak A., Kubis M., Mattern N., Wolf M., Müller K.H. (1998), J. Alloys Compd. 274, 284-293.

191
hP12

U_{0.67}Fe_{4.26}Si_{1.4}

hP12

(191) *P*6/*mmm* – lgea

U₂Fe_{12.8}Si_{4.2} [1]

Structural features: Kagomé-mesh (Fe,Si)₃ layers and (U,Fe₂)(Fe,Si)₂ layers (a (Fe,Si) hexagon mesh, the hexagons of which are centered by a U atom or a Fe₂ dumbbell perpendicular to the layer) alternate along [001] (splitting of the (Fe,Si) site forming the hexagon mesh). Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (disorder). Ordering variant of SmFe_{8.9}.

Berlureau T. et al. (1993) [1]

Fe_{4.24}Si_{1.40}U_{0.67}

a = 0.4834, *c* = 0.4077 nm, *c/a* = 0.843, *V* = 0.0825 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>l</i>	<i>mm</i> 2	0.2957	0.5914	0	0.33	
M2	3 <i>g</i>	<i>mmm</i>	1/2	0	1/2		

Fe3	2e	6mm	0	0	0.2968	0.33
U4	1a	6/mmm	0	0	0	0.67

M1 = 0.7Fe + 0.3Si; M2 = 0.73Fe + 0.27Si

Experimental: single crystal, diffractometer, X-rays, R = 0.023

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

References: [1] Berlureau T., Graveriau P., Chevalier B., Etourneau J. (1993), J. Solid State Chem. 104, 328-337.

191
hP12

WO ₃	hP12	(191) P6/mmm – lgf
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WO₃ hexagonal [1]

Structural features: WO₆ octahedra share vertices to form a 3D-framework with large channels of hexagonal cross-section.

Gerand B. et al. (1979) [1]

O₃W

$a = 0.7298$, $c = 0.3899$ nm, $c/a = 0.534$, $V = 0.1798$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6l	mm2	0.212	0.424	0		non-colinear W ₂
O2	3g	mmm	1/2	0	1/2		colinear W ₂
W3	3f	mmm	1/2	0	0		octahedron O ₆

Experimental: powder, diffractometer, X-rays, R = 0.098

Remarks: Weak spots in selected-area electron diffraction patterns could be indexed with a 2-fold supercell (new axes a,b,2c); no superstructure reflections were detected by X-ray diffraction.

References: [1] Gerand B., Nowogrocki G., Guenot J., Figlarz M. (1979), J. Solid State Chem. 29, 429-434.

191
hP12

BaFe ₂ Al ₉	hP12	(191) P6/mmm – mfca
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BaFe₂Al₉ [1]; SrCo₂Al₉ [1]

Structural features: FeAl₆Al₃ tricapped trigonal prisms share triangular faces and capping atoms to form a 3D-framework; Ba in channels parallel to [001].

Turban K., Schäfer H. (1975) [1]

Al₉BaFe₂

$a = 0.804$, $c = 0.389$ nm, $c/a = 0.484$, $V = 0.2178$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	6m	mm2	0.212	0.424	1/2		10-vertex polyhedron Fe ₂ Al ₈
Al2	3f	mmm	1/2	0	0		10-vertex polyhedron Fe ₂ Al ₈
Fe3	2c	-6m2	1/3	2/3	0		tricapped trigonal prism Al ₉
Ba4	1a	6/mmm	0	0	0		pseudo Frank-Kasper Al ₁₈ Ba ₂

Experimental: single crystal, Weissenberg and precession photographs, X-rays, R = 0.177

References: [1] Turban K., Schäfer H. (1975), J. Less-Common Met. 40, 91-96.

191
hP12

$(\text{Li}_{0.74}\text{Ce}_{0.26})\text{Ga}_2$	<i>hP12</i>	(191) <i>P6/mmm</i> – mfd
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$\text{Li}_{0.74}\text{Ce}_{0.26}\text{Ga}_2$ [1]

Structural features: 3D-framework of fused $\text{Ga}(\text{Li},\text{Ce})_6$ trigonal prisms (partial order Li/Ce). Substitution derivative of AlB_2 , $[(\text{Li},\text{Ce})_3(\text{Ce},\text{Li})]\text{Ga}_8$.

Fedorchuk A.A., Grin' Y.N. (1995) [1]

$\text{Ce}_{0.28}\text{Ga}_2\text{Li}_{0.72}$

$a = 0.8632$, $c = 0.4323$ nm, $c/a = 0.501$, $V = 0.2790$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	6 <i>m</i>	<i>mm2</i>	0.167	0.334	$\frac{1}{2}$		tricapped trigonal prism $\text{Ga}_3\text{Li}_4\text{Ce}_2$
M2	3 <i>f</i>	<i>mmm</i>	$\frac{1}{2}$	0	0		pseudo Frank-Kasper $\text{Ga}_{12}\text{Ce}_2\text{Li}_6$
Ga3	2 <i>d</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Ga_3Li_6
M4	1 <i>a</i>	<i>6/mmm</i>	0	0	0		pseudo Frank-Kasper $\text{Ga}_{12}\text{Li}_6\text{Ce}_2$

M2 = 0.84Li + 0.16Ce; M4 = 0.64Ce + 0.36Li

Experimental: single crystal, diffractometer, X-rays, R = 0.091

Remarks: A refinement in the AlB_2 -type subcell gave R = 0.039. In [1] the *x*-coordinate of former Ga(1) is misprinted as 0.333 instead of 0.167 (from the description of the structure).

References: [1] Fedorchuk A.A., Grin' Y.N. (1995), Inorg. Mater. 31, 120-121 (Neorg. Mater. 31, 132-133).

191
hP12

Ce_2CoSi_3	<i>hP12</i>	(191) <i>P6/mmm</i> – mfd
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Ce_2CoSi_3 [1]

Structural features: 3D-framework of fused CoCe_6 and SiCe_6 trigonal prisms. Planar hexagon-mesh CoSi_3 layers with Si_6 rings. Substitution derivative of AlB_2 .

Gordon R.A. et al. (1997) [1]

Ce_2CoSi_3

$a = 0.8104$, $c = 0.4197$ nm, $c/a = 0.518$, $V = 0.2387$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	6 <i>m</i>	<i>mm2</i>	0.1702	0.3404	$\frac{1}{2}$		tricapped trigonal prism CoSi_2Ce_6
Ce2	3 <i>f</i>	<i>mmm</i>	$\frac{1}{2}$	0	0		pseudo Frank-Kasper $\text{Si}_8\text{Co}_4\text{Ce}_8$
Co3	2 <i>d</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Si_3Ce_6
Ce4	1 <i>a</i>	<i>6/mmm</i>	0	0	0		pseudo Frank-Kasper $\text{Si}_{12}\text{Ce}_8$

Experimental: single crystal, diffractometer, X-rays, R = 0.022, T = 293 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Space group (164) *P-3m1* was tested and rejected. Supersedes a report on Ce_2CoSi_3 with a disordered arrangement of Co and Si in [2] (AlB_2 type).

References: [1] Gordon R.A., Warren C.J., Alexander M.G., DiSalvo F.J., Pöttgen R. (1997), J. Alloys Compd. 248, 24-32. [2] Bodak O.I., Gladyshevskii E.I. (1970), Izv. Akad. Nauk SSSR, Neorg. Mater. 6, 1186.

191
hP12

$\text{LaNi}_2(\text{Ni}_{0.75}\text{Al}_{0.25})_3\text{H}_{0.4}$	<i>hP12</i>	(191) <i>P6/mmm</i> – mgca
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LaNi_{4.25}Al_{0.75}H_x α [1]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (La₂(Ni,Al)₂) voids; partly ordered arrangement of Ni and Al (Al in the Kagomé-mesh layers).

Du H. et al. (2003) [1]

Al_{0.32}D_{0.41}LaNi_{4.68}

$a = 0.5059$, $c = 0.4044$ nm, $c/a = 0.799$, $V = 0.0896$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	6 <i>m</i>	<i>mm</i> 2	0.144	0.288	$\frac{1}{2}$	0.069	non-colinear D ₂
M2	3 <i>g</i>	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		coplanar square D ₄
Ni3	2 <i>c</i>	<i>-6m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	0		hexagonal prism D ₆
La4	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		hexagonal prism D ₁₂

M2 = 0.893Ni + 0.107Al

Experimental: powder, diffractometer, neutrons, $R_p = 0.042$

Remarks: Refinement on a sample of nominal composition LaNi_{4.25}Al_{0.75}D_{1.01}, containing 27 vol.% β-deuteride.

References: [1] Du H., Zhang W., Wang C., Han J., Yang Y., Chen B., Xie C., Sun K., Zhang B. (2003), Solid State Commun. 128, 157-161.

191
hP13

Be ₁₂ Ti	<i>hP13</i>	(191) <i>P6/mmm</i> – iedca
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TiBe₁₂ hexagonal [1]

Structural features: Kagomé-mesh Be₃ layers alternate with TiBe₂ and (Be₂)Be₂ layers (a Be hexagon mesh, the hexagons of which are centered by a Ti atom or a Be₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type slabs in the ratio 1:1.

Raeuchle R.F., Rundle R.E. (1952) [1]

Be₁₂Ti

$a = 0.423$, $c = 0.733$ nm, $c/a = 1.733$, $V = 0.1136$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Be1	6 <i>i</i>	2 <i>mm</i>	$\frac{1}{2}$	0	0.25		icosahedron Be ₁₀ Ti ₂
Be2	2 <i>e</i>	6 <i>mm</i>	0	0	0.28		7-vertex polyhedron TiBe ₆
Be3	2 <i>d</i>	<i>-6m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		15-vertex Frank-Kasper Be ₁₅
Be4	2 <i>c</i>	<i>-6m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron Be ₉ Ti ₃
Ti5	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		pseudo Frank-Kasper Be ₂₀

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Model for short-range order. Additional reflections could be indexed with a 48-fold hexagonal supercell (new axes 8a+4b, -4a+4b, c; see also [2]). Structure doubtful; the authors of [3] suggest the composition be Ti₂Be₁₇ and the structure a member of the Th₂Ni₁₇-Th₂Zn₁₇ structure family. On page 87 of [1] the Wyckoff position of the third Be site is misprinted as 2*c* instead of 2*d* and the *y*-coordinate of the second triplet of Wyckoff position 2*c* as $\frac{1}{2}$ instead of $\frac{1}{3}$.

References: [1] Raeuchle R.F., Rundle R.E. (1952), Acta Crystallogr. 5, 85-93. [2] Murray G.T., Taylor W.E. (1954), Acta Metall. 2, 52-62. [3] Gillam E., Rooksby H.P., Brownlee L.D. (1964), Acta Crystallogr. 17, 762-763.

191
hP13

$(\text{Mn}_{0.57}\text{Fe}_{0.43})_7\text{Ge}_6$	<i>hP13</i>	(191) <i>P6/mmm</i> – iedca
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Mn₄Fe₃Ge₆ [1]

Structural features: Kagomé-mesh (Mn,Fe)₃ layers alternate with (Mn,Fe)Ge₂ and (Ge₂)Ge₂ layers (a Ge hexagon mesh, the hexagons of which are centered by a (Mn,Fe) atom or a Ge₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type slabs in the ratio 1:1. Ordering variant of TiBe₁₂.

Malaman B. et al. (1976) [1]

Fe₃Ge₆Mn₄

$a = 0.5120$, $c = 0.8083$ nm, $c/a = 1.579$, $V = 0.1835$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6i	2mm	$\frac{1}{2}$	0	0.2491		icosahedron Ge ₆ Mn ₆
Ge2	2e	6mm	0	0	0.3377		14-vertex Frank-Kasper Ge ₇ Mn ₇
Ge3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		15-vertex Frank-Kasper Mn ₆ Ge ₉
Ge4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron Mn ₉ Ge ₃
M5	1a	6/mmm	0	0	0		pseudo Frank-Kasper Ge ₈ Mn ₁₂

M1 = 0.571Mn + 0.429Fe; M5 = 0.571Mn + 0.429Fe

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.063

Remarks: Homogeneity range Fe_{7-x}Mn_xGe₆, 1 < x < 4.5. We assigned an approximate value to the Mn/Fe ratio of sites M based on the nominal composition.

References: [1] Malaman B., Roques B., Courtois A., Protas J. (1976), Acta Crystallogr. B 32, 1352-1355.

191
hP13

MgFe ₆ Ge ₆	<i>hP13</i>	(191) <i>P6/mmm</i> – iedca
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MgFe₆Ge₆ [2]; HfFe₆Ge₆ [3]; TmMn₆Sn₆ [4]

Structural features: Kagomé-mesh Fe₃ layers alternate with MgGe₂ and (Ge₂)Ge₂ layers (a Ge hexagon mesh, the hexagons of which are centered by a Mg atom or a Ge₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type slabs in the ratio 1:1. Ordering variant of Mn₄Fe₃Ge₆ and TiBe₁₂. See Fig. III.79.

Buchholz W., Schuster H.U. (1981) [1]

Fe₆Ge₆Mg

$a = 0.5067$, $c = 0.8045$ nm, $c/a = 1.588$, $V = 0.1789$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	6i	2mm	$\frac{1}{2}$	0	0.2496		icosahedron Ge ₆ Fe ₄ Mg ₂
Ge2	2e	6mm	0	0	0.3408		14-vertex Frank-Kasper Ge ₇ Fe ₆ Mg
Ge3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		15-vertex Frank-Kasper Fe ₆ Ge ₉
Ge4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		anticuboctahedron Fe ₆ Mg ₃ Ge ₃

Mg₅ 1a 6/*mmm* 0 0 0 pseudo Frank-Kasper Ge₈Fe₁₂

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

Remarks: Partial disorder was tested for TmMn₆Sn₆ in [4] by refining the occupancy of a second Tm site in Wyckoff position 1b.

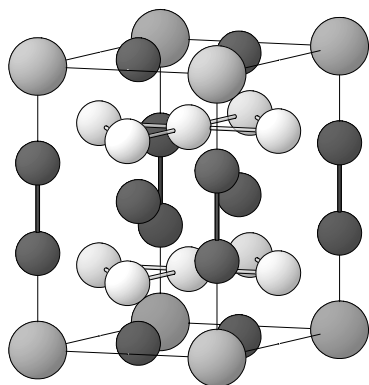


Fig. III.79. **MgFe₆Ge₆**

Arrangement of Mg (large), Fe (light) and Ge (dark) atoms.

References: [1] Buchholz W., Schuster H.U. (1981), Z. Anorg. Allg. Chem. 482, 40-48. [2] Buchholz W., Schuster H.U. (1978), Z. Naturforsch. B 33, 877-880. [3] Olenych R.R., Akselrud L.G., Yarmolyuk Y.P. (1981), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1981(2), 84-88. [4] Lefèvre C., Venturini G., Malaman B. (2003), J. Alloys Compd. 354, 47-53.

191
hP14

Li_{1.67}Cu_{1.67}Al_{3.33}

hP14

(191) *P6/mmm* – ie²dc

LiCuAl₂ [1]

Structural features: Kagomé-mesh (Cu,Al)₃ layers alternate with LiAl₂ and (Al₂)Li₂ layers (an Al or Li hexagon mesh, the hexagons of which are centered by a Li atom or an Al₂ dumbbell perpendicular to the layer, respectively) along [001]. Derivative of TiBe₁₂ and MgFe₆Ge₆ with splitting of the Li site in the LiAl₂ layers.

Van Smaalen S. et al. (1990) [1]

Al_{3.33}Cu_{1.67}Li_{1.67}

a = 0.4954, *c* = 0.9327 nm, *c/a* = 1.883, *V* = 0.1982 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6i	2 <i>mm</i>	1/2	0	0.2363	0.666	icosahedron Cu ₄ Al ₄ Li ₄
Li2	2e	6 <i>mm</i>	0	0	0.051		
Al3	2e	6 <i>mm</i>	0	0	0.3568		14-vertex Frank-Kasper AlCu ₆ Li ₇
Li4	2d	-6 <i>m</i> 2	1/3	2/3	1/2		15-vertex Frank-Kasper Cu ₆ Li ₃ Al ₆
Al5	2c	-6 <i>m</i> 2	1/3	2/3	0		

M1 = 0.556Cu + 0.444Al

Experimental: single crystal, diffractometer, X-rays, R = 0.087, T = 295 K

Remarks: Phase referred to as T1-(AlCuLi). Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies. Supersedes a structure proposal with 12 atoms in the unit cell [2].

References: [1] Van Smaalen S., Meetsma A., De Boer J.L., Bronsveld P.M. (1990), J. Solid State Chem. 85, 293-298. [2] Huang J.C., Ardell A.J. (1987), Mater. Sci. Technol. 3, 176-188.

191
hP14

$K(Al_{0.25}Si_{0.75})_4O_8[H_2O]$	<i>hP14</i>	(191) <i>P6/mmm</i> – ihcba
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KAISi₃O₈·H₂O [1], cymrite-(K)

Structural features: (Si,Al)O₄ tetrahedra share vertices to form infinite double slabs with 6-rings; K and H₂O in channels parallel to [001].

Fasshauer D.W. et al. (1997) [1]

AlH₂KO₉Si₃

$a = 0.53348$, $c = 0.77057$ nm, $c/a = 1.444$, $V = 0.1899$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6i	2mm	1/2	0	0.28631		non-colinear Si ₂
M2	4h	3m.	1/3	2/3	0.21169		tetrahedron O ₄
O3	2c	-6m2	1/3	2/3	0		colinear Si ₂
K4	1b	6/mmm	0	0	1/2		hexagonal prism O ₁₂
(OH ₂)5	1a	6/mmm	0	0	0		coplanar hexagon O ₆

M2 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 1/2

Experimental: powder, diffractometer, X-rays, R_B = 0.106

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

References: [1] Fasshauer D.W., Chatterjee N.D., Marler B. (1997), Phys. Chem. Miner. 24, 455-462.

191
hP14

$Cu_{5.36}Yb_{0.82}$	<i>hP14</i>	(191) <i>P6/mmm</i> – lgeca
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YbCu_{6.5} [1]; Y_{1-x}Co_{5+2x} [2]

Structural features: Kagomé-mesh Cu₃ layers and (Yb,Cu₂)Cu₂ layers (a Cu hexagon mesh, the hexagons of which are centered by an Yb atom or a Cu₂ dumbbell perpendicular to the layer) alternate along [001]; partial splitting of the Cu site forming the hexagon mesh. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (complete substitutional disorder). Variant of TbCu₇ with ideal and split site in the hexagon mesh.

Hornstra J., Buschow K.H.J. (1972) [1]

Cu_{5.36}Yb_{0.82}

$a = 0.5004$, $c = 0.4118$ nm, $c/a = 0.823$, $V = 0.0893$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	6l	mm2	0.30	0.60	0	0.18	
Cu2	3g	mmm	1/2	0	1/2		
Cu3	2e	6mm	0	0	0.32	0.18	
Cu4	2c	-6m2	1/3	2/3	0	0.46	
Yb5	1a	6/mmm	0	0	0	0.82	

Experimental: powder, diffractometer, X-rays, R = 0.066

Remarks: Short interatomic distances for partly occupied site(s). In the legend to table I of [1] the refined *z*-coordinate is misprinted as 0.321 instead of 0.32(1) (given on page 126). Atom coordinates for $Y_{1-x}Co_{5+2x}$ are reported in [3].

References: [1] Hornstra J., Buschow K.H.J. (1972), *J. Less-Common Met.* 27, 123-127. [2] Deportes J., Givord D., Schweizer J., Tasset F. (1976), *IEEE Trans. Magn.* 12, 1000-1002. [3] Schweizer J., Tasset F. (1980), *J. Phys. F: Met. Phys.* 10, 2799-2817.

191
hP15

$[NH_4]_2As_4Cl_2O_6[H_2O]$	<i>hP15</i>	(191) <i>P6/mmm</i> – iheda
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$NH_4As_2O_3Cl \cdot 0.5H_2O$ [1]

Structural features: Double infinite slabs of vertex-linked $:AsO_3$ ψ -tetrahedra separated by water molecules alternate with double layers of Cl atoms separated by NH_4 .

Edstrand M., Blomqvist G. (1955) [1]

$As_4Cl_2H_{10}N_2O_7$

$a = 0.5254$, $c = 1.2574$ nm, $c/a = 2.393$, $V = 0.3006$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6i	2mm	$\frac{1}{2}$	0	0.133		non-colinear As_2
As2	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2119		non-coplanar triangle O_3
Cl3	2e	6mm	0	0	0.323		non-coplanar hexagon As_6
$(NH_4)4$	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper $(NH_4)_3As_2Cl_6$
$(OH_2)5$	1a	6/mmm	0	0	0		hexagonal prism O_{12}

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.110$

Remarks: The description in space group (177) *P622* in [1] does not take into consideration all symmetry elements of the proposed structure. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Edstrand M., Blomqvist G. (1955), *Ark. Kemi* 8, 245-256.

191
hP15

$Sm_{0.67}Fe_{5.66}N_{1.2}$	<i>hP15</i>	(191) <i>P6/mmm</i> – lgfea
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$SmFe_{8.5}N_x$ [1]

Structural features: Filled-up derivative of $TbCu_7$ with N in octahedral (Sm_2Fe_4) voids and splitting of the Fe site forming the hexagon mesh.

Teresiak A. et al. (1999) [1]

$Fe_{5.66}N_{1.20}Sm_{0.67}$

$a = 0.5036$, $c = 0.4225$ nm, $c/a = 0.839$, $V = 0.0928$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	6l	mm2	0.287	0.574	0	0.333	
Fe2	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear N_2
N3	3f	mmm	$\frac{1}{2}$	0	0	0.4	
Fe4	2e	6mm	0	0	0.269	0.333	
Sm5	1a	6/mmm	0	0	0	0.667	

Experimental: powder, diffractometer, X-rays, $R_p = 0.035$

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

References: [1] Teresiak A., Kubis M., Mattern N., Wolf M., Gruner W., Müller K.H. (1999), J. Alloys Compd. 292, 212-220.

191
hP15

$\text{Na}_{0.5}\text{W}_3\text{O}_{9.25}[\text{H}_2\text{O}]_{0.69}$

hP15

(191) *P6/mmm* – lgfea

$\text{Na}_{0.17}\text{WO}_{3.085}\cdot 0.23\text{H}_2\text{O}$ [1], HTB (hexagonal tungsten bronze)

Structural features: WO_6 octahedra share vertices to form a 3D-framework; Na and H_2O (partial orientational disorder) in large channels of hexagonal cross-section parallel to [001].

Reis K.P. et al. (1992) [1]

$\text{D}_{1.14}\text{Na}_{0.51}\text{O}_{9.99}\text{W}_3$

$a = 0.7329$, $c = 0.3891$ nm, $c/a = 0.531$, $V = 0.1810$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6l	<i>mm2</i>	0.2114	0.4228	0		non-colinear W ₂
O2	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear W ₂
W3	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		octahedron O ₆
O4	2e	<i>6mm</i>	0	0	0.412	0.495	
Na5	1a	<i>6/mmm</i>	0	0	0	0.51	colinear O ₂
D6	12o	<i>.m.</i>	0.071	0.142	0.312	0.095	

Experimental: powder, diffractometer, neutrons, $R_p = 0.051$

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] Reis K.P., Prince E., Whittingham M.S. (1992), Chem. Mater. 4, 307-312.

191
hP15

$\text{La}_{0.32}\text{W}_3\text{O}_{9.48}$

hP15

(191) *P6/mmm* – lgfeb

$\text{La}_{0.108}\text{WO}_{3.16}$ [1], HTB (hexagonal tungsten bronze)

Structural features: WO_6 octahedra share vertices to form a 3D-framework; La and additional O in large channels of hexagonal cross-section parallel to [001].

Filonenko V.P. et al. (2002) [1]

$\text{La}_{0.32}\text{O}_{9.49}\text{W}_3$

$a = 0.74089$, $c = 0.37924$ nm, $c/a = 0.512$, $V = 0.1803$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6l	<i>mm2</i>	0.208	0.416	0		non-colinear W ₂
O2	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear W ₂
W3	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		octahedron O ₆
La4	2e	<i>6mm</i>	0	0	0.048	0.162	
O5	1b	<i>6/mmm</i>	0	0	$\frac{1}{2}$	0.486	colinear La ₂

Experimental: powder, diffractometer, X-rays, $R_B = 0.065$

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

References: [1] Filonenko V.P., Grenthe C., Nygren M., Sundberg M., Zibrov I.P. (2002), J. Solid State Chem. 163, 84-92.

191
hP15

CaNi ₅ H _{0.3}	hP15	(191) <i>P6/mmm</i> – mgfca
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CaNi₅H_{0.3} [1]

Structural features: Filled-up derivative of CaCu₅ with H in octahedral (Ca₂Ni₄) and tetrahedral (Ca₂Ni₂) voids.

Yoshikawa A. et al. (1998) [1]

CaD_{0.27}Ni₅

$a = 0.49947$, $c = 0.39596$ nm, $c/a = 0.793$, $V = 0.0855$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	6m	mm2	0.15	0.3	$\frac{1}{2}$	0.03	non-collinear D ₂
Ni2	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		coplanar square D ₄
D3	3f	mmm	$\frac{1}{2}$	0	0	0.03	collinear Ni ₂
Ni4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle D ₃
Ca5	1a	6/mmm	0	0	0		sixcapped hexagonal prism D ₁₈

Experimental: powder, diffractometer, neutrons, R = 0.008

References: [1] Yoshikawa A., Uyenishi Y., Iizumi H., Matsumoto T., Takano N., Terasaki F. (1998), J. Alloys Compd. 280, 204-208.

191
hP16

SmMn ₆ Sn ₆	hP16	(191) <i>P6/mmm</i> – ie ² dcba
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SmMn₆Sn₆ [1]; TbCr₆Ge₆ [2]; LuFe₆Ge₆ [3]

Structural features: Kagomé-mesh Mn₃ layers alternate with SmSn₂ and (Sn₂)Sn₂ layers (a Sn hexagon mesh, the hexagons of which are centered by a Sm atom or a Sn₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type slabs (partial order).

Malaman B. et al. (1997) [1]

Mn₆SmSn₆

$a = 0.5552$, $c = 0.9058$ nm, $c/a = 1.631$, $V = 0.2418$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	6i	2mm	$\frac{1}{2}$	0	0.25		icosahedron Sn ₈ Mn ₄
Sn2	2e	6mm	0	0	0.166	0.25	
Sn3	2e	6mm	0	0	0.33	0.75	
Sn4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism Mn ₆
Sn5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Mn ₆
Sm6	1b	6/mmm	0	0	$\frac{1}{2}$	0.25	
Sm7	1a	6/mmm	0	0	0	0.75	

Experimental: powder, diffractometer, X-rays

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

References: [1] Malaman B., Venturini G., Chafik El Idrissi B., Ressouche E. (1997), J. Alloys Compd. 252, 41-49. [2] Schobinger P., Rodriguez Carvajal J., Buschow K.H.J. (1997), J. Alloys Compd. 255, 67-

73. [3] Schobinger P., Buschow K.H.J., De Boer F.R., Ritter C., Isnard O., Fauth F. (1998), J. Alloys Compd. 267, 59-65.

191
hP16

$\text{Ta}_{0.38}\text{O}_{0.78}$	<i>hP16</i>	(191) <i>P6/mmm</i> – kjcba
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TaO_x hexagonal [1]

Structural features: High degree of disorder.

Khitrova V.I. et al. (1979) [1]

$\text{O}_{0.78}\text{Ta}_{0.38}$

$a = 0.620$, $c = 0.590$ nm, $c/a = 0.952$, $V = 0.1964$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>k</i>	<i>m2m</i>	0.16667	0	$\frac{1}{2}$	0.12	
O2	6 <i>j</i>	<i>m2m</i>	0.33333	0	0	0.40	
Ta3	2 <i>c</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0	0.20	
Ta4	1 <i>b</i>	<i>6/mmm</i>	0	0	$\frac{1}{2}$	0.12	
Ta5	1 <i>a</i>	<i>6/mmm</i>	0	0	0		

Experimental: polycrystalline sample, electron diffraction, $R = 0.176$

Remarks: Idealized coordinates. The description in space group (175) *P6/m* in [1] does not take into consideration all symmetry elements of the proposed structure. Short interatomic distances for partly occupied site(s).

References: [1] Khitrova V.I., Klechkovskaya V.V., Pinsker Z.G. (1979), Sov. Phys. Crystallogr. 24, 537-539 (Kristallografiya 24, 939-944).

191
hP18

$\text{Nd}_3\text{Ni}_{13}\text{B}_2$	<i>hP18</i>	(191) <i>P6/mmm</i> – ihgeca
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Nd₃Ni₁₃B₂ [1]

Structural features: BNi₆ trigonal prisms share edges to form infinite slabs; no B-B contact. Substitution derivative of CaCu₅ (intergrowth of CaCu₅- and CeCo₃B₂-type slabs in the ratio 2:1).

Kuz'ma Y.B., Bilonizhko N.S. (1981) [1]

$\text{B}_2\text{Nd}_3\text{Ni}_{13}$

$a = 0.5005$, $c = 1.0904$ nm, $c/a = 2.179$, $V = 0.2366$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.134		13-vertex polyhedron B ₂ Ni ₇ Nd ₄
Ni2	4 <i>h</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.323		anticuboctahedron Ni ₉ Nd ₃
Ni3	3 <i>g</i>	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		cuboctahedron Ni ₈ Nd ₄
Nd4	2 <i>e</i>	<i>6mm</i>	0	0	0.328		pseudo Frank-Kasper Ni ₁₈ Nd ₂
B5	2 <i>c</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Ni ₆
Nd6	1 <i>a</i>	<i>6/mmm</i>	0	0	0		pseudo Frank-Kasper B ₆ Ni ₁₂ Nd ₂

Experimental: powder, diffractometer, X-rays, $R = 0.125$

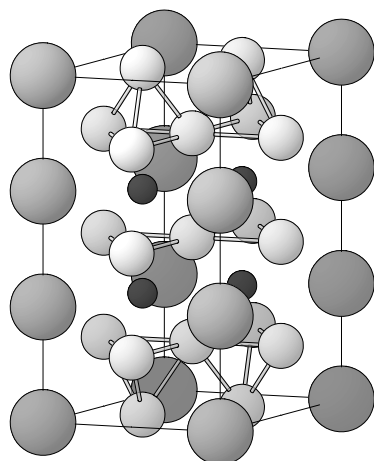
References: [1] Kuz'ma Y.B., Bilonizhko N.S. (1981), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1981(10), 87-90.



hP18

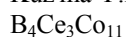
(191) $P6/mmm$ – ihgeca **$\text{Ce}_3\text{Co}_{11}\text{B}_4$ [1]**

Structural features: BCo_6 trigonal prisms share trigonal faces and edges to form infinite double slabs; no B-B contact. Substitution derivative of CaCu_5 (intergrowth of CaCu_5 - and CeCo_3B_2 -type slabs in the ratio 1:2). See Fig. III.80.

Fig. III.80. **$\text{Ce}_3\text{Co}_{11}\text{B}_4$**

Arrangement of Ce (large), Co (light) and B (dark) atoms.

Kuz'ma Y.B., Bilonizhko N.S. (1974) [1]



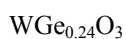
$a = 0.5045$, $c = 0.9925$ nm, $c/a = 1.967$, $V = 0.2188$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6i	2mm	$\frac{1}{2}$	0	0.2		13-vertex polyhedron $\text{B}_2\text{Co}_7\text{Ce}_4$
B2	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.35		trigonal prism Co_6
Co3	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		14-vertex Frank-Kasper $\text{B}_4\text{Co}_6\text{Ce}_4$
Ce4	2e	6mm	0	0	0.333		pseudo Frank-Kasper $\text{Co}_{12}\text{B}_6\text{Ce}_2$
Co5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex polyhedron $\text{Co}_9\text{Ce}_3\text{B}_2$
Ce6	1a	6/mmm	0	0	0		pseudo Frank-Kasper $\text{Co}_{18}\text{Ce}_2$

Experimental: single crystal, rotation photographs, X-rays, $R = 0.140$

Remarks: The same data are also reported in [2].

References: [1] Kuz'ma Y.B., Bilonizhko N.S. (1974), Sov. Phys. Crystallogr. 18, 447-449 (Kristallografiya 18, 710-714). [2] Bilonizhko N.S., Kuz'ma Y.B. (1974), Inorg. Mater. 10, 227-230 (Izv. Akad. Nauk SSSR, Neorg. Mater. 10, 265-269).



hP18

(191) $P6/mmm$ – ljgf **$\text{Ge}_{0.24}\text{WO}_3$ [1], HTB (hexagonal tungsten bronze); SnW_3O_9 [2]**

Structural features: WO_6 octahedra share vertices to form a 3D-framework; Ge in large channels of hexagonal cross-section parallel to $[001]$ (displaced from the channel axis, split site).

Plies V. (1985) [1]

$\text{Ge}_{0.24}\text{O}_3\text{W}$

$a = 0.744$, $c = 0.3817$ nm, $c/a = 0.513$, $V = 0.1830$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6l	$mm2$	0.2117	0.4234	0		non-colinear W_2
Ge2	6j	$m2m$	0.0765	0	0	0.12	
O3	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		colinear W_2
W4	3f	mmm	$\frac{1}{2}$	0	0		octahedron O_6

Transformation from published data ($P622$): origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.062$

Remarks: Short interatomic distances for partly occupied site(s). The description in space group (177) $P622$ in [1] does not take into consideration all symmetry elements of the proposed structure. SnW_3O_9 was reported in space group (191) $P6/mmm$ [2].

References: [1] Plies V. (1985), Z. Anorg. Allg. Chem. 521, 191-198. [2] Xu X.L., Schmalle H.W., Günter J.R. (1995), Solid State Ionics 76, 221-228.

191
hP18

YNi_2Al_3	<i>hP18</i>	(191) $P6/mmm$ – lkfd
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YNi_2Al_3 [2]; CeCo_3Ga_2 [4]; $\text{HoNi}_{2.6}\text{Ga}_{2.4}$ [3]; CaPd_3Al_5 [5]

Structural features: Kagomé-mesh Ni_2Al layers alternate with Al_2 hexagon-mesh layers along $[001]$; Y at the centers of the Ni_6 hexagons of the Kagomé mesh and part of the hexagons of the hexagon mesh. See Fig. III.81.

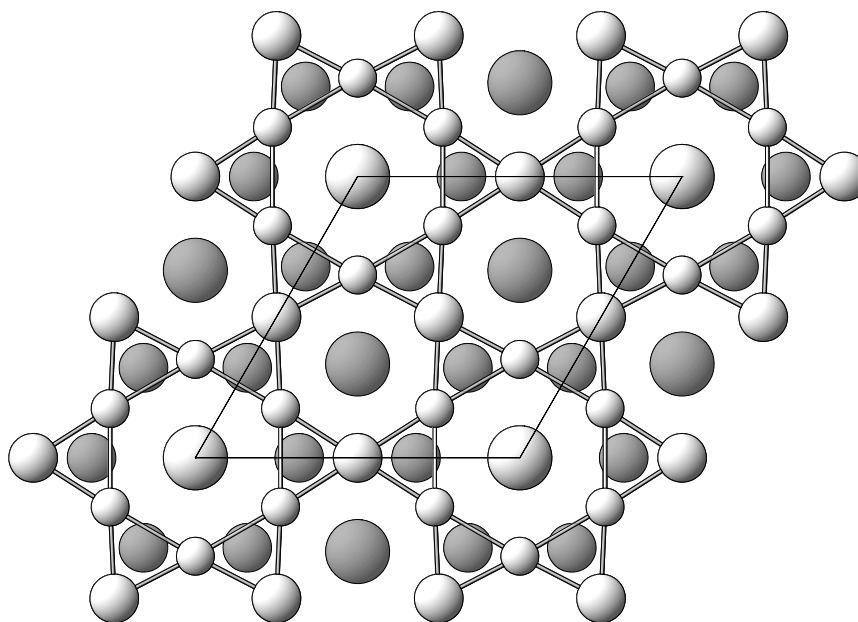


Fig. III.81. YNi_2Al_3

Arrangement of Y (large), Ni (small) and Al (medium) atoms viewed along $[001]$. Light and dark atoms are shifted by $c/2$.

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

 $\text{Al}_3\text{Ni}_2\text{Y}$ $a = 0.9006$, $c = 0.407$ nm, $c/a = 0.452$, $V = 0.2859$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	6l	$mm2$	0.175	0.35	0		pseudo Frank-Kasper $\text{Al}_6\text{Y}_3\text{Ni}_2$
Al2	6k	$m2m$	0.32	0	$\frac{1}{2}$		13-vertex polyhedron $\text{Ni}_4\text{Al}_5\text{Y}_4$
Al3	3f	mmm	$\frac{1}{2}$	0	0		cuboctahedron $\text{Ni}_4\text{Al}_4\text{Y}_4$
Y4	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper $\text{Al}_{12}\text{Ni}_6\text{Y}_2$
Y5	1a	$6/mmm$	0	0	0		coplanar hexagon Ni_6

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays

Remarks: Homogeneity range $\text{YNi}_{5-x}\text{Al}_x$, $2.5 < x < 3$. For CeCo_3Ga_2 [4] mixed Co/Ga occupation is reported for the site in Wyckoff position 6k, $\text{CeCo}_2[(\text{Co},\text{Ga})_2\text{Ga}]$. For CaPd_3Al_5 [5] mixed Pd/Al occupation is reported for the site in Wyckoff position 1a, $[\text{Ca}_2(\text{Pd},\text{Al})]\text{Pd}_6\text{Al}_9$.

References: [1] Sorgic B., Blazina Z., Drasner A. (1998), J. Alloys Compd. 265, 185-189. [2] Zarechnyuk O.S., Rykhal R.M. (1981), Visn. L'viv. Derzh. Univ., Ser. Khim. 23, 45-47. [3] Grin' Y.N., Yarmolyuk Y.P., Pecharskiy V.K. (1983), Russ. Metall. 1983(3), 187-191 (Izv. Akad. Nauk SSSR, Met. 1983, 213-218). [4] Schobinger Papamantellos P., Middleton D.P., Buschow K.H.J. (1994), J. Alloys Compd. 206, 189-193. [5] Cordier G., Dörsam G., Friedrich T., Henseleit R., Röhr C. (1993), J. Alloys Compd. 190, 201-207.

191
hP18

YCo_3Ga_2	<i>hP18</i>	(191) $P6/mmm - 1\text{kfd}a$
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 YCo_3Ga_2 [1]

Structural features: Kagomé-mesh Co_3 layers alternate with hexagon-mesh Ga_2 layers along [001]; Y centers part of the hexagons of the Kagomé mesh and part of the hexagons of the hexagon mesh. Ordering variant of YNi_2Al_3 , $\text{YCo}_2[\text{CoGa}_2]$.

Freymy M.A. et al. (1985) [1]

 $\text{Co}_3\text{Ga}_2\text{Y}$ $a = 0.8819$, $c = 0.4056$ nm, $c/a = 0.460$, $V = 0.2732$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6l	$mm2$	0.1799	0.3598	0		pseudo Frank-Kasper $\text{Co}_4\text{Ga}_4\text{Y}_3$
Ga2	6k	$m2m$	0.2895	0	$\frac{1}{2}$		cuboctahedron $\text{Co}_6\text{Ga}_2\text{Y}_4$
Co3	3f	mmm	$\frac{1}{2}$	0	0		cuboctahedron $\text{Co}_4\text{Ga}_4\text{Y}_4$
Y4	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper $\text{Co}_{12}\text{Ga}_6\text{Y}_2$
Y5	1a	$6/mmm$	0	0	0		sixcapped hexagonal prism $\text{Co}_6\text{Ga}_{12}$

Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.070$

References: [1] Freymy M.A., Gignoux D., Moreau J.M., Paccard D., Paccard L. (1985), J. Less-Common Met. 106, 251-255.

191
hP18

LaNi_5H_3	<i>hP18</i>	(191) $P6/mmm - \text{migca}$
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LaNi₅H₃ [1]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (La₂Ni₂) and trigonal bipyramidal (La₂Ni₃) voids.

Hayakawa H. et al. (1988) [1]

D_{3,12}LaNi₅

$a = 0.5302$, $c = 0.4066$ nm, $c/a = 0.767$, $V = 0.0990$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	6m	mm2	0.131	0.262	$\frac{1}{2}$	0.13	non-colinear D ₂
D2	6i	2mm	$\frac{1}{2}$	0	0.088	0.39	single atom D
Ni3	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		octahedron D ₆
Ni4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism D ₆
La5	1a	6/mmm	0	0	0		hexagonal prism D ₁₂

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

Remarks: The same data are also reported in [4]. Supersedes a structure proposal with Wyckoff position 3f fully occupied by H ([2], [3]).

References: [1] Hayakawa H., Nomura K., Ishido Y., Akiba E., Shin S., Asano H., Izumi F., Watanabe N. (1988), J. Less-Common Met. 143, 315-324. [2] Ono S., Nomura K., Akiba E., Uruno H. (1985), J. Less-Common Met. 113, 113-117. [3] Akiba E., Nomura K., Ono S. (1987), J. Less-Common Met. 129, 159-164. [4] Akiba E., Hayakawa H., Ishido Y., Nomura K., Shin S. (1989), Z. Phys. Chem. 163, 291-296.

191
hP18

NdCo₂(Co_{0.5}Ga_{0.5})₂Ga

hP18

(191) P6/mmm – mjgca

NdCo₃Ga₂ [1]; TbCo₃Ga₂ [2]

Structural features: Kagomé-mesh (Co,Ga)₂Ga layers and NdCo₂ layers (a Co₂ hexagon mesh, the hexagons of which are centered by a Nd atom) alternate along [001]. Substitution derivative of CaCu₅.

Routsi C.D. et al. (1992) [1]

Co₃Ga₂Nd

$a = 0.8886$, $c = 0.4091$ nm, $c/a = 0.46$, $V = 0.2798$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	6m	mm2	0.167	0.334	$\frac{1}{2}$		cuboctahedron Co ₆ Ga ₂ Nd ₄
Co2	6j	m2m	0.333	0	0		icosahedron Co ₇ Ga ₂ Nd ₃
Ga3	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		cuboctahedron Co ₈ Nd ₄
Nd4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		sixcapped hexagonal prism Co ₁₂ Ga ₆
Nd5	1a	6/mmm	0	0	0		sixcapped hexagonal prism Co ₁₈

M1 = 0.5Co + 0.5Ga

Experimental: powder, diffractometer, X-rays, $R_p = 0.065$

References: [1] Routsi C.D., Yakinthos J.K., Gamari Seale E. (1992), J. Magn. Magn. Mater. 116, 99-102. [2] Routsi C.D., Yakinthos J.K., Ressouche E. (1997), J. Alloys Compd. 256, 61-64.

191
hP18

LaNi₅H_{0.4}

hP18

(191) P6/mmm – ngca

LaNi₅H_{0.4} [2]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral (LaNi_3) voids.

Soubeyroux J.L. et al. (1987) [1]

$\text{D}_{0.40}\text{LaNi}_5$

$a = 0.5025$, $c = 0.3991$ nm, $c/a = 0.794$, $V = 0.0873$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	$\dots m$	0.455	0	0.117	0.033	
Ni2	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
Ni3	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		
La4	1a	$6/mmm$	0	0	0		

Experimental: powder, diffractometer, neutrons, $R_B = 0.086$

Remarks: Short interatomic distances for partly occupied site(s). Similar R values are reported for refinements with H in two different sites; the authors exclude the model used in [2] based on geometrical considerations.

References: [1] Soubeyroux J.L., Percheron Guégan A., Achard J.C. (1987), J. Less-Common Met. 129, 181-186. [2] Fischer P., Furrer A., Busch G., Schlapbach L. (1977), Helv. Phys. Acta 50, 421-430.

191
hP18

U_2RuSi_3	hP18	(191) $P6/mmm - ofda$
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U_2RuSi_3 [1]

Structural features: 3D-framework of fused RuU_6 and SiU_6 trigonal prisms. Slightly puckered hexagon-mesh RuSi_3 layers with Si_6 rings. Substitution derivative of AlB_2 with split Si site.

Pöttgen R. et al. (1994) [1]

RuSi_3U_2

$a = 0.8145$, $c = 0.38496$ nm, $c/a = 0.473$, $V = 0.2212$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	12o	$\dots m$	0.166	0.332	0.4432	0.5	
U2	3f	mmm	$\frac{1}{2}$	0	0		
Ru3	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		
U4	1a	$6/mmm$	0	0	0		

Experimental: single crystal, diffractometer, X-rays, $wR = 0.024$

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for split site Si1. Short interatomic distances for partly occupied site(s).

References: [1] Pöttgen R., Gravereau P., Darriet B., Chevalier B., Hickey E., Etourneau J. (1994), J. Mater. Chem. 4, 463-467.

191
hP18

LaNi_5H_6	hP18	(191) $P6/mmm - ogca$
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LaNi_5H_6 [1]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral (LaNi_3) voids.

Halstead T.K. (1974) [1]

 H_6LaNi_5 $a = 0.544$, $c = 0.4308$ nm, $c/a = 0.792$, $V = 0.1104$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
H1	12o	\bar{m}	0.2	0.4	0.27	0.5	non-coplanar triangle Ni ₃
Ni2	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		square prism (cube) H ₈
Ni3	2c	$\bar{6}m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism H ₆
La4	1a	$6/mmm$	0	0	0		hexagonal prism H ₁₂

Remarks: Structure determination based on NMR measurements. Other structure models in space group (191) $P6/mmm$ were tested and rejected.

References: [1] Halstead T.K. (1974), J. Solid State Chem. 11, 114-119.

191
hP19

 $\text{Ba}(\text{Al}_{0.5}\text{Si}_{0.5})_4\text{O}_8$

hP19

(191) $P6/mmm$ – nhda**"BaAl₂Si₂O₈ hexagonal α " [1]**

Structural features: (Al,Si)O₄ tetrahedra share vertices to form infinite double slabs with 6-rings; Ba between the slabs in channels parallel to [001].

Takeuchi Y. (1958) [1]

 $\text{Al}_2\text{BaO}_8\text{Si}_2$ $a = 0.5293$, $c = 0.779$ nm, $c/a = 1.472$, $V = 0.1890$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12n	\bar{m}	0.45	0	0.209	0.5	
M2	4h	$3m$	$\frac{1}{3}$	$\frac{2}{3}$	0.288		
O3	2d	$\bar{6}m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		colinear Al ₂
Ba4	1a	$6/mmm$	0	0	0		hexagonal prism O ₁₂

M2 = 0.50Al + 0.50Si

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

Remarks: Phase stable at T < 723 K. Short interatomic distances for partly occupied site(s). Average structure; the authors state that true symmetry is probably orthorhombic body-centered (new axes a, a+2b, 2c). Phase referred to as celsian in [1], however, the structural features correspond to cymrite, BaAl₂Si₂O₈·H₂O, which was later refined in space group (6) Pm [2].

References: [1] Takeuchi Y. (1958), Mineral. J. 2, 311-332. [2] Bolotina N.B., Rastsvetaeva R.K., Andrianov V.I., Kashaev A.A. (1991), Sov. Phys. Crystallogr. 36, 190-194 (Kristallografiya 36, 361-368).

191
hP22

 $\text{Tb}_2(\text{Fe}_{0.83}\text{Al}_{0.17})_{17}$

hP22

(191) $P6/mmm$ – mjhgca**Tb₂(Fe_{0.832}Al_{0.168})₁₇ [1]**

Structural features: Kagomé-mesh (Fe,Al)₃ layers and [Tb₂(Fe,Al)₂](Fe,Al)₂ layers (a (Fe,Al) hexagon mesh, the hexagons of which are centered by a Tb atom or a (Fe,Al)₂ dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (partial disorder).

Boller H., Oesterreicher H. (1976) [1]

$\text{Al}_{2.86}\text{Fe}_{14.14}\text{Tb}_2$

$a = 0.8532$, $c = 0.4175$ nm, $c/a = 0.489$, $V = 0.2632$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	6m	mm2	0.16667	0.33333	1/2		
M2	6j	m2m	0.33333	0	0		
M3	4h	3m.	1/3	2/3	0.28	0.5	
M4	3g	mmm	1/2	0	1/2		
Tb5	2c	-6m2	1/3	2/3	0	0.5	
Tb6	1a	6/mmm	0	0	0		sixcapped hexagonal prism Fe ₁₈

M1 = 0.832Fe + 0.168Al; M2 = 0.832Fe + 0.168Al; M3 = 0.832Fe + 0.168Al; M4 = 0.832Fe + 0.168Al

Transformation from published data (P622): origin shift 0 0 1/2

Experimental: powder, film, X-rays

Remarks: Idealized coordinates for sites M1 and M2. Short interatomic distances for partly occupied site(s). The description in space group (177) *P622* in [1] does not take into consideration all symmetry elements of the proposed model (see [3]); the true symmetry is, however, probably lower. A partly ordered model with site M4 occupied exclusively by Al was tested and rejected. In [2] the Fe/Al ratio is misprinted as 0.8235/0.1765 instead of 0.8325/0.1675.

References: [1] Boller H., Oesterreicher H. (1976), J. Less-Common Met. 45, 103-109. [2] (1978), Structure Reports 42A, 7. [3] Cenxual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439.

191
hP24

$\text{Ce}_2\text{Co}_7\text{B}_3$	hP24	(191) <i>P6/mmm</i> – i ² hedcba
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Ce₂Co₇B₃ [1]

Structural features: BCo₆ trigonal prisms share triangular faces and edges to form infinite triple slabs; no B-B contact. Substitution derivative of CaCu₅ (intergrowth of CaCu₅- and CeCo₃B₂-type slabs in the ratio 1:3).

Kuz'ma Y.B., Bilonizhko N.S. (1974) [1]

$\text{B}_3\text{Ce}_2\text{Co}_7$

$a = 0.5053$, $c = 1.297$ nm, $c/a = 2.567$, $V = 0.2868$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	6i	2mm	1/2	0	0.125		14-vertex Frank-Kasper B ₄ Co ₆ Ce ₄
Co2	6i	2mm	1/2	0	0.35		13-vertex polyhedron B ₂ Co ₇ Ce ₄
B3	4h	3m.	1/3	2/3	0.238		trigonal prism Co ₆
Ce4	2e	6mm	0	0	0.25		pseudo Frank-Kasper Co ₁₂ B ₆ Ce ₂
Co5	2d	-6m2	1/3	2/3	1/2		14-vertex polyhedron Co ₉ Ce ₃ B ₂
B6	2c	-6m2	1/3	2/3	0		trigonal prism Co ₆
Ce7	1b	6/mmm	0	0	1/2		pseudo Frank-Kasper Co ₁₈ Ce ₂
Ce8	1a	6/mmm	0	0	0		pseudo Frank-Kasper B ₆ Co ₁₂ Ce ₂

Transformation from published data: origin shift 0 0 1/2

Experimental: powder, X-rays, R_B = 0.104

Remarks: The same data are also reported in [2].

References: [1] Kuz'ma Y.B., Bilonizhko N.S. (1974), Sov. Phys. Crystallogr. 18, 447-449 (Kristallografiya 18, 710-714). [2] Bilonizhko N.S., Kuz'ma Y.B. (1974), Inorg. Mater. 10, 227-230 (Izv. Akad. Nauk SSSR, Neorg. Mater. 10, 265-269).

191
hP24

Ba ₁₀ Ge ₇ O ₃	hP24	(191) P6/mmm – I ² kgda
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Ba₁₀Ge₇O₃ [1]

Structural features: OBa₆ octahedra share vertices to form an HTB-type framework (split O site); additional Ba and planar Ge₆ rings in channels parallel to [001], additional Ge in trigonal prismatic (Ba₆) voids.

Von Schnering H.G. et al. (1996) [1]

Ba₁₀Ge₇O₃

$a = 1.1701$, $c = 0.5095$ nm, $c/a = 0.435$, $V = 0.6041$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	6l	mm2	0.21321	0.42642	0		non-colinear O ₂
O2	6l	mm2	0.5163	0.0326	0	0.5	
Ge3	6k	m2m	0.21152	0	$\frac{1}{2}$		non-colinear Ge ₂
Ba4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
Ge5	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.5	tricapped trigonal prism Ba ₉
Ba6	1a	6/mmm	0	0	0		sixcapped hexagonal prism Ge ₁₂ Ba ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.045, T = 293 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s).

References: [1] Von Schnering H.G., Bolle U., Curda J., Peters K., Carrillo Cabrera W., Somer M., Schultheiss M., Wedig U. (1996), Angew. Chem. Int. Ed. Engl. 35, 984-986.

191
hP24

LaGaBi ₂	hP24	(191) P6/mmm – mkjgca
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LaGaBi₂ [1]

Structural features: LaBi₆Bi₂ bicapped trigonal prisms share prism bases, edges and capping atoms to form a 3D-framework; planar Ga₆ rings alternating with additional Bi atoms in channels parallel to [001]. See Fig. III.82.

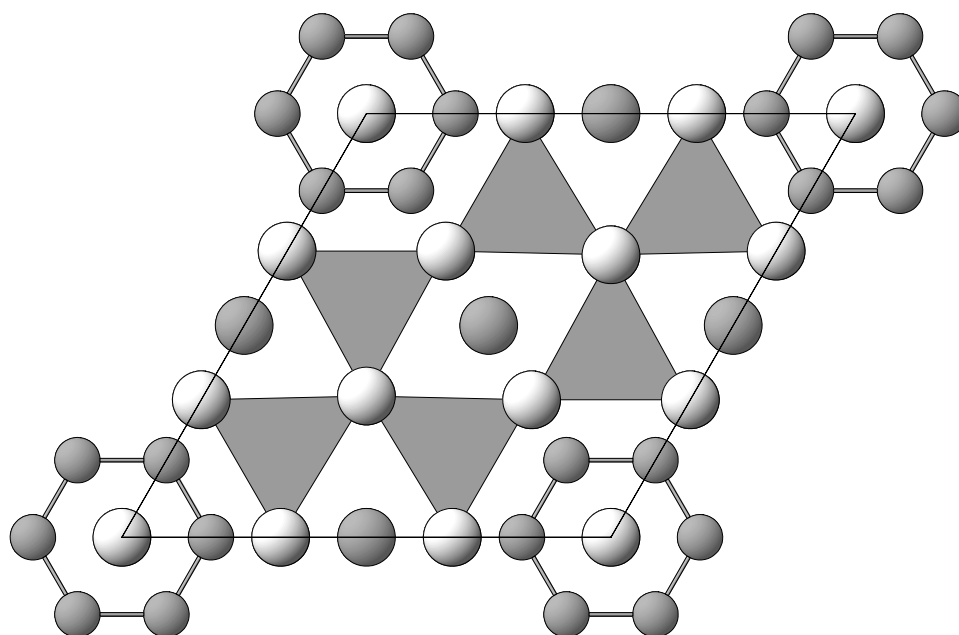
Morgan M.G. et al. (2003) [1]

Bi₂GaLa

$a = 1.35483$, $c = 0.43937$ nm, $c/a = 0.324$, $V = 0.6984$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
La1	6m	mm2	0.2253	0.45059	$\frac{1}{2}$		10-vertex polyhedron Bi ₈ Ga ₂
Ga2	6k	m2m	0.18199	0	$\frac{1}{2}$		non-colinear Ga ₂
Bi3	6j	m2m	0.32457	0	0		square prism (cube) Ga ₂ Bi ₂ La ₄
Bi4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		square prism (cube) Bi ₄ La ₄
Bi5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism La ₆
Bi6	1a	6/mmm	0	0	0		hexagonal prism Ga ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 295 K

Fig. III.82. **LaGaBi₂**

Arrangement of LaBi₆ trigonal prisms (Bi atoms large), Ga₆ rings (Ga atoms small) and additional Bi atoms viewed along [001]. Light and dark atoms are shifted by $c/2$.

References: [1] Morgan M.G., Wang M., Chan W.Y., Mar A. (2003), Inorg. Chem. 42, 1549-1555.

191
hP24

Ce(Mn_{0.08}Co_{0.15}Ni_{0.71}Al_{0.06})₅H_{1.3}

hP24

(191) *P6/mmm* – nm \bar{g} ca

CeMn_{0.4}Co_{0.75}Ni_{3.55}Al_{0.3}H_{1.3} [1]; LaNi_{4.25}Al_{0.75}H_{3.1} [2]; La(Ni,Co,Mn,Al)₅H_{4.7} [3]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (La₂M₂) and trigonal bipyramidal (La₂M₃) voids.

Joubert J.M. et al. (1998) [1]

Al_{0.30}CeCo_{0.75}D_{1.26}Mn_{0.40}Ni_{3.55}

$a = 0.4978$, $c = 0.4116$ nm, $c/a = 0.827$, $V = 0.0883$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	$\bar{6}m$	0.46	0	0.1	0.03	
D2	6m	$mm2$	0.14	0.28	$\frac{1}{2}$	0.15	non-colinear D ₂
M3	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
M4	2c	$\bar{6}m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		
Ce5	1a	6/ mmm	0	0	0		24-vertex polyhedron D ₂₄

M3 = 0.71Ni + 0.15Co + 0.08Mn + 0.06Al; M4 = 0.71Ni + 0.15Co + 0.08Mn + 0.06Al

Experimental: powder, diffractometer, neutrons, $R_B = 0.130$

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

References: [1] Joubert J.M., Latroche M., Percheron Guégan A., Bourée Vigneron F. (1998), J. Alloys Compd. 275/277, 118-122. [2] Du H., Zhang W., Wang C., Han J., Yang Y., Chen B., Xie C., Sun K.,

Zhang B. (2003), Solid State Commun. 128, 157-161. [3] Georgiev P.A., Liu J., Ross D.K., Andersen K.H., Otto A. (2003), J. Alloys Compd. 349, 325-333.

191
hP25

$K_2Ba[NO_2]_4$	<i>hP25</i>	(191) <i>P6/mmm</i> – njgcba
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$K_2Ba(NO_2)_4$ ht [1]

Structural features: $K_2(NO_2)$ layers (K_2N triangle mesh, O-N-O linear units perpendicular to [001], partial orientational disorder) and $Ba(NO_2)_3$ layers (BaN_2 triangle mesh, linear O-N-O units perpendicular to [120], partial orientational disorder) alternate along [001].

Kirpichnikova L.F. et al. (2002) [1]

$BaK_2N_4O_8$

$a = 0.66677$ nm, $c = 0.6137$ nm, $c/a = 0.920$, $V = 0.2363$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12n	<i>..m</i>	0.4297	0	0.332	0.5	
O2	6j	<i>m2m</i>	0.1468	0	0	0.333	
N3	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		
K4	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		
Ba5	1b	<i>6/mmm</i>	0	0	$\frac{1}{2}$		
N6	1a	<i>6/mmm</i>	0	0	0		

Experimental: single crystal, diffractometer, X-rays, $R = 0.016$, $T = 432$ K

Remarks: Phase stable at $T > 420$ K. Short interatomic distances: $d(N6-O2) = 0.098$ nm. Short interatomic distances for partly occupied site(s).

References: [1] Kirpichnikova L.F., Shakhmatov V.S., Pietraszko A. (2002), Crystallogr. Rep. 47, 1031-1035 (Kristallografiya 47, 1100-1104).

191
hP25

$P_8[C_{60}]$	<i>hP25</i>	(191) <i>P6/mmm</i> – o ² a
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$C_{60}(P_4)_2$ [1]

Structural features: Pseudo-spherical C_{60} fullerene units (twelve 5- and twenty 6-membered rings; orientational disorder) and P_4 tetrahedra (partial orientational disorder) in an AlB_2 -type arrangement.

Locke I.W. et al. (1994) [1]

$P_{8.16}C_{60}$

$a = 1.00838$ nm, $c = 1.01048$ nm, $c/a = 1.002$, $V = 0.8898$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	12o	<i>.m.</i>	0.291	0.582	0.372	0.38	
P2	12o	<i>.m.</i>	0.594	0.188	0.467	0.3	
$(C_{60})_3$	1a	<i>6/mmm</i>	0	0	0		hexagonal prism P_{12}

Experimental: powder, diffractometer, X-rays, synchrotron, $R_B = 0.065$, $T = 300$ K

Remarks: Positions of P atoms and centers of C_{60} units determined. Short interatomic distances for partly occupied site(s). Refinement incorporating spherical shell functions for the description of disordered molecules. Space group (147) *P-3* (orientational ordering of the C_{60} units) was tested and rejected.

References: [1] Locke I.W., Darwish A.D., Kroto H.W., Prassides K., Taylor R., Walton D.R.M. (1994), Chem. Phys. Lett. 225, 186-190.

191
hP25

$\text{TaPb}_{0.24}(\text{O}_{0.75}\text{F}_{0.25})_{3.12}$	<i>hP25</i>	(191) <i>P6/mmm</i> – olgfb
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Pb_{0.24}Ta(O,F)_{3.12} [1]

Structural features: Ta(O,F)₆ octahedra share vertices to form an HTB-type framework; Pb and additional (O,F) in hexagonal channels parallel to [001].

Sälvborg Ö. (1985) [1]

$\text{F}_{0.78}\text{O}_{2.34}\text{Pb}_{0.24}\text{Ta}$

$a = 0.7548$, $c = 0.3941$ nm, $c/a = 0.522$, $V = 0.1944$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Pb1	12 <i>o</i>	. <i>m</i> .	0.0193	0.0387	0.0734	0.059	
M2	6 <i>l</i>	<i>mm2</i>	0.2108	0.4217	0		non-collinear Ta ₂
M3	3 <i>g</i>	<i>mmm</i>	1/2	0	1/2		collinear Ta ₂
Ta4	3 <i>f</i>	<i>mmm</i>	1/2	0	0		octahedron O ₆
M5	1 <i>b</i>	6/ <i>mmm</i>	0	0	1/2	0.36	

M2 = 0.75O + 0.25F; M3 = 0.75O + 0.25F; M5 = 0.75O + 0.25F

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

Remarks: We assigned an approximate value to the O/F ratio of sites M based on the nominal composition, assuming Pb(II) and Ta(V). Short interatomic distances for partly occupied site(s).

References: [1] Sälvborg Ö. (1985), J. Solid State Chem. 57, 160-165.

191
hP26

$\text{La}_{0.81}\text{Rh}_3\text{B}_2$	<i>hP26</i>	(191) <i>P6/mmm</i> – jihge ² ca
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La_{1-x}Rh₃B₂ [1]

Structural features: Kagomé-mesh Rh₃ layers and LaB₂ layers (a B hexagon mesh, most hexagons of which are centered by La atoms, in part displaced from the hexagon centers) alternate along [001]. Infinite columns of base-linked BRh₆ trigonal prisms share edges to form a 3D-framework; no B-B contact. Derivative of CeCo₃B₂ with partly ordered La vacancies and site splitting.

Ku H.C. et al. (1985) [1]

$\text{B}_2\text{La}_{0.81}\text{Rh}_3$

$a = 0.5642$, $c = 0.8546$ nm, $c/a = 1.515$, $V = 0.2356$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
La1	6 <i>j</i>	<i>m2m</i>	0.118	0	0	0.055	
Rh2	6 <i>i</i>	<i>2mm</i>	1/2	0	0.1637		coplanar square B ₄
B3	4 <i>h</i>	3. <i>m</i> .	1/3	2/3	0.331		trigonal prism Rh ₆
Rh4	3 <i>g</i>	<i>mmm</i>	1/2	0	1/2		coplanar square B ₄
La5	2 <i>e</i>	6 <i>mm</i>	0	0	0.2732	0.255	
La6	2 <i>e</i>	6 <i>mm</i>	0	0	0.324	0.669	
B7	2 <i>c</i>	-6 <i>m2</i>	1/3	2/3	0		trigonal prism Rh ₆
La8	1 <i>a</i>	6/ <i>mmm</i>	0	0	0	0.264	

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

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

References: [1] Ku H.C., Ma L.J., Tai M.F., Wang Y., Horng H.E. (1985), J. Less-Common Met. 109, 219-228.

191
hP26

$\text{La}_{0.9}\text{Ni}_{2.2}(\text{Ni}_{0.83}\text{Al}_{0.17})_3\text{H}_{4.5}$	<i>hP26</i>	(191) <i>P6/mmm</i> – mligeca
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LaNi_{4.5}Al_{0.5}H_{4.5} [1]

Structural features: Filled-up derivative of CaCu_5 (PrNi_2Al_3) with H in tetrahedral ($\text{La}_2(\text{Ni},\text{Al})_2$) and trigonal bipyramidal ($\text{La}_2\text{Ni}_2(\text{Ni},\text{Al})$) voids; partial disorder La/Ni₂ and splitting of the Ni site forming the hexagon mesh.

Crowder C. et al. (1982) [1]

$\text{Al}_{0.50}\text{D}_{4.55}\text{La}_{0.93}\text{Ni}_{4.63}$

$a = 0.5341$, $c = 0.4236$ nm, $c/a = 0.793$, $V = 0.1046$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	6 <i>m</i>	<i>mm2</i>	0.139	0.278	$\frac{1}{2}$	0.379	non-collinear D ₂
Ni2	6 <i>l</i>	<i>mm2</i>	0.29	0.58	0	0.022	
D3	6 <i>i</i>	2 <i>mm</i>	$\frac{1}{2}$	0	0.12	0.379	single atom D
M4	3 <i>g</i>	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		octahedron D ₆
Ni5	2 <i>e</i>	6 <i>mm</i>	0	0	0.31	0.066	
Ni6	2 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0	0.934	
La7	1 <i>a</i>	6/ <i>mmm</i>	0	0	0	0.934	

M4 = 0.833Ni + 0.167Al

Experimental: powder, diffractometer, neutrons, R = 0.041, T = 298 K

Remarks: We assigned approximate values to the Ni/Al ratio of site M4 and the site occupancies, based on the refined composition reported in [1]. Short interatomic distances for partly occupied site(s). Space group (157) *P31m*, proposed in [2], was tested and rejected (R = 0.045).

References: [1] Crowder C., James W.J., Yelon W. (1982), J. Appl. Phys. 53, 2637-2639. [2] Fischer P., Furrer A., Busch G., Schlapbach L. (1977), Helv. Phys. Acta 50, 421-430.

191
hP27

$\text{Ca}_7\text{Mg}_6\text{Si}_{14}$	<i>hP27</i>	(191) <i>P6/mmm</i> – mlk ² ca
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Ca₇Mg₆Si₁₄ [1]

Structural features: Infinite columns of base-linked SiMg_6Ca_3 tricapped trigonal prisms and columns where planar Si_{12} units (a Si_6 hexagon with an additional Si bonded to each atom) alternate with additional Ca atoms.

Zmii O.F., Gladyshevskii E.I. (1974) [1]

$\text{Ca}_7\text{Mg}_6\text{Si}_{14}$

$a = 1.271$, $c = 0.437$ nm, $c/a = 0.344$, $V = 0.6114$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	6 <i>m</i>	<i>mm2</i>	0.59	0.18	$\frac{1}{2}$		octahedron Si ₄ Mg ₂
Ca2	6 <i>l</i>	<i>mm2</i>	0.19	0.38	0		pseudo Frank-Kasper Si ₉ Mg ₄ Ca ₅
Si3	6 <i>k</i>	2 <i>m2</i>	0.19	0	$\frac{1}{2}$		coplanar triangle Si ₃
Si4	6 <i>k</i>	2 <i>m2</i>	0.37	0	$\frac{1}{2}$		coplanar triangle SiMg ₂

Si5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	tricapped trigonal prism Mg ₆ Ca ₃
Ca6	1a	6/mmm	0	0	0	pseudo Frank-Kasper Si ₁₂ Ca ₈

Experimental: single crystal, X-rays

Remarks: The composition was later corrected to Ca₇Mg_{7.5}Si₁₄ [2].

References: [1] Zmii O.F., Gladyshevskii E.I. (1974), Vses. Konf. Kristallokhim. Internet. Soeden., 2nd, L'vov 1974, Coll. Abstr. p. 23. [2] Nesper R., Currao A., Wengert S. (1998), Chem. Eur. J. 4, 2251-2257.

191
hP28

La(Fe _{0.2} Ni _{0.8}) ₅ H _{5.1}	hP28	(191) P6/mmm – nmhgca
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LaFeNi₄H_{5.1} [1]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (La₂(Ni,Fe)₂ and (Ni,Fe)₄) and trigonal bipyramidal (La₂(Ni,Fe)₃) voids.

Lamloumi J. et al. (1987) [1]

D_{5.06}FeLaNi₄

$a = 0.5376$, $c = 0.421$ nm, $c/a = 0.783$, $V = 0.1054$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	..m	0.475	0	0.09	0.21	
D2	6m	mm2	0.144	0.288	$\frac{1}{2}$	0.35	non-colinear D ₂
D3	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.382	0.11	single atom D
M4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
M5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		
La6	1a	6/mmm	0	0	0		24-vertex polyhedron D ₂₄

M4 = 0.8Ni + 0.2Fe; M5 = 0.8Ni + 0.2Fe

Experimental: powder, diffractometer, neutrons, R_B = 0.057

Remarks: Refinement using scattering lengths for Ni, occ(M4) = 0.980 and occ(M5) = 0.977. We assigned an approximate value to the Fe/Ni ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Lamloumi J., Percheron Guégan A., Lartigue C., Achard J.C., Jehanno G. (1987), J. Less-Common Met. 130, 111-122.

191
hP30

Lu ₅ Ni ₁₉ B ₆	hP30	(191) P6/mmm – i ² h ² ge ² ca
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Lu₅Ni₁₉B₆ [1]

Structural features: BNi₆ trigonal prisms share triangular faces and edges to form infinite triple slabs; no B-B contact. Ordering variant of CaCu₅ (intergrowth of CaCu₅- and CeCo₃B₂-type slabs in the ratio 2:3).

Kuz'ma Y.B. et al. (1985) [1]

B₆Lu₅Ni₁₉

$a = 0.4943$, $c = 1.7161$ nm, $c/a = 3.472$, $V = 0.3631$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	6i	2mm	$\frac{1}{2}$	0	0.082		13-vertex polyhedron B ₂ Ni ₇ Lu ₄
Ni2	6i	2mm	$\frac{1}{2}$	0	0.315		13-vertex polyhedron B ₂ Ni ₇ Lu ₄
Ni3	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.201		icosahedron Ni ₉ Lu ₃

B4	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.407	trigonal prism Ni ₆
Ni5	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$	rhombic dodecahedron B ₄ Ni ₆ Lu ₄
Lu6	2e	6mm	0	0	0.204	pseudo Frank-Kasper Ni ₁₈ Lu ₂
Lu7	2e	6mm	0	0	0.407	pseudo Frank-Kasper B ₆ Ni ₁₂ Lu ₂
B8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	trigonal prism Ni ₆
Lu9	1a	6/mmm	0	0	0	pseudo Frank-Kasper Ni ₁₂ B ₆ Lu ₂

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, R = 0.120

References: [1] Kuz'ma Y.B., Dub O.M., Chaban N.F. (1985), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1985(7), 36-39.

191
hP32

LaNi ₄ AlH _{4.8}	hP32	(191) P6/mmm – nmlgeca
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LaNi₄AlH_{4.8} [1]

Structural features: Filled-up derivative of CaCu₅ (PrNi₂Al₃) with H in tetrahedral (La₂(Ni,Al)₂) and trigonal bipyramidal (La₂Ni₂(Ni,Al)) voids; partial disorder La/Ni₂ and splitting of the Ni site forming the hexagon mesh.

Percheron Guégan A. et al. (1980) [1]

Al_{0.94}D_{4.79}La_{0.99}Ni_{4.08}

$a = 0.5313$, $c = 0.4242$ nm, $c/a = 0.798$, $V = 0.1037$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	..m	0.471	0	0.103	0.228	non-collinear D ₂
D2	6m	mm2	0.137	0.274	$\frac{1}{2}$	0.343	
Ni3	6l	mm2	0.283	0.566	0	0.007	
M4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
Ni5	2e	6mm	0	0	0.305	0.007	
Ni6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.979	
La7	1a	6/mmm	0	0	0	0.993	

M4 = 0.687Ni + 0.313Al

Experimental: powder, diffractometer, neutrons, R = 0.071, T = 293 K

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

References: [1] Percheron Guégan A., Lartigue C., Achard J.C., Germi P., Tasset F. (1980), J. Less-Common Met. 74, 1-12.

191
hP33

Ba ₉ Cu ₇ Cl ₂ O ₁₅	hP33	(191) P6/mmm – nmlgfda
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Ba₉Cu₇O₁₅Cl₂ [1]

Structural features: OBa₆ octahedra share vertices to form an HTB-type framework; Cu₇O₁₂ columns (O forms fused hexagonal prisms, Cu alternatively at the prism centers and at the centers of the six square prism faces) in channels parallel to [001]. See Fig. III.83.

Kipka R., Müller Buschbaum H. (1976) [1]

Ba₉Cl₂Cu₇O₁₅

$a = 1.1257$, $c = 0.5853$ nm, $c/a = 0.520$, $V = 0.6423$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12n	.m	0.25	0	0.283		non-colinear Cu ₂
Cu2	6m	mm2	0.131	0.262	1/2		non-coplanar square O ₄
Ba3	6l	mm2	0.207	0.414	0		trigonal prism O ₆
Ba4	3g	mmm	1/2	0	1/2		8-vertex polyhedron O ₆ Cl ₂
O5	3f	mmm	1/2	0	0		bicapped square antiprism Ba ₆ O ₄
Cl6	2d	-6m2	1/3	2/3	1/2		coplanar triangle Ba ₃
Cu7	1a	6/mmm	0	0	0		hexagonal prism O ₁₂

Transformation from published data: origin shift 0 0 1/2

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

Remarks: In table I of [1] the Wyckoff position of former O(II) is misprinted as 12b instead of 12n.

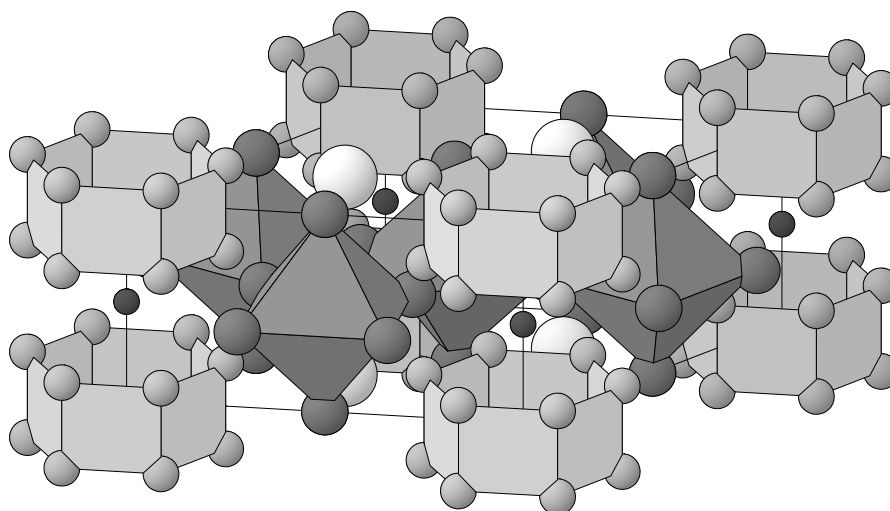


Fig. III.83. **Ba₉Cu₇O₁₅Cl₂**

Arrangement of CuO₄ squares (O atoms medium light), OBa₆ octahedra (Ba atoms medium dark), Cl (large) and additional Cu (small) atoms.

References: [1] Kipka R., Müller Buschbaum H. (1976), Z. Naturforsch. B 31, 1067-1069.

191
hP34

LaNi₂(Ni_{0.92}Al_{0.08})₃H_{3.6}

hP34

(191) *P6/mmm* – nmlhgea

LaNi_{4.75}Al_{0.25}H_x β [1]

Structural features: Filled-up derivative of CaCu₅ (PrNi₂Al₃) with H in tetrahedral (La₂Ni₂ and Ni₄) and trigonal prismatic (La₂Ni₃, partial Al substitution ignored) voids; partial disorder La/Ni₂ and splitting of the Ni site forming the hexagon mesh.

Du H. et al. (2003) [1]

Al_{0.12}D_{3.65}La_{0.99}Ni_{4.89}

a = 0.5375, *c* = 0.42 nm, *c/a* = 0.781, *V* = 0.1051 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	..m	0.483	0	0.0814	0.158	
D2	6m	mm2	0.139	0.278	$\frac{1}{2}$	0.246	non-collinear D ₂
Ni3	6l	mm2	0.3272	0.6544	0	0.333	
D4	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.396	0.069	
M5	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
Ni6	2e	6mm	0	0	0.286	0.007	
La7	1a	6/mmm	0	0	0	0.986	

M5 = 0.961Ni + 0.039Al

Experimental: powder, diffractometer, neutrons, R_p = 0.055

Remarks: Refinement on a sample of nominal composition LaNi_{4.75}Al_{0.25}D_{1.10}, containing 66 vol.% α-deuteride. Short interatomic distances for partly occupied site(s). Splitting of site Ni3 does not seem to be justified, however, the published standard uncertainty does not include the ideal value.

References: [1] Du H., Zhang W., Wang C., Han J., Yang Y., Chen B., Xie C., Sun K., Zhang B. (2003), Solid State Commun. 128, 157-161.

191
hP35

La(Mn _{0.4} Ni _{0.6}) ₅ H _{4.8}	hP35	(191) P6/mmm – nmlgfeca
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LaMn₂Ni₃H_{4.8} [1]

Structural features: Filled-up derivative of CaCu₅ (PrNi₂Al₃) with H in tetrahedral (La₂(Mn,Ni)₂ and LaNi₂(Mn,Ni)) and octahedral (La₂Ni₂(Mn,Ni)₂) voids; partial disorder La/Ni₂ and splitting of the site forming the hexagon mesh.

Percheron Guégan A. et al. (1980) [1]

D_{4.80}La_{0.98}Mn_{1.79}Ni_{3.24}

a = 0.5451, c = 0.4344 nm, c/a = 0.797, V = 0.1118 nm³, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12n	..m	0.455	0	0.118	0.142	
D2	6m	mm2	0.127	0.254	$\frac{1}{2}$	0.342	non-collinear D ₂
Ni3	6l	mm2	0.278	0.556	0	0.017	
M4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
D5	3f	mmm	$\frac{1}{2}$	0	0	0.347	
Ni6	2e	6mm	0	0	0.301	0.017	
M7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.949	
La8	1a	6/mmm	0	0	0	0.983	

M4 = 0.548Mn + 0.452Ni; M7 = 0.922Ni + 0.078Mn

Experimental: powder, diffractometer, neutrons, R = 0.079, T = 293 K

Remarks: The atom coordinates and occupancies of the metal atom sites were determined on an unhydrogenated sample. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). In table 3 of [1] the x-coordinate of the H site in Wyckoff position 12n is misprinted as 0.445 instead of 0.455 (see [2]).

References: [1] Percheron Guégan A., Lartigue C., Achard J.C., Germi P., Tasset F. (1980), J. Less-Common Met. 74, 1-12. [2] (1982), Structure Reports 46A, 70.

191
hP36

$\text{Co}_3\text{Ge}_2\text{Sb}$	<i>hP36</i>	(191) <i>P6/mmm</i> – okjihe
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Co₃Ge₂Sb [1]; Fe₃Ge₂Sb [2]

Structural features: Kagomé-mesh Co₉ layers alternate with $\square_2(\text{Sb}_2)\text{Ge}_6$ and $\square(\text{Sb}_2)_2\text{Ge}_6$ layers (a Ge hexagon mesh, the hexagons of which are either vacant or centered by a Sb₂ dumbbell perpendicular to the layer) along [001].

Mills A.M. et al. (1998) [1]

 $\text{Co}_3\text{Ge}_2\text{Sb}_{0.95}$ $a = 0.89128$, $c = 0.76312$ nm, $c/a = 0.856$, $V = 0.5250$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	12 <i>o</i>	<i>.m.</i>	0.16701	0.334	0.24288		bicapped square antiprism Ge ₄ Co ₄ Sb ₂
Ge2	6 <i>k</i>	<i>m2m</i>	0.31623	0	$\frac{1}{2}$		trigonal prism Co ₆
Ge3	6 <i>j</i>	<i>m2m</i>	0.34759	0	0		trigonal prism Co ₆
Co4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.2638		bicapped square antiprism Ge ₄ Co ₄ Sb ₂
Sb5	4 <i>h</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.31106	0.92	7-vertex polyhedron Co ₆ Sb
Sb6	2 <i>e</i>	<i>6mm</i>	0	0	0.1853		7-vertex polyhedron Co ₆ Sb

Experimental: single crystal, diffractometer, X-rays, $R = 0.039$, $T = 295$ K

References: [1] Mills A.M., Lam R., Mar A. (1998), Can. J. Chem. 76, 1588-1594. [2] Mills A.M., Mar A. (2000), J. Alloys Compd. 298, 82-92.

191
hP39

$\text{U}_{20}\text{Si}_{16}\text{C}_3$	<i>hP39</i>	(191) <i>P6/mmm</i> – nmlihfba
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U₂₀Si₁₆C₃ [2]

Structural features: SiU₆U₃ and SiU₆(USi₂) tricapped trigonal prisms share atoms to form a 3D-framework; C in octahedral (U₆) voids. Planar Si₆ rings and single Si atoms.

Pöttgen R. et al. (1993) [1]

 $\text{C}_3\text{Si}_{16}\text{U}_{20}$ $a = 1.0377$, $c = 0.8005$ nm, $c/a = 0.771$, $V = 0.7465$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	12 <i>n</i>	<i>.m</i>	0.229	0	0.246		non-colinear Si ₂
U2	6 <i>m</i>	<i>mm2</i>	0.2126	0.4252	$\frac{1}{2}$		7-capped pentagonal prism Si ₆ U ₁₁
U3	6 <i>l</i>	<i>mm2</i>	0.2152	0.4304	0		square antiprism C ₂ Si ₆
U4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.2862		single atom C
Si5	4 <i>h</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.252		tricapped trigonal prism U ₉
C6	3 <i>f</i>	<i>mmm</i>	$\frac{1}{2}$	0	0		octahedron U ₆
U7	1 <i>b</i>	<i>6/mmm</i>	0	0	$\frac{1}{2}$		pseudo Frank-Kasper Si ₁₂ U ₈
U8	1 <i>a</i>	<i>6/mmm</i>	0	0	0		pseudo Frank-Kasper Si ₁₂ U ₈

Experimental: single crystal, diffractometer, X-rays, $wR = 0.030$

Remarks: Refinement of the site occupancies showed no significant deviation from unity.

References: [1] Pöttgen R., Kaczorowski D., Jeitschko W. (1993), J. Mater. Chem. 3, 253-258. [2] Blum P.L., Silvestre G. (1966), C. R. Seances Acad. Sci., Ser. B 263, 709-711.

191
hP39

LiFe ₆ Ge ₆	hP39	(191) <i>P6/mmm</i> – okjiheda
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LiFe₆Ge₆ [1]

Structural features: Kagomé-mesh Fe₉ layers alternate with Li₂(Ge₂)Ge₆ and Li(Ge₂)₂Ge₆ layers (a Ge hexagon mesh, the hexagons of which are centered by a Li atom or a Ge₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks in the ratio 1:1.

Welk E., Schuster H.U. (1976) [1]

Fe₆Ge₆Li $a = 0.8744$, $c = 0.8033$ nm, $c/a = 0.919$, $V = 0.5319$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	12 <i>o</i>	. <i>m</i> .	0.166	0.332	0.254		icosahedron Ge ₆ Fe ₄ Li ₂
Ge2	6 <i>k</i>	<i>m2m</i>	0.333	0	$\frac{1}{2}$		pseudo Frank-Kasper Fe ₆ Ge ₅ Li ₂
Ge3	6 <i>j</i>	<i>m2m</i>	0.333	0	0		14-vertex Frank-Kasper Fe ₆ Ge ₇ Li
Fe4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.25		icosahedron Ge ₆ Fe ₄ Li ₂
Ge5	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1514		14-vertex Frank-Kasper Ge ₇ Fe ₆ Li
Ge6	2 <i>e</i>	6 <i>mm</i>	0	0	0.3486		14-vertex Frank-Kasper Ge ₇ Fe ₆ Li
Li7	2 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper Ge ₈ Fe ₁₂
Li8	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		pseudo Frank-Kasper Ge ₈ Fe ₁₂

Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.078$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Welk E., Schuster H.U. (1976), *Z. Anorg. Allg. Chem.* 424, 193-197.191
hP39

Ag ₄ EuIn ₈	hP39	(191) <i>P6/mmm</i> – okjiheda
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EuAg₄In₈ [2]

Structural features: Kagomé-mesh Ag₆In₃ layers alternate with Eu₂(In₂)In₆ and Eu(In₂)₂In₆ layers (an In hexagon mesh, the hexagons of which are centered by a Eu atom or an In₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks in the ratio 1:1. Ordering variant of LiFe₆Ge₆, Eu[Ag₄In₂]In₆.

Sysa L.V. et al. (1994) [1]

Ag₄EuIn₈ $a = 0.9925$, $c = 0.9727$ nm, $c/a = 0.980$, $V = 0.8298$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	12 <i>o</i>	. <i>m</i> .	0.167	0.334	0.2416		icosahedron Ag ₂ In ₈ Eu ₂
In2	6 <i>k</i>	<i>m2m</i>	0.3008	0	$\frac{1}{2}$		pseudo Frank-Kasper Ag ₄ In ₇ Eu ₂
In3	6 <i>j</i>	<i>m2m</i>	0.3469	0	0		14-vertex Frank-Kasper Ag ₄ In ₉ Eu
In4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.2764		icosahedron Ag ₄ In ₆ Eu ₂
In5	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1487		14-vertex Frank-Kasper In ₁₀ Ag ₃ Eu
In6	2 <i>e</i>	6 <i>mm</i>	0	0	0.3434		14-vertex Frank-Kasper Ag ₆ In ₇ Eu
Eu7	2 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper In ₁₄ Ag ₆
Eu8	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		pseudo Frank-Kasper In ₈ Ag ₁₂

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

Remarks: The same data are reported in [2].

References: [1] Sysa L.V., Kalychak Y.M., Stets' I.N., Galadzhun Y.V. (1994), Crystallogr. Rep. 39, 743-746 (Kristallografiya 39, 821-824). [2] Sysa L.V., Kalychak Y.M. (1992), Sov. Kristallokhim. Neorg. Koord. Soeden., 6th, L'vov 1992, Coll. Abstr. p. 234.

191
hP40

$\text{Cs}_3\text{Mo}[\text{SCN}]_6$	hP40	(191) $P6/mmm - o^3fa$
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$\text{Cs}_3\text{Mo}(\text{NCS})_6$ [1]

Structural features: $\text{Mo}(\text{NCS})_6$ octahedral units (MoN_6 octahedron in 2-fold rotational disorder about [001], NCS linear units) and Cs atoms in a simple hexagonal arrangement (MoCs_3 triangle mesh).

Delfs C.D. et al. (1989) [1]

$\text{C}_6\text{Cs}_3\text{MoN}_6\text{S}_6$

$a = 1.097$, $c = 0.5008$ nm, $c/a = 0.457$, $V = 0.5219$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12o	.m.	0.0923	0.1846	0.2263	0.5	single atom C
C2	12o	.m.	0.1465	0.293	0.3344	0.5	single atom N
S3	12o	.m.	0.22365	0.4473	0.4803	0.5	
Cs4	3f	mmm	$\frac{1}{2}$	0	0		
Mo5	1a	6/mmm	0	0	0		hexagonal prism N_{12}

Experimental: single crystal, diffractometer, X-rays, $R = 0.030$, $T = 295$ K

Remarks: Short interatomic distances for partly occupied site(s). Electron density studied on diffraction data collected at 115 K.

References: [1] Delfs C.D., Figgis B.N., Kucharski E.S., Reynolds P.A. (1989), J. Chem. Soc., Dalton Trans. 1989, 1779-1785.

191
hP40

$\text{La}(\text{Mn}_{0.08}\text{Co}_{0.15}\text{Ni}_{0.71}\text{Al}_{0.06})_5\text{H}_{5.57}$	hP40	(191) $P6/mmm - \text{onmhcga}$
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$\text{La}(\text{Ni}, \text{Co}, \text{Mn}, \text{Al})_5\text{H}_{5.57}$ [2]; $\text{LaNi}_{4.6}\text{Sn}_{0.4}\text{H}_{5.8}$ [3]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral (La_2M_2 , LaM_3 and M_4) and trigonal bipyramidal (La_2M_3) voids.

Georgiev P.A. et al. (2003) [1]

$\text{Al}_{0.30}\text{Ce}_{0.30}\text{Co}_{0.75}\text{D}_{4.83}\text{La}_{0.50}\text{Mn}_{0.40}\text{Nd}_{0.10}\text{Ni}_{3.55}\text{Pr}_{0.10}$

$a = 0.5333$, $c = 0.4248$ nm, $c/a = 0.797$, $V = 0.1046$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12o	.m.	0.2148	0.4296	0.2825	0.04	non-colinear D_2
D2	12n	..m	0.4768	0	0.0989	0.205	
D3	6m	mm2	0.1385	0.277	$\frac{1}{2}$	0.305	tetrahedron D_4
D4	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.389	0.016	tetrahedron D_4
M5	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
M6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		

M7	1a	6/ <i>mmm</i>	0	0	0	hexagonal prism D ₁₂
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$$\text{M5} = 0.71\text{Ni} + 0.15\text{Co} + 0.08\text{Mn} + 0.06\text{Al}; \text{M6} = 0.71\text{Ni} + 0.15\text{Co} + 0.08\text{Mn} + 0.06\text{Al}; \text{M7} = 0.5\text{La} + 0.3\text{Ce} + 0.1\text{Nd} + 0.1\text{Pr}$$

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_p = 0.033$

Remarks: We assigned approximate values to the cation ratios of sites M based on the nominal composition given as $\text{LaMMNi}_{3.55}\text{Co}_{0.75}\text{Mn}_{0.4}\text{Al}_{0.3}\text{D}_{5.1}$, where $\text{LaMM} = (\text{La}, \text{Ce}, \text{Nd}, \text{Pr})$. Short interatomic distances for partly occupied site(s).

References: [1] Georgiev P.A., Liu J., Ross D.K., Andersen K.H., Otto A. (2003), *J. Alloys Compd.* 349, 325-333. [2] Latroche M., Rodriguez Carvajal J., Percheron Guégan A., Bourée Vigneron F. (1995), *J. Alloys Compd.* 218, 64-72. [3] Joubert J.M., Latroche M., Cerny R., Bowman R.C., Yvon K., Percheron Guégan A. (1999), *J. Alloys Compd.* 293/295, 124-129.

191
hP41

Ba₇Cd₃₁ *hP*41 (191) *P*6/*mmm* – omjijhgec

BaCd_{4.43} [1]

Structural features: Ba₂(Ba₂)Cd₉ layers (a Cd hexagon mesh, the hexagons of which are centered by a Ba atom or a Ba₂ dumbbell perpendicular to the layer) and Ba₃Cd₃ layers (a Ba Kagomé mesh, the hexagons of which are centered by a Cd₃ triangle); additional Cd between the layers.

Bruzzone G., Fornasini M.L. (1974) [1]

Ba₇Cd₃₁
$$a = 1.0740, c = 1.0200 \text{ nm}, c/a = 0.950, V = 1.0189 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	12 <i>o</i>	<i>.m.</i>	0.1852	0.3704	0.2604	0.5	pentagonal pyramid Cd ₆
Cd2	6 <i>m</i>	<i>mm</i> 2	0.1038	0.2076	1/2		non-colinear Cd ₂
Cd3	6 <i>j</i>	<i>m</i> 2 <i>m</i>	0.2708	0	0		icosahedron Cd ₈ Ba ₄
Cd4	6 <i>i</i>	2 <i>mm</i>	1/2	0	0.1619		icosahedron Cd ₉ Ba ₃
Cd5	4 <i>h</i>	3 <i>m.</i>	1/3	2/3	0.3499		pseudo Frank-Kasper Cd ₇ Ba ₄
Ba6	3 <i>g</i>	<i>mmm</i>	1/2	0	1/2		18-vertex polyhedron Cd ₁₈
Ba7	2 <i>e</i>	6 <i>mm</i>	0	0	0.2135		pseudo Frank-Kasper Cd ₁₈ Ba
Ba8	2 <i>c</i>	-6 <i>m</i> 2	1/3	2/3	0		pseudo Frank-Kasper Cd ₂₀

Experimental: single crystal, precession photographs, X-rays, R = 0.146

Remarks: Short interatomic distances for partly occupied site(s). Additional reflections could be indexed with an 8-fold supercell (new axes 2a,2b,2c).

References: [1] Bruzzone G., Fornasini M.L. (1974), *Acta Crystallogr. B* 30, 317-319.

191
hP41

La(Ni_{0.8}Al_{0.2})₅H₄ *hP41* (191) *P6/mmm* – onmgfeca

LaNi₄AlH₄ [1]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral $(\text{La}_2(\text{Ni},\text{Al})_2)$ and $\text{La}(\text{Ni},\text{Al})_3$ and octahedral $(\text{La}_2(\text{Ni},\text{Al})_4)$ voids; partial disorder La/Ni_2 .

Achard J.C. et al. (1979) [1]

$$\text{Al}_{1.06}\text{D}_{5.10}\text{La}_{0.98}\text{Ni}_{3.99}$$
$$a = 0.531, c = 0.4249 \text{ nm}, c/a = 0.8, V = 0.1038 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12o	.m.	0.233	0.466	0.34	0.038	single atom D
D2	12n	..m	0.438	0	0.112	0.22	
D3	6m	mm2	0.132	0.264	$\frac{1}{2}$	0.313	tetrahedron D ₄
M4	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		square prism (cube) D ₈
D5	3f	mmm	$\frac{1}{2}$	0	0	0.043	
Ni6	2e	6mm	0	0	0.31	0.024	8-vertex polyhedron LaD ₆ Ni
M7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle D ₃
La8	1a	6/mmm	0	0	0	0.976	

M4 = 0.6867Ni + 0.3133Al; M7 = 0.94Ni + 0.06Al

Experimental: powder, diffractometer, neutrons, R = 0.025

Remarks: The z-coordinate of the Ni site in Wyckoff position 2e is omitted in [1], we took an approximate value from the literature. Short interatomic distances for partly occupied site(s). In table II of [1] the H content from the refinement is misprinted as 4.8 instead of 5.1 atoms per formula unit.

References: [1] Achard J.C., Givord F., Percheron Guégan A., Soubeyroux J.L., Tasset F. (1979), J. Phys. (Paris) 40, 218-220.

191
hP42

Ca ₇ Mg _{7.52} Si ₁₄	hP42	(191) P6/mmm – m ² l ² k ² fca
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Ca₇Mg_{7.52}Si₁₄ [1]

Structural features: Infinite columns of base-linked SiMg₆Ca₃ tricapped trigonal prisms and columns where planar Si₁₂ units (a Si₆ hexagon with an additional Si bonded to each atom) alternate with additional Ca atoms.

Nesper R. et al. (1998) [1]

Ca₇Mg_{7.52}Si₁₄

$a = 1.2696$, $c = 0.44025$ nm, $c/a = 0.347$, $V = 0.6146$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	6m	mm2	0.2716	0.5432	$\frac{1}{2}$	0.178	
Mg2	6m	mm2	0.5891	0.1782	$\frac{1}{2}$	0.591	
Ca3	6l	mm2	0.1819	0.3638	0		
Mg4	6l	mm2	0.5317	0.0634	0	0.409	
Si5	6k	m2m	0.182	0	$\frac{1}{2}$		coplanar triangle Si ₃
Si6	6k	m2m	0.3648	0	$\frac{1}{2}$		
Mg7	3f	mmm	$\frac{1}{2}$	0	0	0.15	
Si8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		
Ca9	1a	6/mmm	0	0	0		hexagonal prism Si ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.042, T = 298 K

Remarks: Short interatomic distances for partly occupied site(s). Supersedes a refinement for so-called Ca₇Mg₆Si₁₄ in [2].

References: [1] Nesper R., Currao A., Wengert S. (1998), Chem. Eur. J. 4, 2251-2257. [2] Zmii O.F., Gladyshevskii E.I. (1974), Vses. Konf. Kristallokhim. Intermet. Soeden., 2nd, L'vov 1974, Coll. Abstr. p. 23.

191
hP42

$\text{Zn}_{11.78}\text{Sm}_{1.11}$	<i>hP42</i>	(191) <i>P6/mmm</i> – okjihedcba
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SmZn₁₁ ht [1]

Structural features: Kagomé-mesh Zn₃ layers alternate with (Sm,Zn₂)Zn₂ layers (a Zn hexagon mesh, the hexagons of which are centered by a Sm atom or a Zn₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (partial disorder).

Mason J.T. et al. (1970) [1]

 $\text{Sm}_{1.11}\text{Zn}_{11.77}$ $a = 0.8974$, $c = 0.8918$ nm, $c/a = 0.994$, $V = 0.6220$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	12 <i>o</i>	. <i>m</i> .	0.1671	0.3342	0.2585		bicapped square prism Zn ₁₀
Zn2	6 <i>k</i>	<i>m2m</i>	0.3552	0	$\frac{1}{2}$		
Zn3	6 <i>j</i>	<i>m2m</i>	0.2944	0	0		
Zn4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.2258		bicapped square prism Zn ₁₀
Zn5	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3543	0.85	
Zn6	2 <i>e</i>	6 <i>mm</i>	0	0	0.1456	0.96	
Sm7	2 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.15	
Sm8	2 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		pseudo Frank-Kasper Zn ₂₀
Sm9	1 <i>b</i>	6/ <i>mmm</i>	0	0	$\frac{1}{2}$		pseudo Frank-Kasper Zn ₂₀
Sm10	1 <i>a</i>	6/ <i>mmm</i>	0	0	0	0.04	

Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.056$

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

References: [1] Mason J.T., Harsha K.S.S., Chiotti P. (1970), Acta Crystallogr. B 26, 356-361.

191
hP45

$\text{Cr}_{0.8}\text{Fe}_{5.3}\text{Ge}_{5.2}\text{Sb}_{0.8}$	<i>hP45</i>	(191) <i>P6/mmm</i> – okjih ² e ² da
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Cr_{0.8}Fe_{5.3}Ge_{5.2}Sb_{0.8} [1]

Structural features: Idealized, Kagomé-mesh Fe₉ layers (some hexagons centered by a Ge atom) alternate with Cr₂(Sb₂)Ge₆ and Cr(Sb₂)₂Ge₆ layers (a Ge hexagon mesh, the hexagons of which are centered by a Cr atom or a Sb₂ dumbbell perpendicular to the layer) along [001].

Mills A.M. et al. (2001) [1]

 $\text{Cr}_{0.81}\text{Fe}_{5.34}\text{Ge}_{5.16}\text{Sb}_{0.84}$ $a = 0.88504$, $c = 0.80246$ nm, $c/a = 0.907$, $V = 0.5444$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>o</i>	. <i>m</i> .	0.168	0.336	0.25374		
Ge2	6 <i>k</i>	<i>m2m</i>	0.34356	0	$\frac{1}{2}$		trigonal prism Fe ₆
Ge3	6 <i>j</i>	<i>m2m</i>	0.31992	0	0		trigonal prism Fe ₆
M4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.24288		
M5	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1737	0.66	
Ge6	4 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2523	0.338	
Ge7	2 <i>e</i>	6 <i>mm</i>	0	0	0.259	0.15	
M8	2 <i>e</i>	6 <i>mm</i>	0	0	0.3231	0.86	
Cr9	2 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.14	colinear Ge ₂

Cr₁₀ 1a 6/*mmm* 0 0 0 0.16 colinear Ge₂

M1 = 0.89Fe + 0.11Cr; M4 = 0.89Fe + 0.11Cr; M5 = 0.545Sb + 0.455Ge; M8 = 0.628Sb + 0.372Ge

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 295 K

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

References: [1] Mills A.M., Anderson E.J., Mar A. (2001), J. Alloys Compd. 322, 103-112.

191
hP45

Zn _{11.74} U _{1.13}	hP45	(191) <i>P6/mmm</i> – okjih ² edca
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UZn₁₂ [1]

Structural features: Kagomé-mesh Zn₃ layers alternate with (U,Zn₂)Zn₂ layers (a Zn hexagon mesh, the hexagons of which are centered by a U atom or a Zn₂ dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu₅- and Zr₄Al₃-type blocks (partial disorder).

Mason J.T., Chiotti P. (1971) [1]

U_{1.13}Zn_{11.75}

$a = 0.895$, $c = 0.8902$ nm, $c/a = 0.995$, $V = 0.6175$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	12 <i>o</i>	. <i>m</i> .	0.1683	0.3366	0.2390		11-vertex polyhedron Zn ₁₁
Zn2	6 <i>k</i>	<i>m2m</i>	0.2953	0	$\frac{1}{2}$		icosahedron Zn ₁₀ U ₂
Zn3	6 <i>j</i>	<i>m2m</i>	0.355	0	0		tricapped trigonal prism Zn ₇ U ₂
Zn4	6 <i>i</i>	<i>2mm</i>	$\frac{1}{2}$	0	0.2753		icosahedron Zn ₁₂
Zn5	4 <i>h</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1472	0.76	
Zn6	4 <i>h</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.3492	0.05	
Zn7	2 <i>e</i>	6 <i>mm</i>	0	0	0.3537		14-vertex Frank-Kasper Zn ₁₃ U
U8	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.95	
U9	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.24	
U10	1 <i>a</i>	6/ <i>mmm</i>	0	0	0		pseudo Frank-Kasper Zn ₂₀

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

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

References: [1] Mason J.T., Chiotti P. (1971), Acta Crystallogr. B 27, 1789-1792.

191
hP45

La(Mn _{0.2} Ni _{0.8}) ₅ H ₆	hP45	(191) <i>P6/mmm</i> – onmhgfeca
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LaMnNi₄H₆ [1]

Structural features: Filled-up derivative of CaCu₅ with H in tetrahedral (La₂(Ni,Mn)₂, La(Ni,Mn)₃ and (Ni,Mn)₄) and trigonal bipyramidal (La₂(Ni,Mn)₃) voids; partial disorder La/Ni₂.

Achard J.C. et al. (1979) [1]

D_{5.96}La_{0.98}Mn_{0.95}Ni_{4.10}

$a = 0.5437$, $c = 0.4332$ nm, $c/a = 0.797$, $V = 0.1109$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	12 <i>o</i>	. <i>m</i> .	0.227	0.454	0.38	0.085	non-coplanar triangle D ₃
D2	12 <i>n</i>	.. <i>m</i>	0.452	0	0.117	0.175	

D3	6m	mm2	0.133	0.266	$\frac{1}{2}$	0.32	non-colinear D ₂
D4	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.38	0.082	4-vertex polyhedron D ₄
M5	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		square prism (cube) D ₈
D6	3f	mmm	$\frac{1}{2}$	0	0	0.196	
Ni7	2e	6mm	0	0	0.31	0.021	8-vertex polyhedron LaD ₆ Ni
M8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		coplanar triangle D ₃
La9	1a	6/mmm	0	0	0	0.98	

M5 = 0.885Ni + 0.115Mn; M8 = 0.70Ni + 0.30Mn

Experimental: powder, diffractometer, neutrons, R = 0.081

Remarks: The z-coordinate of the Ni site in Wyckoff position 2e is omitted in [1], we took an approximate value from the literature. Short interatomic distances for partly occupied site(s).

References: [1] Achard J.C., Givord F., Percheron Guégan A., Soubeyroux J.L., Tasset F. (1979), J. Phys. (Paris) 40, C5 218-220.

191
hP48

Ta_{0.36}O_{0.52} hP48 (191) P6/mmm – oli²hgfe²cba

TaO_x δ'(II) [1]

Structural features: Mixed Ta-O layers alternate with O layers along [001].

Khitrova V.I., Klechkovskaya V.V. (1980) [1]

O_{0.52}Ta_{0.36}

a = 0.716, c = 1.152 nm, c/a = 1.609, V = 0.5115 nm³, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12o	.m.	0.16667	0.33333	0.33333	0.10	
O2	6l	mm2	0.16667	0.33333	0	0.15	
O3	6i	2mm	$\frac{1}{2}$	0	0.16667	0.15	colinear Ta ₂
Ta4	6i	2mm	$\frac{1}{2}$	0	0.33333	0.45	8-vertex polyhedron O ₈
O5	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.33333	0.25	
O6	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$	0.10	colinear Ta ₂
Ta7	3f	mmm	$\frac{1}{2}$	0	0	0.10	8-vertex polyhedron O ₈
O8	2e	6mm	0	0	0.16667	0.40	colinear Ta ₂
Ta9	2e	6mm	0	0	0.33333	0.15	8-vertex polyhedron O ₈
O10	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.30	
O11	1b	6/mmm	0	0	$\frac{1}{2}$	0.50	colinear Ta ₂
Ta12	1a	6/mmm	0	0	0		8-vertex polyhedron O ₈

Experimental: thin film, electron diffraction, R = 0.167

Remarks: Idealized coordinates. Short interatomic distances: d(Ta4-Ta12) = 0.207 nm. The same atom sites are occupied in so-called TaO_x δ'(III).

References: [1] Khitrova V.I., Klechkovskaya V.V. (1980), Sov. Phys. Crystallogr. 25, 669-672 (Kristallografiya 25, 1169-1175).

191
hP48

La(Mn_{0.07}Ni_{0.93})₅H_{6.6} hP48 (191) P6/mmm – onmlhgeca

LaMn_{0.34}Ni_{4.72}H_{6.6} [1]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral ($\text{La}_2(\text{Ni},\text{Mn})_2$, $\text{La}(\text{Ni},\text{Mn})_3$ and $(\text{Ni},\text{Mn})_4$) and trigonal bipyramidal ($\text{La}_2(\text{Ni},\text{Mn})_3$) voids; partial disorder La/Ni_2 and splitting of the site forming the hexagon mesh.

Percheron Guégan A. et al. (1980) [1]

$\text{D}_{6,62}\text{La}_{0,99}\text{Mn}_{0,31}\text{Ni}_{4,71}$

$a = 0.5392$, $c = 0.4296$ nm, $c/a = 0.797$, $V = 0.1082$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12o	.m.	0.225	0.45	0.316	0.107	non-colinear D_2
D2	12n	.m	0.466	0	0.102	0.232	
D3	6m	mm2	0.138	0.276	$\frac{1}{2}$	0.368	tetrahedron D_4
Ni4	6l	mm2	0.285	0.57	0	0.011	
D5	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.408	0.085	tetrahedron D_4
M6	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		
Ni7	2e	6mm	0	0	0.31	0.011	
M8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.967	
La9	1a	6/mmm	0	0	0	0.989	

$\text{M6} = 0.915\text{Ni} + 0.085\text{Mn}$; $\text{M8} = 0.970\text{Ni} + 0.030\text{Mn}$

Experimental: powder, diffractometer, neutrons, $R = 0.059$, $T = 293$ K

Remarks: The positional coordinates and occupancies of the metal atom sites were determined on an unhydrogenated sample. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). In table 1 of [1] the normalized composition of the alloy is misprinted as $\text{LaNi}_{4,76}\text{Mn}_{0,92}$ instead of $\text{LaNi}_{4,76}\text{Mn}_{0,32}$; in table 3 the refined composition of the deuteride is misprinted as $\text{La}_{0,99}\text{Ni}_{4,68}\text{Mn}_{0,34}\text{D}_{6,60}$ instead of $\text{La}_{0,99}\text{Ni}_{4,71}\text{Mn}_{0,32}\text{D}_{6,60}$.

References: [1] Percheron Guégan A., Lartigue C., Achard J.C., Germi P., Tasset F. (1980), J. Less-Common Met. 74, 1-12.

191
hP50

$\text{La}_{13}\text{Ga}_8\text{Sb}_{21}$	hP50	(191) $P6/mmm - \text{nm}^2\text{lkjhfa}$
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$\text{La}_{13}\text{Ga}_8\text{Sb}_{21}$ [1]

Structural features: Columns of directly superposed Ga_6 rings are interconnected via Sb bands (5-atom broad square mesh) to form a 3D-framework; La_6GaSb_3 columns (a central column of base-linked GaLa_6 trigonal prisms sharing rectangular faces with three surrounding columns of base-linked SbLa_6 trigonal prisms) in large channels parallel to [001].

Mills A.M., Mar A. (2000) [1]

$\text{Ga}_{7,56}\text{La}_{12,86}\text{Sb}_{21}$

$a = 1.7657$, $c = 0.43378$ nm, $c/a = 0.246$, $V = 1.1712$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	12n	.m	0.1343	0	0.443	0.471	
La2	6m	mm2	0.168	0.336	$\frac{1}{2}$		
La3	6m	mm2	0.58274	0.16547	$\frac{1}{2}$		
Sb4	6l	mm2	0.24818	0.49636	0		
Sb5	6k	m2m	0.37508	0	$\frac{1}{2}$		square prism (cube) Sb_4La_4
Sb6	6j	m2m	0.24697	0	0		
Ga7	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0663	0.478	
Sb8	3f	mmm	$\frac{1}{2}$	0	0		square prism (cube) Sb_4La_4

La9	1a	6/ <i>mmm</i>	0	0	0	0.859
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Experimental: single crystal, diffractometer, X-rays, R = 0.034, T = 295 K

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

References: [1] Mills A.M., Mar A. (2000), *Inorg. Chem.* 39, 4599-4607.

191
hP51

LaNi ₅ H _{6.5}	<i>hP51</i>	(191) <i>P6/mmm</i> – onmlhgfeca
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LaNi_{5.13}H_{6.5} [1]

Structural features: Filled-up derivative of CaCu_5 with H in tetrahedral (La_2Ni_2 , LaNi_3 and Ni_4) and octahedral (La_2Ni_4) voids; partial disorder La/ Ni_2 and splitting of the Ni site forming the hexagon mesh.

Percheron Guégan A. et al. (1980) [1]

D_{6.50}La_{0.98}Ni_{5.03}
$$a = 0.5399, c = 0.429 \text{ nm}, c/a = 0.795, V = 0.1083 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12 <i>o</i>	<i>.m.</i>	0.204	0.408	0.354	0.108	single atom D
D2	12 <i>n</i>	<i>.m</i>	0.455	0	0.117	0.178	
D3	6 <i>m</i>	<i>mm2</i>	0.136	0.272	$\frac{1}{2}$	0.318	non-colinear D ₂
Ni4	6 <i>l</i>	<i>mm2</i>	0.287	0.574	0	0.017	
D5	4 <i>h</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.369	0.13	tetrahedron D ₄
Ni6	3 <i>g</i>	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		
D7	3 <i>f</i>	<i>mmm</i>	$\frac{1}{2}$	0	0	0.213	
Ni8	2 <i>e</i>	6 <i>mm</i>	0	0	0.313	0.017	
Ni9	2 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0	0.949	
La10	1 <i>a</i>	6/ <i>mmm</i>	0	0	0	0.983	

Experimental: powder, diffractometer, neutrons, $R = 0.073$, $T = 293$ K

Remarks: The positional coordinates and occupancies of the metal atom sites were determined on an unhydrogenated sample. Short interatomic distances for partly occupied site(s). A model in space group (186) $P6_3mc$ with double c -parameter was later proposed by the same authors [2].

References: [1] Percheron Guégan A., Lartigue C., Achard J.C., Germi P., Tasset F. (1980), *J. Less-Common Met.* 74, 1-12. [2] Lartigue C., Percheron Guégan A., Achard J.C., Soubeyroux J.L. (1985), *J. Less-Common Met.* 113, 127-148.

191
hP52

ScNi ₆ Ge ₆	<i>hP52</i>	(191) <i>P6/mmm</i> – onmligedca
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ScNi₆Ge₆ [1]

Structural features: Kagomé-mesh Ni_9 layers alternate with $\text{Sc}_2(\text{Ge}_2)\text{Ge}_6$ and $\text{Sc}(\text{Ge}_2)_2\text{Ge}_6$ layers (a Ge hexagon mesh, the hexagons of which are centered by a Sc atom or a Ge_2 dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu_5 - and Zr_4Al_3 -type blocks in the ratio 1:1.

Buchholz W., Schuster H.U. (1981) [1]

Ge₆Ni₆Sc
$$a = 1.0152, c = 0.7813 \text{ nm}, c/a = 0.770, V = 0.6974 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12o	.m.	0.247	0.494	0.25		icosahedron Ge ₆ Ni ₄ Sc ₂
Ni2	12n	..m	0.238	0	0.258		icosahedron Ge ₆ Ni ₄ Sc ₂
Ge3	6m	mm2	0.162	0.324	1/2		pseudo Frank-Kasper Ni ₆ Ge ₅ Sc ₂
Ge4	6l	mm2	0.16	0.32	0		14-vertex Frank-Kasper Ni ₆ Ge ₇ Sc
Ge5	6i	2mm	1/2	0	0.158		14-vertex Frank-Kasper Ge ₇ Ni ₆ Sc
Sc6	3g	mmm	1/2	0	1/2		pseudo Frank-Kasper Ge ₈ Ni ₁₂
Ge7	2e	6mm	0	0	0.34		14-vertex Frank-Kasper Ni ₆ Ge ₇ Sc
Ge8	2d	-6m2	1/3	2/3	1/2		icosahedron Ni ₆ Sc ₃ Ge ₃
Ge9	2c	-6m2	1/3	2/3	0		15-vertex Frank-Kasper Ni ₆ Ge ₉
Sc10	1a	6/mmm	0	0	0		pseudo Frank-Kasper Ge ₈ Ni ₁₂

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Buchholz W., Schuster H.U. (1981), Z. Anorg. Allg. Chem. 482, 40-48.

191
hP55

Ta _{2.32} O _{7.40}	hP55	(191) P6/mmm – oli ³ hgfe ³ ca
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TaO_x δ'(I) [1]

Structural features: Mixed Ta-O layers alternate with O layers along [001].

Khitrova V.I., Klechkovskaya V.V. (1980) [1]

O_{7.40}Ta_{2.32}

$a = 0.716$, $c = 1.152$ nm, $c/a = 1.609$, $V = 0.5115$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12o	.m.	0.16667	0.33333	0.33333	0.15	
O2	6l	mm2	0.16667	0.33333	0	0.15	
O3	6i	2mm	1/2	0	0.1	0.15	
O4	6i	2mm	1/2	0	0.233	0.15	
Ta5	6i	2mm	1/2	0	0.33333	0.12	
O6	4h	3m.	1/3	2/3	0.33333	0.20	
O7	3g	mmm	1/2	0	1/2	0.20	colinear Ta ₂
Ta8	3f	mmm	1/2	0	0	0.10	
O9	2e	6mm	0	0	0.16667	0.20	colinear Ta ₂
Ta10	2e	6mm	0	0	0.33333	0.15	
O11	2e	6mm	0	0	0.433	0.25	
O12	2c	-6m2	1/3	2/3	0	0.30	
Ta13	1a	6/mmm	0	0	0		8-vertex polyhedron O ₈

Experimental: thin film, electron diffraction, R = 0.207

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

References: [1] Khitrova V.I., Klechkovskaya V.V. (1980), Sov. Phys. Crystallogr. 25, 669-672 (Kristallografiya 25, 1169-1175).

191
hP55

Ag ₇ Te ₄	hP55	(191) P6/mmm – qonlkfec
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Ag₇Te₄ [1]

Structural features: Te forms infinite columns where planar Te₆ rings are interconnected via bridging Te atoms; additional Te at longer distances between the columns.

Imamov R.M., Pinsker Z.G. (1966) [1]

Ag₇Te₄

$a = 1.348$, $c = 0.849$ nm, $c/a = 0.630$, $V = 1.3360$ nm³, $Z = 5$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12 q	$m..$	0.120	0.454	$\frac{1}{2}$		8-vertex polyhedron Te ₃ Ag ₅
Ag2	12 o	$.m.$	0.237	0.474	0.181		7-vertex polyhedron Te ₃ Ag ₄
Te3	12 n	$..m$	0.330	0	0.181		9-vertex polyhedron Ag ₇ Te ₂
Ag4	6 l	$mm2$	0.125	0.250	0		10-vertex polyhedron Te ₄ Ag ₆
Te5	6 k	$m2m$	0.217	0	$\frac{1}{2}$		octahedron Ag ₂ Te ₄
Ag6	3 f	mmm	$\frac{1}{2}$	0	0		coplanar square Te ₄
Ag7	2 e	$6mm$	0	0	0.181		pseudo Frank-Kasper Ag ₇ Te ₁₂
Te8	2 c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Ag ₆

Experimental: thin film, electron diffraction, $R = 0.232$

Remarks: In Table 1 of [1] the y -coordinates of former Ag(II) and Ag(III) are misprinted as 0 instead of $2x$ (agreement with Wyckoff positions 12 o and 6 l , respectively; checked on the drawing in fig. 9). A refinement in space group (189) $P-62m$ with a 2-fold supercell was reported for so-called Ag_{11.67}Te₇ in [2].

References: [1] Imamov R.M., Pinsker Z.G. (1966), Sov. Phys. Crystallogr. 11, 182-188 (Kristallografiya 11, 182-190). [2] Peters J., Conrad O., Bremer B., Krebs B. (1996), Z. Anorg. Allg. Chem. 622, 1823-1832.

191
hP57

LaMn₃Ni₂H_{5.6}

hP57

(191) $P6/mmm$ – pomlkjgfd

LaMn₃Ni₂H_{5.6} [1]

Structural features: Filled-up derivative of YNi₂Al₃ with H in octahedral (La₂Mn₄), tetrahedral (La₂Mn₂, La₂NiMn and LaMn₂Ni) and square pyramidal (LaMn₂Ni₂) voids.

Guénée L., Yvon K. (2003) [1]

D_{5.64}LaMn₃Ni₂

$a = 0.98379$, $c = 0.43038$ nm, $c/a = 0.437$, $V = 0.3607$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12 p	$m..$	0.2079	0.5404	0	0.431	non-colinear D ₂
D2	12 o	$.m.$	0.2019	0.4038	0.357	0.246	single atom D
D3	6 m	$mm2$	0.068	0.136	$\frac{1}{2}$	0.288	non-colinear D ₂
Ni4	6 l	$mm2$	0.1847	0.3694	0		octahedron D ₆
Mn5	6 k	$m2m$	0.2856	0	$\frac{1}{2}$		tricapped trigonal prism D ₉
D6	6 j	$m2m$	0.2542	0	0	0.68	non-colinear Ni ₂
D7	3 g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		coplanar square Mn ₄
Mn8	3 f	mmm	$\frac{1}{2}$	0	0		coplanar square D ₄
La9	2 d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		21-vertex polyhedron D ₂₁
La10	1 a	$6/mmm$	0	0	0		sixcapped hexagonal prism D ₁₈

Experimental: powder, diffractometer, neutrons, $R_B = 0.057$

References: [1] Guénée L., Yvon K. (2003), J. Alloys Compd. 348, 176-183.

191
hP63

YbGa _{2.64}	hP63	(191) <i>P6/mmm</i> – o ³ mlkjda
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YbGa_{2.64} [1]

Structural features: Hexagon-mesh Ga₁₈ layers alternate with Yb₇(Ga₃)₂ and Yb₈(Ga₃) layers (the Yb atoms and the centers of coplanar Ga₃ triangles in partial orientational disorder form a triangle mesh) along [001] (partial vacancies ignored). Derivative of AlB₂ with part of the Yb atoms replaced by Ga₃ triangles.

Cirafici S., Fornasini M.L. (1990) [1]

Ga_{2.63}Yb_{0.99}

$a = 1.3025$, $c = 0.836$ nm, $c/a = 0.642$, $V = 1.2283$ nm³, $Z = 15$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	12o	.m.	0.1118	0.2236	0.201		4-vertex polyhedron Ga ₄
Ga2	12o	.m.	0.223	0.446	0.244	0.62	coplanar triangle Ga ₃
Ga3	12o	.m.	0.555	0.110	0.265		4-vertex polyhedron Ga ₄
Ga4	6m	mm2	0.067	0.134	$\frac{1}{2}$	0.50	
Ga5	6l	mm2	0.603	0.206	0	0.84	tetrahedron Ga ₄
Yb6	6k	m2m	0.3367	0	$\frac{1}{2}$		
Yb7	6j	m2m	0.348	0	0		
Yb8	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		hexagonal prism Ga ₁₂
Yb9	1a	6/mmm	0	0	0	0.86	hexagonal prism Ga ₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.080

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

References: [1] Cirafici S., Fornasini M.L. (1990), J. Less-Common Met. 163, 331-338.

191
hP88

Ba ₆ (Ti _{0.25} Mn _{0.70} Fe _{0.05}) ₃ Si ₆ Cl _{4.5} O ₁₈ (O _{0.5} [OH] _{0.5})([OH] _{0.5} [H ₂ O] _{0.5}) _{3.5}	hP88	(191) <i>P6/mmm</i> – ro ² ml ² kjide
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[(Mn,Ti,Fe)₆(Si₄O₁₂)₃(OH,O)₂][Ba₁₂(OH,H₂O)₇Cl]₉ [1], verplanckite

Structural features: Units of three apex-linked (Mn,Ti,Fe)O₅ square pyramids share vertices with rings of four vertex-linked SiO₄ tetrahedra to form a 3D-framework; Ba and Cl in large channels parallel to [001].

Kampf A.R. et al. (1973) [1]

Ba₆Cl_{4.60}Fe_{0.15}H_{0.50}Mn_{2.10}O₁₉Si₆Ti_{0.75}

$a = 1.6398$, $c = 0.72$ nm, $c/a = 0.439$, $V = 1.6767$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.16	0.499	0.303		non-colinear SiMn
Cl2	12o	.m.	0.142	0.284	0.382	0.3	single atom Cl
Si3	12o	.m.	0.556	0.112	0.226		tetrahedron O ₄
M4	6m	mm2	0.2606	0.5212	$\frac{1}{2}$		square pyramid O ₅
Ba5	6l	mm2	0.2164	0.4328	0		non-coplanar square O ₄
O6	6l	mm2	0.559	0.118	0		non-colinear Si ₂
Ba7	6k	m2m	0.3484	0	$\frac{1}{2}$		10-vertex polyhedron O ₆ Cl ₄
Cl8	6j	m2m	0.301	0	0	0.6	non-colinear Ba ₂
O9	6i	2mm	$\frac{1}{2}$	0	0.294		non-colinear Si ₂

M10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	coplanar triangle Mn ₃
Cl11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	coplanar triangle O ₃

M4 = 0.70Mn + 0.25Ti + 0.05Fe; M10 = 0.5O + 0.5OH

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.102

Remarks: Natural specimen from the Esquire mine, Big Creek, Fresno County, California. Composition Ba_{11.27}Mn_{4.06}Ti_{1.5}Fe_{0.29}Si₁₂O₃₆O_{2.2}Cl_{8.84}(H₂O)_{7.05} from electron microprobe analysis. H₂O and part of OH not located. We assigned an approximate value to the cation ratio of site M4 based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kampf A.R., Khan A.A., Baur W.H. (1973), Acta Crystallogr. B 29, 2019-2021.

191
hP91

K ₂₃ Na ₈ Cd ₁₂ In ₄₈	hP91	(191) P6/mmm – po ² n ² m ² lkhea
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K₂₃Na₈Cd₁₂In₄₈ [1]

Structural features: In₁₂ icosahedra, In₃ trigonal clusters and Cd₁₂In₆ double hexagonal antiprisms (containing two Na atoms) are interconnected via exo-bonds to form a 3D-framework. The double antiprisms center large (In₈₄Cd₁₂) fullerene-like cages. See Fig. III.84.

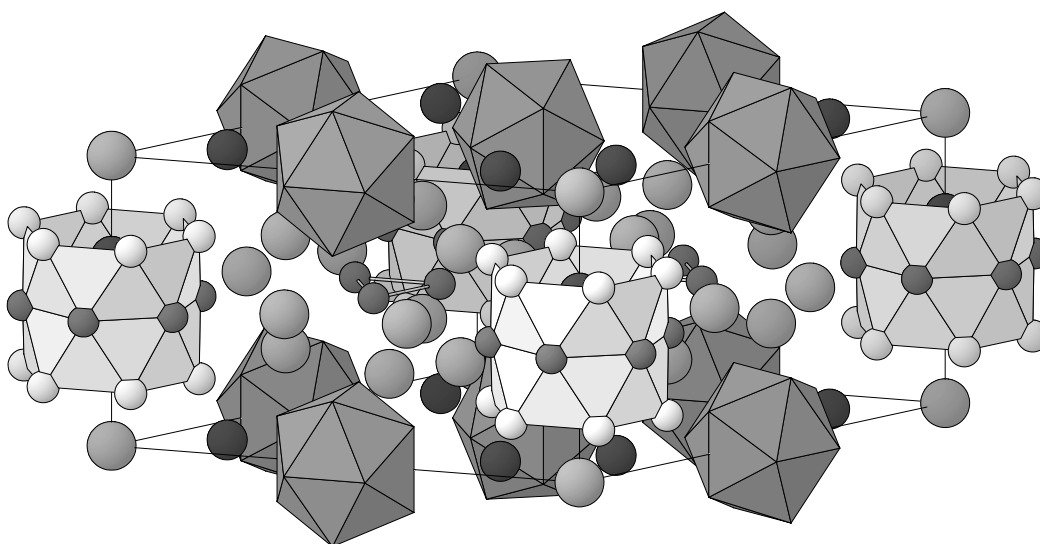


Fig. III.84. K₂₃Na₈Cd₁₂In₄₈

Arrangement of Cd₁₂In₆ double hexagonal antiprisms (light; Cd atoms small light, In atoms small dark), In₁₂ icosahedra (dark), In₃ triangles, K (large light) and Na (large dark) atoms.

Flot D.M. et al. (1996) [1]

Cd₁₂In₄₈K₂₃Na₈

$a = 1.7114$, $c = 1.0442$ nm, $c/a = 0.610$, $V = 2.6486$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	12p	$m..$	0.16062	0.49358	0		11-vertex polyhedron In ₆ NaK ₄

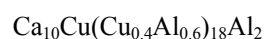
K2	12o	.m.	0.2088	0.4176	0.305	16-vertex Frank-Kasper In ₉ NaCd ₂ K ₄
In3	12o	.m.	0.55025	0.1005	0.2502	11-vertex polyhedron In ₆ K ₅
Cd4	12n	..m	0.187	0	0.2549	icosahedron In ₃ Cd ₂ Na ₃ K ₄
In5	12n	..m	0.35363	0	0.1477	11-vertex polyhedron In ₅ CdK ₃ Na ₂
In6	6m	mm2	0.10663	0.21326	¹ / ₂	icosahedron Cd ₄ In ₂ Na ₂ K ₄
In7	6m	mm2	0.60631	0.21262	¹ / ₂	icosahedron In ₄ K ₈
Na8	6l	mm2	0.1387	0.2774	0	15-vertex Frank-Kasper Cd ₄ In ₆ K ₃ Na ₂
K9	6k	m2m	0.3692	0	¹ / ₂	7-capped pentagonal prism In ₁₀ K ₅ Cd ₂
K10	4h	3m.	¹ / ₃	² / ₃	0.1991	16-vertex Frank-Kasper In ₁₂ K ₄
Na11	2e	6mm	0	0	0.347	14-vertex Frank-Kasper NaCd ₆ In ₆ K
K12	1a	6/mmm	0	0	0	pseudo Frank-Kasper Na ₈ Cd ₁₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.033

Remarks: Atomic ratio 1Na:2.94(3)K:1.46(3)Cd:5.91(9)In from atomic absorption spectroscopy.

References: [1] Flot D.M., Tillard Charbonnel M., Belin C.H.E. (1996), J. Am. Chem. Soc. 118, 5229-5235.

191
hP93



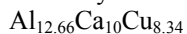
hP93

(191) $P6/mmm - q_0^2 n^2 m l^2 j h g e$

Ca(Cu,Al)_{2.1} [1]

Structural features: Ca(Al,Cu)₁₂ truncated tetrahedra and related Ca(Al,Cu)₁₁ and Ca(Al,Cu)₁₀ polyhedra share atoms to form a dense 3D-framework.

Zarechnyuk O.S. et al. (1988) [1]



$a = 1.5298$, $c = 0.9289$ nm, $c/a = 0.607$, $V = 1.8827$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12q	m..	0.1623	0.4928	¹ / ₂		icosahedron CuAl ₆ Ca ₅
Ca2	12o	.m.	0.2104	0.4208	0.2021		16-vertex Frank-Kasper Al ₉ Cu ₂ Ca ₅
M3	12o	.m.	0.5502	0.1005	0.2530		icosahedron CuAl ₆ Ca ₅
M4	12n	..m	0.2088	0	0.2132		pseudo Frank-Kasper Al ₃ Ca ₆ Cu ₂
M5	12n	..m	0.3561	0	0.3521		icosahedron Cu ₂ Al ₅ Ca ₅
Ca6	6m	mm2	0.1318	0.2638	¹ / ₂		14-vertex Frank-Kasper Cu ₄ Al ₆ Ca ₄
M7	6l	mm2	0.1116	0.2232	0		cuboctahedron Cu ₄ Al ₂ Ca ₆
Al8	6l	mm2	0.6041	0.2082	0		icosahedron Al ₄ Ca ₈
Ca9	6j	m2m	0.3805	0	0		7-capped pentagonal prism Al ₁₀ Cu ₂ Ca ₅
Ca10	4h	3m.	¹ / ₃	² / ₃	0.308		16-vertex Frank-Kasper Al ₁₂ Ca ₄
Cu11	3g	mmm	¹ / ₂	0	¹ / ₂		icosahedron Al ₁₂
Ca12	2e	6mm	0	0	0.228		pseudo Frank-Kasper Cu ₆ Al ₆ Ca ₇

M1 = 0.58Al + 0.42Cu; M3 = 0.58Al + 0.42Cu; M4 = 0.58Cu + 0.42Al; M5 = 0.75Al + 0.25Cu; M7 = 0.67Al + 0.33Cu

Transformation from published data: origin shift 0 0 ¹/₂

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

Remarks: The structure was refined independently on so-called CaCuAl in [2], where two additional, partly occupied sites were found.

References: [1] Zarechnyuk O.S., Manyako N.B., Yanson T.I., Bruskov V.A. (1988), Sov. Phys. Crystallogr. 33, 196-199 (Kristallografiya 33, 336-340). [2] Fornasini M.L., Merlo F. (1988), Acta Crystallogr. C 44, 1351-1355.

191
hP94

$\text{Na}_{15.2}(\text{Ag}_{0.2}\text{Ga}_{0.8})_6\text{Ga}_{24}$	<i>hP94</i>	(191) $P6/mmm - \text{qo}^2\text{n}^2\text{ml}^2\text{jhe}^3$
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Na_{30.5}Ag_xGa_{60-x} [1]

Structural features: Ga₁₂ icosahedra, Ga₃ trigonal clusters and (Ga,Ag)₁₈ double hexagonal antiprisms are interconnected via exo-bonds to form a 3D-framework. Variant of K₂₃Na₈Cd₁₂In₄₈.

Henning R.W., Corbett J.D. (2002) [1]

Ag_{1.32}Ga_{28.68}Na₁₅

$a = 1.5161$, $c = 0.9267$ nm, $c/a = 0.611$, $V = 1.8447$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	12 <i>q</i>	<i>m.</i>	0.1613	0.4938	$\frac{1}{2}$		11-vertex polyhedron Ga ₆ Na ₅
Na2	12 <i>o</i>	<i>m.</i>	0.2109	0.4218	0.1911		16-vertex Frank-Kasper Ga ₁₁ Na ₅
Ga3	12 <i>o</i>	<i>m.</i>	0.551	0.102	0.2467		11-vertex polyhedron Ga ₆ Na ₅
M4	12 <i>n</i>	<i>m.</i>	0.1969	0	0.2303		
Ga5	12 <i>n</i>	<i>m.</i>	0.35508	0	0.3507		11-vertex polyhedron Ga ₆ Na ₅
Na6	6 <i>m</i>	<i>mm2</i>	0.1354	0.2708	$\frac{1}{2}$		
Ga7	6 <i>l</i>	<i>mm2</i>	0.1121	0.2242	0		
Ga8	6 <i>l</i>	<i>mm2</i>	0.60575	0.2115	0		icosahedron Ga ₄ Na ₈
Na9	6 <i>j</i>	<i>m2m</i>	0.3742	0	0		7-capped pentagonal prism Ga ₁₂ Na ₅
Na10	4 <i>h</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.3001		16-vertex Frank-Kasper Ga ₁₂ Na ₄
Na11	2 <i>e</i>	6 <i>mm</i>	0	0	0.131	0.25	
Na12	2 <i>e</i>	6 <i>mm</i>	0	0	0.199	0.5	
Na13	2 <i>e</i>	6 <i>mm</i>	0	0	0.446	0.25	

M4 = 0.78Ga + 0.22Ag

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.034, T = 296 K

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

References: [1] Henning R.W., Corbett J.D. (2002), Z. Anorg. Allg. Chem. 628, 2715-2723.

191
hP96

$\text{CaCu}_{0.98}\text{Al}_{1.12}$	<i>hP96</i>	(191) $P6/mmm - \text{qo}^2\text{n}^2\text{ml}^2\text{jhge}^2\text{a}$
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CaCuAl [1]

Structural features: Ca(Al,Cu)₁₂ truncated tetrahedra and related Ca(Al,Cu)₁₁ and Ca(Al,Cu)₁₀ polyhedra share atoms to form a dense framework.

Fornasini M.L., Merlo F. (1988) [1]

Al_{1.12}CaCu_{0.98}

$a = 1.5256$, $c = 0.9252$ nm, $c/a = 0.606$, $V = 1.8649$ nm³, $Z = 30$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>q</i>	<i>m.</i>	0.1628	0.493	$\frac{1}{2}$		icosahedron Cu ₃ Al ₄ Ca ₅
Ca2	12 <i>o</i>	<i>m.</i>	0.2099	0.4198	0.2029		16-vertex Frank-Kasper Al ₇ Cu ₄ Ca ₅
M3	12 <i>o</i>	<i>m.</i>	0.5506	0.1012	0.2526		icosahedron Cu ₂ Al ₅ Ca ₅
M4	12 <i>n</i>	<i>m.</i>	0.2109	0	0.2134		non-coplanar triangle Al ₃
M5	12 <i>n</i>	<i>m.</i>	0.3557	0	0.3524		icosahedron Cu ₄ Al ₃ Ca ₅
Ca6	6 <i>m</i>	<i>mm2</i>	0.1322	0.2644	$\frac{1}{2}$		16-vertex Frank-Kasper Cu ₄ Al ₆ Ca ₆
M7	6 <i>l</i>	<i>mm2</i>	0.1101	0.2202	0		non-coplanar square Cu ₄

M8	6l	mm2	0.6047	0.2094	0		icosahedron Cu ₂ Al ₂ Ca ₈
Ca9	6j	m2m	0.3808	0	0		7-capped pentagonal prism Cu ₆ Al ₆ Ca ₅
Ca10	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.3068		16-vertex Frank-Kasper Cu ₃ Al ₉ Ca ₄
Cu11	3g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		icosahedron Al ₈ Cu ₄
Ca12	2e	6mm	0	0	0.2231	0.801	
Ca13	2e	6mm	0	0	0.3673	0.199	
M14	1a	6/mmm	0	0	0	0.199	colinear Ca ₂

M1 = 0.518Al + 0.482Cu; M3 = 0.636Cu + 0.364Al; M4 = 0.719Cu + 0.281Al; M5 = 0.780Al + 0.220Cu; M7 = 0.818Al + 0.182Cu; M8 = 0.895Al + 0.105Cu; M14 = 0.749Al + 0.251Cu

Experimental: single crystal, diffractometer, X-rays, R = 0.038, T = 293 K

Remarks: Short interatomic distances for partly occupied site(s). The structure was refined independently on so-called Ca(Cu,Al)_{2.1} in [2], where no partly occupied sites were detected.

References: [1] Fornasini M.L., Merlo F. (1988), Acta Crystallogr. C 44, 1351-1355. [2] Zarechnyuk O.S., Manyako N.B., Yanson T.I., Bruskov V.A. (1988), Sov. Phys. Crystallogr. 33, 196-199 (Kristallografiya 33, 336-340).

191
hP102

SiO ₂	hP102	(191) P6/mmm – ro ³ nlkjhc
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SiO₂ dodecasil-1H [1], zeolite DOH

Structural features: SiO₄ tetrahedra share vertices to form a DOH-type zeolite framework with 12-face (pentagonal dodecahedra and 4³5⁶6³ polyhedra) and 20-face cages (5¹²6⁸ polyhedra).

Flot D.M. et al. (1984) [1]

O₂Si

$a = 1.3783$, $c = 1.119$ nm, $c/a = 0.812$, $V = 1.8410$ nm³, $Z = 34$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1052	0.3933	0.3031		non-colinear Si ₂
O2	12o	.m.	0.1702	0.3404	0.1139		non-colinear Si ₂
Si3	12o	.m.	0.2093	0.4186	0.2252		tetrahedron O ₄
O4	12o	.m.	0.2715	0.543	0.1836		non-colinear Si ₂
Si5	12n	..m	0.3868	0	0.3627		tetrahedron O ₄
Si6	6l	mm2	0.1314	0.2628	0		tetrahedron O ₄
O7	6k	m2m	0.3601	0	$\frac{1}{2}$		non-colinear Si ₂
O8	6j	m2m	0.1865	0	0		non-colinear Si ₂
O9	6i	2mm	$\frac{1}{2}$	0	0.3451		non-colinear Si ₂
Si10	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1384		tetrahedron O ₄
O11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		colinear Si ₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.086

Remarks: Non-framework species not located (N₂ in the smaller, piperidine in the larger cages). When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Flot D.M., Tillard Charbonnel M., Belin C.H.E. (1984), Z. Kristallogr. 166, 11-22.

191
hP108

BaTa ₂ O ₆	hP108	(191) P6/mmm – qp ³ m ² l ⁴ kj ² gda
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BaTa₂O₆ [1]

Structural features: Units of two edge-linked TaO₆ octahedra share vertices with single TaO₆ octahedra to form infinite slabs, which are interconnected via common vertices to form a 3D-framework.

Layden G.K. (1968) [1]

BaO₆Ta₂

$a = 2.114$, $c = 0.3917$ nm, $c/a = 0.185$, $V = 1.5160$ nm³, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 q	$m..$	0.17	0.51	$\frac{1}{2}$		non-colinear Ta ₂
O2	12 p	$m..$	0.07	0.41	0		non-colinear Ta ₂
O3	12 p	$m..$	0.08	0.28	0		non-colinear Ta ₂
Ta4	12 p	$m..$	0.16	0.5	0		octahedron O ₆
O5	6 m	$mm2$	0.1	0.2	$\frac{1}{2}$		colinear Ta ₂
Ba6	6 m	$mm2$	0.187	0.374	$\frac{1}{2}$		tricapped trigonal prism O ₉
Ta7	6 l	$mm2$	0.1	0.2	0		octahedron O ₆
O8	6 l	$mm2$	0.24	0.48	0		non-colinear Ta ₂
O9	6 l	$mm2$	0.55	0.1	0		non-colinear Ta ₂
O10	6 l	$mm2$	0.62	0.24	0		non-colinear Ta ₂
O11	6 k	$m2m$	0.31	0	$\frac{1}{2}$		non-colinear Ta ₂
O12	6 j	$m2m$	0.125	0	0		non-colinear Ta ₂
Ta13	6 j	$m2m$	0.313	0	0		octahedron O ₆
Ba14	3 g	mmm	$\frac{1}{2}$	0	$\frac{1}{2}$		coplanar square O ₄
Ba15	2 d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism O ₆
Ba16	1 a	6/ mmm	0	0	0		coplanar hexagon O ₆

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_p = 0.260$

References: [1] Layden G.K. (1968), Mater. Res. Bull. 3, 349-359.

191
hP113

Y _{0.915} Ni _{4.12} B	hP113	(191) $P6/mmm - \text{ronm}^3\text{l}^3\text{kje}^3\text{dca}$
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Y_{0.915}Ni_{4.12}B [1]

Structural features: Kagomé-mesh Ni₉ layers alternate with (Y,□)₃Ni₄B₂ and (Y,□)₃Ni₂B₄ layers (a Ni₂B or NiB₂ hexagon mesh, part of the hexagons of which are centered by an Y atom) along [001]; additional Y and Ni along 0 0 z (disorder). Derivative of CaCu₅.

Belger A. et al. (1999) [1]

BNi_{4.12}Y_{0.91}

$a = 1.49143$, $c = 0.69123$ nm, $c/a = 0.463$, $V = 1.3316$ nm³, $Z = 18$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	24 r	1	0.16544	0.49779	0.29744		pseudo Frank-Kasper B ₂ Ni ₇ Y ₄
Ni2	12 o	$.m.$	0.16506	0.33011	0.2673		pseudo Frank-Kasper B ₂ Ni ₇ Y ₄
Ni3	12 n	$.m$	0.17083	0	0.1866		non-colinear B ₂
Ni4	6 m	$mm2$	0.09151	0.18301	$\frac{1}{2}$		
B5	6 m	$mm2$	0.2152	0.4304	$\frac{1}{2}$		trigonal prism Ni ₆
B6	6 m	$mm2$	0.554	0.1081	$\frac{1}{2}$		trigonal prism Ni ₆
B7	6 l	$mm2$	0.1237	0.2475	0		trigonal prism Ni ₆
Ni8	6 l	$mm2$	0.22324	0.4465	0		icosahedron Ni ₈ BY ₃
Ni9	6 l	$mm2$	0.55977	0.11955	0		14-vertex Frank-Kasper Ni ₉ Y ₃ B ₂

Y10	6k	<i>m2m</i>	0.32074	0	$\frac{1}{2}$		pseudo Frank-Kasper $B_4Ni_{14}Y_2$
Y11	6j	<i>m2m</i>	0.34448	0	0		pseudo Frank-Kasper $Ni_{16}B_2Y_2$
Ni12	6i	<i>2mm</i>	$\frac{1}{2}$	0	0.2904		pseudo Frank-Kasper $B_2Ni_7Y_4$
Ni13	2e	<i>6mm</i>	0	0	0.096	0.325	
Ni14	2e	<i>6mm</i>	0	0	0.326	0.53	
Ni15	2e	<i>6mm</i>	0	0	0.4	0.25	
Y16	2d	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper $Ni_{12}B_6Y_2$
Y17	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		pseudo Frank-Kasper $Ni_{18}Y_2$
Y18	1a	<i>6/mmm</i>	0	0	0	0.465	

Experimental: single crystal, diffractometer, X-rays, $R = 0.041$, $T = 298$ K

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

References: [1] Belger A., Zahn G., Wehner B., Paufler P., Graw G., Behr G. (1999), J. Alloys Compd. 283, 26-33.

191
hP116

$Er_{0.917}Ni_{4.09}B$	<i>hP116</i>	(191) <i>P6/mmm</i> – $ronm^3l^3kjie^4dcba$
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$Er_{0.917}Ni_{4.09}B$ [1]

Structural features: Kagomé-mesh Ni_9 layers alternate with $(Er, \square)_3Ni_4B_2$ and $(Er, \square)_3Ni_2B_4$ layers (a Ni_2B or NiB_2 hexagon mesh, part of the hexagons of which are centered by an Er atom) along [001]; additional Er and Ni along 0 0 z (disorder). Derivative of $CaCu_5$.

Kuz'ma Y.B. et al. (2004) [1]

$B_{Er_{0.92}Ni_{4.09}}$

$a = 1.48399$, $c = 0.69194$ nm, $c/a = 0.466$, $V = 1.3197$ nm³, $Z = 18$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	24r	1	0.16562	0.49803	0.2976		non-colinear B_2
Ni2	12o	.m.	0.16538	0.33076	0.2667		non-colinear B_2
Ni3	12n	.m	0.1708	0	0.1883		non-colinear B_2
Ni4	6m	<i>mm2</i>	0.0934	0.1868	$\frac{1}{2}$	0.922	
B5	6m	<i>mm2</i>	0.2113	0.4226	$\frac{1}{2}$		trigonal prism Ni_6
B6	6m	<i>mm2</i>	0.5541	0.1082	$\frac{1}{2}$		trigonal prism Ni_6
B7	6l	<i>mm2</i>	0.1239	0.2478	0		trigonal prism Ni_6
Ni8	6l	<i>mm2</i>	0.2238	0.4476	0		icosahedron $Ni_8B_{Er_3}$
Ni9	6l	<i>mm2</i>	0.5603	0.1206	0		trigonal prism Ni_6
Er10	6k	<i>m2m</i>	0.3217	0	$\frac{1}{2}$		pseudo Frank-Kasper $B_4Ni_{14}Er_2$
Er11	6j	<i>m2m</i>	0.3439	0	0		pseudo Frank-Kasper $Ni_{16}B_2Er_2$
Ni12	6i	<i>2mm</i>	$\frac{1}{2}$	0	0.2859		non-colinear B_2
Ni13	2e	<i>6mm</i>	0	0	0.048	0.265	
Ni14	2e	<i>6mm</i>	0	0	0.117	0.18	
Ni15	2e	<i>6mm</i>	0	0	0.346	0.38	
Ni16	2e	<i>6mm</i>	0	0	0.393	0.16	
Er17	2d	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		pseudo Frank-Kasper $Ni_{12}B_6Er_2$
Er18	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0	0.949	pseudo Frank-Kasper $Ni_{18}Er_2$
Ni19	1b	<i>6/mmm</i>	0	0	$\frac{1}{2}$	0.19	
Er20	1a	<i>6/mmm</i>	0	0	0	0.615	

Experimental: single crystal, diffractometer, X-rays, $wR = 0.054$

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

References: [1] Kuz'ma Y.B., Babizhetskij V., Veremchuk I., Chaban N. (2004), J. Solid State Chem. 177, 425-430.

191
hP117

$\text{Be}_{1.11}\text{Al}_{0.07}\text{B}_{3.38}$			$hP117$			$(191) P6/mmm - \text{po}^4\text{n}^3\text{m}^2\text{lea}$	
$\text{Al}_{0.06}\text{BeB}_{3.05}$ [1]; " BeB_3 " [1]							
Structural features: B forms a 3D-framework with B_{12} icosahedra (interconnected via exo-bonds) and B_{12} truncated tetrahedra.							
Mattes R. et al. (1975) [1]							
$\text{Al}_{0.06}\text{B}_{3.36}\text{Be}$							
$a = 0.98, c = 0.9532 \text{ nm}, c/a = 0.973, V = 0.7928 \text{ nm}^3, Z = 24$							
site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	$12p$	$m..$	0.1641	0.4931	0		
M2	$12o$	$.m.$	0.119	0.238	0.3576		
B3	$12o$	$.m.$	0.2283	0.4566	0.4041		8-vertex polyhedron B_4Be_4
B4	$12o$	$.m.$	0.5532	0.1064	0.1531		pentagonal pyramid B_6
B5	$12o$	$.m.$	0.6053	0.2106	0.3064		8-vertex polyhedron B_5Be_3
B6	$12n$	$..m$	0.1878	0	0.1865		
B7	$12n$	$..m$	0.349	0	0.0948		
Be8	$12n$	$..m$	0.3655	0	0.3205		13-vertex polyhedron B_{10}Be_3
M9	$6m$	$mm2$	0.062	0.124	$\frac{1}{2}$	0.502	
Be10	$6m$	$mm2$	0.5604	0.1208	$\frac{1}{2}$		7-vertex polyhedron B_6Be
Al11	$6l$	$mm2$	0.193	0.386	0	0.083	
Al12	$2e$	$6mm$	0	0	0.1051	0.167	
Al13	$1a$	$6/mmm$	0	0	0	0.18	

$\text{M2} = 0.5\text{B} + 0.5\text{Be}$; $\text{M9} = 0.86\text{B} + 0.14\text{Al}$

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

Remarks: 26-27 Be per unit cell expected from density measurements, the authors state that remaining Be is probably located in site B6. Short interatomic distances: $d(\text{Al11-B1}) = 0.122$ nm. Short interatomic distances for partly occupied site(s). The same data are also reported in [4]. Preliminary data in [2]. Identical to the phase BeB_2 in [3]. A refinement on Al-free BeB_3 ($\text{Be}_{1.09}\text{B}_3$) is reported in [5]. In table 2 of [1] the Wyckoff positions of former sites 7 and 13 are misprinted as $5m$ and $6i$ instead of $6m$ and $6l$, respectively.

References: [1] Mattes R., Tebbe K.F., Neidhard H., Rethfeld H. (1975), Z. Anorg. Allg. Chem. 413, 1-9. [2] Mattes R., Neidhard H., Rethfeld H., Tebbe K.F. (1973), Inorg. Nucl. Chem. Lett. 9, 1021-1024. [3] Sands D.E., Cline C.F., Zalkin A., Hoenig C.L. (1961), Acta Crystallogr. 14, 309-310. [4] Mattes R., Tebbe K.F., Neidhard H., Rethfeld H. (1976), J. Less-Common Met. 47, 29-32. [5] Chan J.Y., Fronczek F.R., Young D.P., DiTusa J.F., Adams P.W. (2002), J. Solid State Chem. 163, 385-389.

191
hP119

$\text{K}_9(\text{Ga}_{0.25}\text{Si}_{0.75})_{36}\text{O}_{72}$			hP119			(191) $P6/mmm - \text{r}^2\text{qpo}^2\text{lkjfc}$	
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$\text{K}_9\text{Ga}_9\text{Si}_{27}\text{O}_{72}$ [1], zeolite LTL(Ga)-K

Structural features: $(\text{Si,Ga})\text{O}_4$ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to $[001]$; K at the centers of cancrinite-type cages (B positions), between non-planar 6-rings (C) and at the centers of 8-rings (D).

Newsam J.M. (1986) [1]

 $\text{Ga}_9\text{K}_{10.10}\text{O}_{72}\text{Si}_{27}$ $a = 1.858$, $c = 0.74894$ nm, $c/a = 0.403$, $V = 2.2391$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1014	0.4135	0.1799		non-colinear Si ₂
M2	24r	1	0.1673	0.4991	0.2868		tetrahedron O ₄
O3	12q	<i>m..</i>	0.1446	0.4767	$\frac{1}{2}$		non-colinear Si ₂
M4	12p	<i>m..</i>	0.0925	0.3556	0		tetrahedron O ₄
O5	12o	<i>.m.</i>	0.2658	0.5316	0.2407		non-colinear Si ₂
O6	12o	<i>.m.</i>	0.5734	0.1468	0.2257		non-colinear Si ₂
O7	6l	<i>mm2</i>	0.1654	0.3308	0		non-colinear Si ₂
K8	6k	<i>m2m</i>	0.3234	0	$\frac{1}{2}$	0.85	non-colinear O ₂
O9	6j	<i>m2m</i>	0.2753	0	0		non-colinear Si ₂
K10	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		coplanar square O ₄
K11	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆

M2 = 0.75Si + 0.25Ga; M4 = 0.75Si + 0.25Ga

Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: powder, diffractometer, neutrons, $R_B = 0.050$, $T = 298$ K

Remarks: We assigned an approximate value to the Ga/Si ratio of sites M based on the nominal composition. No significant electron density was detected in Wyckoff positions 2c and 3f (2d and 3g after standardization).

References: [1] Newsam J.M. (1986), Mater. Res. Bull. 21, 661-672.

191
hP120

$\text{Be}_{3.9}(\text{Be}_{0.5}\text{B}_{0.5})_2\text{B}_{12.5}$	hP120	(191) $P6/mmm - po^4n^3m^2lhe$
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Be_{1.09}B₃ [1]Structural features: B forms a 3D-framework with B₁₂ icosahedra (interconnected via exo-bonds) and B₁₂ truncated tetrahedra.

Chan J.Y. et al. (2002) [1]

 $\text{B}_{13.50}\text{Be}_{4.92}$ $a = 0.97738$, $c = 0.95467$ nm, $c/a = 0.977$, $V = 0.7898$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	12p	<i>m..</i>	0.164	0.4926	0		pentagonal pyramid B ₆
M2	12o	<i>.m.</i>	0.1191	0.2382	0.3582		
B3	12o	<i>.m.</i>	0.2285	0.457	0.4046		8-vertex polyhedron B ₄ Be ₄
B4	12o	<i>.m.</i>	0.553	0.106	0.153		7-vertex polyhedron B ₆ Be
B5	12o	<i>.m.</i>	0.605	0.21	0.3071		7-vertex polyhedron B ₅ Be ₂
B6	12n	<i>..m</i>	0.1884	0	0.188		9-vertex polyhedron B ₅ Be ₄
B7	12n	<i>..m</i>	0.348	0	0.0953		pentagonal pyramid B ₆
Be8	12n	<i>..m</i>	0.3644	0	0.3213		12-vertex polyhedron B ₁₀ Be ₂
B9	6m	<i>mm2</i>	0.0619	0.1238	$\frac{1}{2}$	0.5	
Be10	6m	<i>mm2</i>	0.5605	0.121	$\frac{1}{2}$		7-vertex polyhedron B ₆ Be
Be11	6l	<i>mm2</i>	0.1244	0.2488	0	0.5	14-vertex polyhedron B ₁₀ Be ₄
Be12	4h	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.125	0.125	12-vertex polyhedron B ₁₂

Be13 2e 6mm 0 0 0.1067 13-vertex polyhedron B₆Be₇

M2 = 0.50B + 0.50Be

Experimental: single crystal, diffractometer, X-rays, R = 0.047, T = 120 K

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

References: [1] Chan J.Y., Fronczek F.R., Young D.P., DiTusa J.F., Adams P.W. (2002), J. Solid State Chem. 163, 385-389.

191
hP122

(Na_{0.5}Mg_{0.5})₅Ga₉ hP122 (191) P6/mmm – po²n⁵mlkhe²

Na_{2.5}Mg_{2.5}Ga₉ [1]

Structural features: Ga forms a 3D-framework with Ga₁₂ icosahedra and Ga₁₂ truncated tetrahedra.

Nesper R. (1989) [1]

Ga₉Mg_{2.50}Na_{2.50}

$a = 1.543$, $c = 0.8998$ nm, $c/a = 0.583$, $V = 1.8553$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	12p	m..	0.1596	0.4911	0		
M2	12o	.m.	0.2088	0.418	0.309		
Ga3	12o	.m.	0.5499	0.0998	0.2422		
Ga4	12n	..m	0.168	0	0.2700	0.10	
Ga5	12n	..m	0.2000	0	0.3400	0.18	
Ga6	12n	..m	0.2062	0	0.3000	0.72	
Ga7	12n	..m	0.351	0	0.1700	0.42	
Ga8	12n	..m	0.353	0	0.14	0.58	
Ga9	6m	mm2	0.6042	0.2085	¹ / ₂		icosahedron Ga ₄ Mg ₈
M10	6l	mm2	0.130	0.260	0		
M11	6k	m2m	0.387	0	¹ / ₂		
M12	4h	3m.	¹ / ₃	² / ₃	0.194		16-vertex Frank-Kasper Ga ₁₂ Mg ₄
M13	2e	6mm	0	0	0.160	0.88	
M14	2e	6mm	0	0	0.240	0.12	

M2 = 0.5Mg + 0.5Na; M10 = 0.5Mg + 0.5Na; M11 = 0.5Mg + 0.5Na; M12 = 0.5Mg + 0.5Na; M13 = 0.5Mg + 0.5Na; M14 = 0.5Mg + 0.5Na

Transformation from published data: origin shift 0 0 ¹/₂

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

Remarks: Homogeneity range Na_xMg_{5-x}Ga₉, 2 < x < 3. No attempt was made to distinguish Na and Mg (misprinted as Na and Ga) in [1]; we arbitrarily set Na/Mg = 1 (composition of the sample not given). Laue symmetry 6/mmm modulated by composition-dependent superstructures. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s).

References: [1] Nesper R. (1989), Angew. Chem. 101, 99-101.

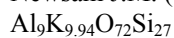
191
hP122

K₉(Al_{0.25}Si_{0.75})₃₆O₇₂ hP122 (191) P6/mmm – r²qpo²lkjgfc

K₉Al₉Si₂₇O₇₂ [1], zeolite LTL-K

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions), between non-planar 6-rings (C) and at the centers of 8-rings (D, E).

Newsam J.M. (1989) [1]



$a = 1.8466$, $c = 0.74763$ nm, $c/a = 0.405$, $V = 2.2078$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1022	0.4142	0.1817		non-colinear Si ₂
M2	24r	1	0.166	0.4989	0.2879		tetrahedron O ₄
O3	12q	$m..$	0.1442	0.4772	$1/2$		non-colinear Si ₂
M4	12p	$m..$	0.0943	0.3584	0		tetrahedron O ₄
O5	12o	$.m.$	0.2657	0.5314	0.244		non-colinear Si ₂
O6	12o	$.m.$	0.5749	0.1498	0.2249		non-colinear Si ₂
O7	6l	$mm2$	0.1659	0.3318	0		non-colinear Si ₂
K8	6k	$m2m$	0.3197	0	$1/2$	0.797	non-colinear O ₂
O9	6j	$m2m$	0.2754	0	0		non-colinear Si ₂
K10	3g	mmm	$1/2$	0	$1/2$	0.053	coplanar square O ₄
K11	3f	mmm	$1/2$	0	0		coplanar square O ₄
K12	2c	$-6m2$	$1/3$	$2/3$	0		trigonal prism O ₆

M2 = 0.75Si + 0.25Al; M4 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 $1/2$

Experimental: powder, diffractometer, neutrons, $R_B = 0.035$, $T = 296$ K

Remarks: Composition Na_{0.027}K_{9.272}Si_{26.701}Al_{9.299}O₇₂·17H₂O from inductively coupled plasma method before dehydration.

References: [1] Newsam J.M. (1989), J. Phys. Chem. 93, 7689-7694.

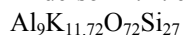
191
hP131

K ₁₂ (Al _{0.25} Si _{0.75}) ₃₆ O ₇₂	hP131	(191) $P6/mmm - r^2qpo^3lkjfc$
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K₁₂Al₉Si₂₇O₇₂ [1], zeolite LTL-K₉/K₃

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K⁺ at the centers of cancrinite-type cages (B positions), between non-planar 6-rings (C) and at the centers of 8-rings (D), K₃ clusters (partial positive charge) in the channels.

Anderson P.A. et al. (1997) [1]



$a = 1.83893$, $c = 0.74828$ nm, $c/a = 0.407$, $V = 2.1914$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1011	0.4139	0.182		non-colinear Si ₂
M2	24r	1	0.1677	0.4991	0.2887		tetrahedron O ₄
O3	12q	$m..$	0.1462	0.4776	$1/2$		non-colinear Si ₂
M4	12p	$m..$	0.0922	0.3561	0		tetrahedron O ₄
K5	12o	$.m.$	0.082	0.164	0.151	0.13	
O6	12o	$.m.$	0.2647	0.5294	0.2475		non-colinear Si ₂
O7	12o	$.m.$	0.5734	0.1468	0.2265		non-colinear Si ₂

O8	6l	<i>mm</i> 2	0.1645	0.329	0		non-colinear Si ₂
K9	6k	<i>m</i> 2 <i>m</i>	0.3117	0	$\frac{1}{2}$	0.86	6-vertex polyhedron O ₆
O10	6j	<i>m</i> 2 <i>m</i>	0.2729	0	0		non-colinear Si ₂
K11	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		hexagonal prism O ₁₂
K12	2c	<i>-6m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆

M2 = 0.75Si + 0.25Al; M4 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.040$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s).

References: [1] Anderson P.A., Armstrong A.R., Porch A., Edwards P.P., Woodall L.J. (1997), J. Phys. Chem. B 101, 9892-9900.

191
hP149

Cs_{3.7}K_{5.3}(Al_{0.25}Si_{0.75})₃₆O₇₂[H₂O]₂₁ *hP*149 (191) *P*6/*mmm* – $r^2qpo^4lk^2jfc$

Cs_{3.7}K_{5.3}Al₉Si₂₇O₇₂·*x*H₂O [1], zeolite LTL-Cs,K hydrated

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions) and between non-planar 6-rings (C), Cs at the centers of 8-rings (D), H₂O in the channels.

Sato M. et al. (1990) [1]

Al₉Cs_{3.66}H_{16.44}K₅O_{80.22}Si₂₇

$a = 1.8411$, $c = 0.7558$ nm, $c/a = 0.411$, $V = 2.2187$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>r</i>	1	0.1078	0.4251	0.186		non-colinear Si ₂
M2	24 <i>r</i>	1	0.165	0.4995	0.294		trigonal bipyramid O ₄ (OH ₂)
O3	12 <i>q</i>	<i>m</i> ..	0.1472	0.4799	$\frac{1}{2}$		non-colinear Si ₂
M4	12 <i>p</i>	<i>m</i> ..	0.0938	0.3508	0		tetrahedron O ₄
(OH ₂)5	12 <i>o</i>	<i>m</i> .	0.0765	0.153	0.187	0.44	non-colinear (OH ₂) ₂
(OH ₂)6	12 <i>o</i>	<i>m</i> .	0.239	0.478	0.312	0.14	single atom O
O7	12 <i>o</i>	<i>m</i> .	0.266	0.532	0.2352		single atom (OH ₂)
O8	12 <i>o</i>	<i>m</i> .	0.57	0.14	0.2244		non-colinear Si ₂
O9	6l	<i>mm</i> 2	0.1617	0.3234	0		non-colinear Si ₂
(OH ₂)10	6k	<i>m</i> 2 <i>m</i>	0.107	0	$\frac{1}{2}$	0.21	non-colinear (OH ₂) ₂
Cs11	6k	<i>m</i> 2 <i>m</i>	0.2779	0	$\frac{1}{2}$	0.61	7-vertex polyhedron (OH ₂)O ₆
O12	6j	<i>m</i> 2 <i>m</i>	0.2738	0	0		non-colinear Si ₂
K13	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		coplanar square O ₄
K14	2c	<i>-6m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆

M2 = 0.75Si + 0.25Al; M4 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.044$

Remarks: Part of H₂O not located. Approximate composition, we took the amount of Cs from the refinement and adjusted the charge balance in the formula given above by adding K. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the *y*-coordinate of former O(2) and the *x*-coordinate of former H₂O(3) are misprinted as 0.3245

and 0.765 instead of 0.3234 and 0.0765, respectively (agreement with Wyckoff positions *6m* and *12o*; checked on interatomic distances).

References: [1] Sato M., Morikawa K., Kurosawa S. (1990), *Eur. J. Mineral.* 2, 851-859.

191
hP155

$K_{2.7}Ba_{7.65}(Al_{0.5}Si_{0.5})_{36}O_{72}[H_2O]_{23}$	hP155	(191) <i>P6/mmm</i> – $r^2qpo^3nmlk^2jfc$
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$K_{2.7}Ba_{7.65}Al_{18}Si_{18}O_{72} \cdot 23H_2O$ [1], zeolite LTL-Ba hydrated

Structural features: (Al,Si) O_4 tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; Ba at the centers of cancrinite-type cages (B positions) and between non-planar 6-rings (C), (Ba,K) at the centers of 8-rings (D), H_2O in the channels.

Baerlocher C., Barrer R.M. (1972) [1]

$Al_{18}Ba_{6.68}H_{55.20}K_{2.19}O_{99.60}Si_{18}$

$a = 1.8701$, $c = 0.7501$ nm, $c/a = 0.401$, $V = 2.2718$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>r</i>	1	0.098	0.4045	0.1775		non-colinear Al ₂
M2	24 <i>r</i>	1	0.1665	0.498	0.2825		
O3	12 <i>q</i>	<i>m..</i>	0.154	0.4825	$\frac{1}{2}$		non-colinear Al ₂
M4	12 <i>p</i>	<i>m..</i>	0.089	0.35	0		tetrahedron O ₄
(OH ₂)5	12 <i>o</i>	<i>.m.</i>	0.111	0.222	0.291	0.4	non-coplanar triangle (OH ₂) ₃
O6	12 <i>o</i>	<i>.m.</i>	0.269	0.538	0.2235		non-colinear Al ₂
O7	12 <i>o</i>	<i>.m.</i>	0.5685	0.1375	0.2455		
(OH ₂)8	12 <i>n</i>	<i>.m</i>	0.1455	0	0.158		non-colinear (OH ₂) ₂
(OH ₂)9	6 <i>m</i>	<i>mm2</i>	0.145	0.29	$\frac{1}{2}$	0.95	non-colinear (OH ₂) ₂
O10	6 <i>l</i>	<i>mm2</i>	0.1635	0.327	0		non-colinear Al ₂
(OH ₂)11	6 <i>k</i>	<i>m2m</i>	0.178	0	$\frac{1}{2}$	0.85	non-coplanar square (OH ₂) ₄
M12	6 <i>k</i>	<i>m2m</i>	0.325	0	$\frac{1}{2}$	0.73	single atom (OH ₂)
O13	6 <i>j</i>	<i>m2m</i>	0.2675	0	0		non-colinear Al ₂
Ba14	3 <i>f</i>	<i>mmm</i>	$\frac{1}{2}$	0	0	0.83	
Ba15	2 <i>c</i>	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆

M2 = 0.50Al + 0.50Si; M4 = 0.50Al + 0.50Si; M12 = 0.50Ba + 0.50K

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.130$

Remarks: Major part of non-framework species refined as O, part of non-framework cations not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Baerlocher C., Barrer R.M. (1972), *Z. Kristallogr.* 136, 245-254.

191
hP155

$K_3Na_6(Al_{0.25}Si_{0.75})_{36}O_{72}[H_2O]_{21}$	hP155	(191) <i>P6/mmm</i> – $r^2qpo^4lk^2j^2fc$
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$K_3Na_6Al_9Si_{27}O_{72} \cdot 21H_2O$ [1], zeolite LTL-Na,K hydrated

Structural features: (Si,Al) O_4 tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B

positions) and between non-planar 6-rings (C), Na at the centers of 8-rings (D), H₂O in the channels. See Fig. III.85.

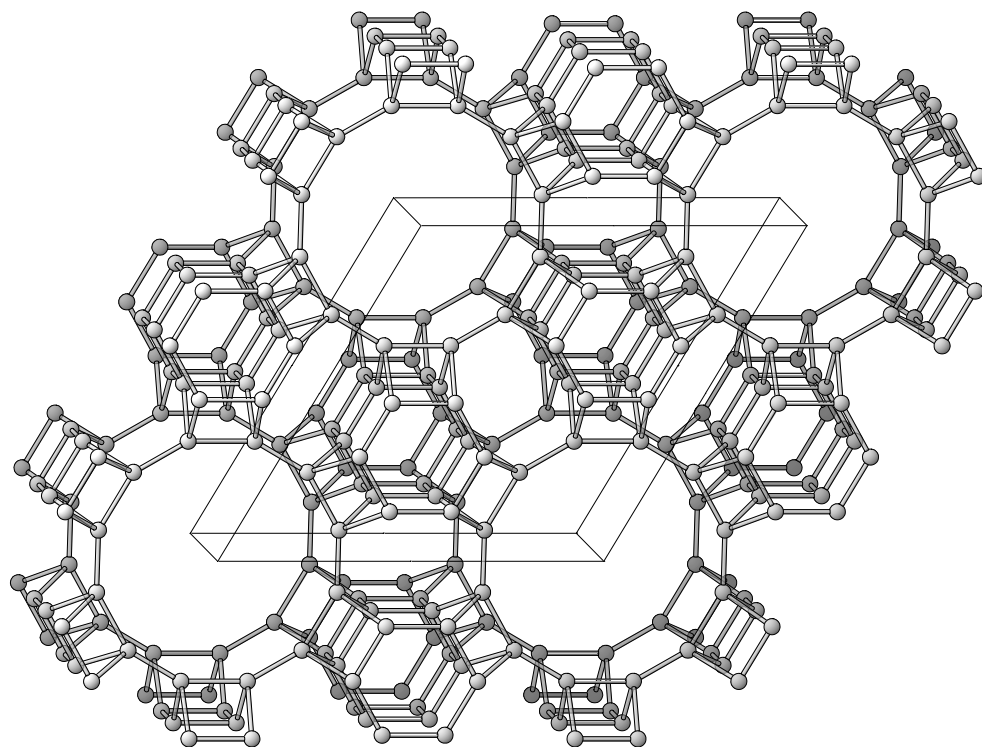


Fig. III.85. **K₃Na₆Al₉Si₂₇O₇₂·21H₂O**

LTL-type (Si,Al) framework.

Sato M. et al. (1990) [1]

Al₉H_{38.64}K_{4.63}Na₆O_{91.32}Si₂₇

$a = 1.8358$, $c = 0.7521$ nm, $c/a = 0.410$, $V = 2.1951$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1058	0.4173	0.1841		non-colinear Si ₂
M2	24r	1	0.1712	0.5055	0.2866		tetrahedron O ₄
O3	12q	$m..$	0.1547	0.4798	$\frac{1}{2}$		non-colinear Si ₂
M4	12p	$m..$	0.0927	0.3578	0		tetrahedron O ₄
(OH ₂)5	12o	$.m.$	0.0694	0.1389	0.218	0.67	square pyramid (OH ₂) ₅
(OH ₂)6	12o	$.m.$	0.1277	0.2554	0.426	0.42	single atom (OH ₂)
O7	12o	$.m.$	0.2581	0.5162	0.254		non-colinear Si ₂
O8	12o	$.m.$	0.5708	0.1416	0.227		non-colinear Si ₂
O9	6l	$mm2$	0.1606	0.3212	0		non-colinear Si ₂
(OH ₂)10	6k	$m2m$	0.211	0	$\frac{1}{2}$	0.59	square pyramid Na(OH ₂) ₄
Na11	6k	$m2m$	0.3056	0	$\frac{1}{2}$		single atom (OH ₂)
(OH ₂)12	6j	$m2m$	0.109	0	0	0.45	6-vertex polyhedron (OH ₂) ₆
O13	6j	$m2m$	0.2886	0	0		non-colinear Si ₂
K14	3f	mmm	$\frac{1}{2}$	0	0	0.91	coplanar square O ₄

K15 2c -6m2 $\frac{1}{3}$ $\frac{2}{3}$ 0 0.95 trigonal prism O₆

M2 = 0.75Si + 0.25Al; M4 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, R_B = 0.031

Remarks: Approximate composition, we took the amount of Na from the refinement and adjusted the charge balance in the formula given above by removing K. 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] Sato M., Morikawa K., Kurosawa S. (1990), Eur. J. Mineral. 2, 851-859.

191
hP157

HAsF ₆ [H ₂ O] ₆	hP157	(191) <i>P6/mmm</i> – r ² qpo ² n ² l ² jh ² ge ³ c
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HAsF₆·6H₂O [1]

Structural features: H₂O molecules are interconnected via hydrogen bonding to form a clathrate-like framework (not all O have a complete tetrahedral environment); AsF₆ octahedra (partial orientational disorder) in 4²5⁸(6)⁴, 5¹²6³ and 5¹²6² cages.

Wiebcke M., Mootz D. (1988) [1]

AsF_{5.33}H_{11.43}O_{5.71}

a = 1.1714, *c* = 1.3841 nm, *c/a* = 1.182, *V* = 1.6448 nm³, *Z* = 7

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24r	1	0.042	0.153	0.199	0.18	
F2	24r	1	0.059	0.401	0.455	0.25	
F3	12q	<i>m.</i>	0.144	0.489	$\frac{1}{2}$	0.5	
F4	12p	<i>m.</i>	0.19	0.523	0	0.33	
(OH ₂)5	12o	<i>m.</i>	0.128	0.256	0.412	0.5	non-collinear F ₂
(OH ₂)6	12o	<i>m.</i>	0.2069	0.4138	0.2627		
(OH ₂)7	12n	<i>.m</i>	0.372	0	0.1581		non-coplanar triangle (OH ₂) ₃
F8	12n	<i>.m</i>	0.442	0	0.386	0.5	
F9	6l	<i>mm2</i>	0.251	0.502	0	0.33	
F10	6l	<i>mm2</i>	0.584	0.168	0	0.33	
(OH ₂)11	6j	<i>m2m</i>	0.24	0	0		non-collinear (OH ₂) ₂
F12	4h	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.117		single atom As
(OH ₂)13	4h	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.326		4-vertex polyhedron (OH ₂) ₃ F
As14	3g	<i>mmm</i>	$\frac{1}{2}$	0	$\frac{1}{2}$		
F15	2e	6 <i>mm</i>	0	0	0.068	0.55	collinear AsF
M16	2e	6 <i>mm</i>	0	0	0.1938		
M17	2e	6 <i>mm</i>	0	0	0.326		single atom As
As18	2c	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		collinear F ₂

M16 = 0.55As + 0.45F; M17 = 0.55F + 0.45As

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.129, T = 148 K

Remarks: Part of F delocalized. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Average structure; additional reflections could be indexed with a 4-fold supercell (new axes 2a,2b,c).

References: [1] Wiebcke M., Mootz D. (1988), Z. Kristallogr. 183, 1-13.

191
hP159

HSbF ₆ [H ₂ O] ₆	hP159	(191) <i>P6/mmm</i> – r ² qpo ² n ² l ² j ² h ² ge ⁴ c
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HSbF₆·6H₂O [1]

Structural features: H₂O molecules are interconnected via hydrogen bonding to form a clathrate-like framework (not all O have a complete tetrahedral environment); SbF₆ octahedra (partial orientational disorder) in 4²5⁸(6)⁴, 5¹²6³ and 5¹²6² cages.

Wiebcke M., Mootz D. (1988) [1]

F_{5.30}H_{11.98}O_{5.99}Sb*a* = 1.184, *c* = 1.39 nm, *c/a* = 1.174, *V* = 1.6875 nm³, *Z* = 7

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24r	1	0.035	0.161	0.198	0.2	
F2	24r	1	0.067	0.388	0.45	0.25	non-colinear F ₂
F3	12q	<i>m.</i>	0.169	0.525	1/2	0.5	single atom F
F4	12p	<i>m.</i>	0.173	0.506	0	0.33	
(OH ₂)5	12o	<i>m.</i>	0.134	0.268	0.403	0.66	non-colinear F ₂
(OH ₂)6	12o	<i>m.</i>	0.2104	0.4208	0.2644		non-colinear (OH ₂) ₂
(OH ₂)7	12n	<i>m.</i>	0.3767	0	0.112		non-coplanar triangle (OH ₂)F ₂
F8	12n	<i>m.</i>	0.441	0	0.375	0.5	4-vertex polyhedron F ₃ Sb
F9	6l	<i>mm</i> 2	0.241	0.482	0	0.33	
F10	6l	<i>mm</i> 2	0.575	0.15	0	0.33	
(OH ₂)11	6j	<i>m</i> 2 <i>m</i>	0.243	0	0		non-colinear (OH ₂) ₂
F12	4h	3 <i>m.</i>	1/3	2/3	0.132		single atom Sb
(OH ₂)13	4h	3 <i>m.</i>	1/3	2/3	0.327		4-vertex polyhedron (OH ₂) ₃ F
Sb14	3g	<i>mmm</i>	1/2	0	1/2		16-vertex Frank-Kasper F ₁₆
F15	2e	6 <i>mm</i>	0	0	0.061	0.6	colinear FSb
Sb16	2e	6 <i>mm</i>	0	0	0.1918	0.6	
Sb17	2e	6 <i>mm</i>	0	0	0.2841	0.4	
F18	2e	6 <i>mm</i>	0	0	0.335	0.6	
Sb19	2c	-6 <i>m</i> 2	1/3	2/3	0		

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.098, T = 108 K

Remarks: Part of F delocalized. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Average structure; additional reflections could be indexed with a 4-fold supercell (new axes 2a,2b,c).

References: [1] Wiebcke M., Mootz D. (1988), Z. Kristallogr. 183, 1-13.

191
hP167

Na ₂₆ Cd ₁₄₁	hP167	(191) <i>P6/mmm</i> – rqp ⁴ nm ² l ² k ² j ² ieca
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Na₂₆Cd₁₄₁ [1]

Structural features: Three kinds of atom layer are stacked along [001]; Cd forms a 3D-framework.

Todorov E., Sevov S.C. (1998) [1]

Cd₁₄₁Na₂₆*a* = 2.1306, *c* = 0.9625 nm, *c/a* = 0.452, *V* = 3.7839 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	24r	1	0.11074	0.45432	0.27575		icosahedron Cd ₉ Na ₃
Cd2	12q	m..	0.08384	0.31683	1/2		pseudo Frank-Kasper Cd ₁₀ Na ₃
Cd3	12p	m..	0.12939	0.40832	0		icosahedron Cd ₉ Na ₃
Cd4	12o	.m.	0.09439	0.18877	0.2627		pseudo Frank-Kasper Cd ₁₀ Na ₃
Cd5	12o	.m.	0.17908	0.35816	0.2564		icosahedron Cd ₉ Na ₃
Cd6	12o	.m.	0.26176	0.52352	0.1545		icosahedron Cd ₉ Na ₃
Cd7	12o	.m.	0.61929	0.23858	0.3386		icosahedron Cd ₉ Na ₃
Na8	12n	..m	0.2766	0	0.1914		7-capped pentagonal prism Cd ₁₆ Na
Na9	6m	mm2	0.2415	0.4831	1/2		pseudo Frank-Kasper Cd ₁₈
Cd10	6m	mm2	0.5537	0.1074	1/2		pseudo Frank-Kasper Cd ₁₁ Na ₂
Cd11	6l	mm2	0.13653	0.27306	0		icosahedron Cd ₈ Na ₄
Na12	6l	mm2	0.5754	0.1509	0		7-capped pentagonal prism Cd ₁₇
Cd13	6k	m2m	0.15021	0	1/2		icosahedron Cd ₈ Na ₄
Cd14	6k	m2m	0.39367	0	1/2		cuboctahedron Cd ₁₀ Na ₂
Cd15	6j	m2m	0.13729	0	0		pseudo Frank-Kasper Cd ₉ Na ₂
Cd16	6j	m2m	0.42041	0	0		pseudo Frank-Kasper Cd ₉ Na ₄
Cd17	6i	2mm	1/2	0	0.2541		cuboctahedron Cd ₁₀ Na ₂
Na18	2e	6mm	0	0	0.324		14-vertex Frank-Kasper Cd ₁₃ Na
Cd19	2c	-6m2	1/3	2/3	0		15-vertex Frank-Kasper Cd ₁₂ Na ₃
Cd20	1a	6/mmm	0	0	0		8-vertex polyhedron Cd ₆ Na ₂

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.030, T = 293 K

Remarks: In fig. 4 of [1] the drawings of the layers called B and C are interchanged.

References: [1] Todorov E., Sevov S.C. (1998), Inorg. Chem. 37, 6341-6345.

191
hP168

Y ₁₃ Pd ₄₀ Sn ₃₁	hP168	(191) P6/mmm – rqp ⁴ nm ² l ² k ² j ² iedc
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Y₁₃Pd₄₀Sn₃₁ [1]; TaCo₄Si₃ [2]

Structural features: Intergrowth of ternary CaCu₅- and MnCu₂Al-type columns; columns of alternating single PdSn₆ and SnPd₆ trigonal prisms in channels.

Cenzual K., Parthé E. (1984) [1]

Pd₄₀Sn₃₁Y₁₃

a = 1.9891, *c* = 0.9246 nm, *c/a* = 0.465, *V* = 3.1681 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pd1	24r	1	0.1058	0.4476	0.2211		pseudo Frank-Kasper Sn ₅ Pd ₅ Y ₃
Sn2	12q	m..	0.1264	0.4111	1/2		icosahedron Pd ₆ Y ₃ Sn ₃
Pd3	12p	m..	0.0857	0.3209	0		pseudo Frank-Kasper Sn ₄ Pd ₆ Y ₃
Pd4	12o	.m.	0.0884	0.1768	0.2419		pseudo Frank-Kasper Sn ₅ Pd ₅ Y ₃
Sn5	12o	.m.	0.1776	0.3552	0.2333		icosahedron Pd ₇ Sn ₂ Y ₃
Pd6	12o	.m.	0.2603	0.5206	0.348		icosahedron Sn ₆ Pd ₃ Y ₃
Sn7	12o	.m.	0.6073	0.2146	0.1869		14-vertex Frank-Kasper Pd ₆ Y ₃ Sn ₅
Y8	12n	..m	0.2712	0	0.2895		7-capped pentagonal prism Pd ₉ Sn ₇ Y
Pd9	6m	mm2	0.141	0.282	1/2		icosahedron Sn ₆ Pd ₂ Y ₄
Y10	6m	mm2	0.5761	0.1522	1/2		7-capped pentagonal prism Pd ₁₀ Sn ₇
Y11	6l	mm2	0.2433	0.4866	0		pseudo Frank-Kasper Pd ₁₁ Sn ₈
Pd12	6l	mm2	0.5452	0.0904	0		11-vertex polyhedron Sn ₆ Pd ₅

Sn13	6k	m2m	0.1459	0	$\frac{1}{2}$	bicapped square prism Pd ₆ Sn ₂ Y ₂
Pd14	6k	m2m	0.4225	0	$\frac{1}{2}$	pseudo Frank-Kasper Sn ₄ Y ₄ Pd ₅
Sn15	6j	m2m	0.1621	0	0	trigonal prism Pd ₆
Sn16	6j	m2m	0.3862	0	0	icosahedron Pd ₈ Sn ₂ Y ₂
Sn17	6i	2mm	$\frac{1}{2}$	0	0.2584	14-vertex Frank-Kasper Pd ₈ Sn ₄ Y ₂
Y18	2e	6mm	0	0	0.194	pseudo Frank-Kasper Pd ₆ YSn ₁₂
Sn19	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	15-vertex Frank-Kasper Pd ₆ Y ₃ Sn ₆
Pd20	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0	tricapped trigonal prism Sn ₆ Y ₃

Experimental: single crystal, diffractometer, X-rays, wR = 0.067, T = 293 K

Remarks: Refinement fixing the displacement parameter of site Y18 gave occ = 0.83(5). The Ta site on the c-axis (occ = 0.78) in TaCo₄Si₃ [2] is shifted along 0 0 z so that it is located in a different hexagonal antiprism. In table 1 of [2] the x-coordinate of site Si(2) is misprinted as $\frac{1}{3}$ instead of $\frac{1}{2}$.

References: [1] Cenxual K., Parthé E. (1984), Acta Crystallogr. C 40, 1127-1131. [2] Vilasi M., Venturini G., Steinmetz J., Malaman B. (1995), J. Alloys Compd. 227, 32-36.

191
hP169

Sc_{12.3}Ni_{40.7}Ge₃₁ hP169 (191) P6/mmm – rqp⁴nm²l²k²j²iedca

Sc_{12.3}Ni_{40.7}Ge₃₁ [1]

Structural features: Intergrowth of ternary CaCu₅- and MnCu₂Al-type columns; columns of alternating single NiGe₆ and GeNi₆ trigonal prisms in channels. Variant of Y₁₃Pd₄₀Sn₃₁ with a different atom arrangement along 0 0 z (partial disorder).

Bodak O.I. et al. (1990) [1]

Ge₃₁Ni_{40.67}Sc_{12.32}

a = 1.7865, c = 0.822 nm, c/a = 0.460, V = 2.2720 nm³, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	24r	1	0.1052	0.4491	0.2764		pseudo Frank-Kasper Ge ₅ Ni ₅ Sc ₃
Ni2	12q	m..	0.0859	0.322	$\frac{1}{2}$		pseudo Frank-Kasper Ge ₄ Ni ₆ Sc ₃
Ge3	12p	m..	0.1273	0.4118	0		icosahedron Ni ₆ Sc ₃ Ge ₃
Ni4	12o	.m.	0.0883	0.1766	0.2611		14-vertex Frank-Kasper Ge ₅ Ni ₆ Sc ₃
Ge5	12o	.m.	0.178	0.356	0.2699		icosahedron Ni ₇ Ge ₂ Sc ₃
Ni6	12o	.m.	0.2609	0.5218	0.1545		icosahedron Ge ₆ Ni ₃ Sc ₃
Ge7	12o	.m.	0.6063	0.2126	0.3159		14-vertex Frank-Kasper Ni ₆ Sc ₃ Ge ₅
Sc8	12n	.m	0.2721	0	0.2058		7-capped pentagonal prism Ni ₉ Ge ₇ Sc
Sc9	6m	mm2	0.2446	0.4892	$\frac{1}{2}$		15-vertex polyhedron Ni ₉ Ge ₆
Ni10	6m	mm2	0.5434	0.0868	$\frac{1}{2}$		pentacapped trigonal prism Ge ₆ Ni ₅
Ni11	6l	mm2	0.142	0.284	0		icosahedron Ge ₆ Ni ₂ Sc ₄
Sc12	6l	mm2	0.5763	0.1526	0		7-capped pentagonal prism Ge ₇ Ni ₁₀
Ge13	6k	m2m	0.1656	0	$\frac{1}{2}$		trigonal prism Ni ₆
Ge14	6k	m2m	0.3856	0	$\frac{1}{2}$		square prism (cube) Ni ₈
Ge15	6j	m2m	0.1457	0	0		pseudo Frank-Kasper Ni ₆ Ge ₂ Sc ₃
Ni16	6j	m2m	0.42	0	0		pseudo Frank-Kasper Ge ₄ Sc ₄ Ni ₅
Ge17	6i	2mm	$\frac{1}{2}$	0	0.2337		8-vertex polyhedron Ni ₈
Ni18	2e	6mm	0	0	0.33	0.67	8-vertex polyhedron ScNi ₇
Ni19	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Ge ₆ Sc ₃
Ge20	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		tricapped trigonal prism Ni ₆ Sc ₃
Sc21	1a	6/mmm	0	0	0	0.64	8-vertex polyhedron Ge ₆ Ni ₂

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Bodak O.I., Pavlyuk V.V., Andrusyak R.I., Kotur B.Y., Pecharskii V.K., Bruskov V.A. (1990), Sov. Phys. Crystallogr. 35, 173-175 (Kristallografiya 35, 312-315).

191
hP170

$K_{9.5}(Al_{0.26}Si_{0.74})_{36}O_{72}[H_2O]_{5.1}$	<i>hP170</i>	(191) <i>P6/mmm</i> – $r^2qpo^3nml^2k^2j^2feca$
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$K_{9.5}Al_{9.5}Si_{26.5}O_{72} \cdot xH_2O$ [1], zeolite LTL-K residual water

Structural features: (Si,Al) O_4 tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions), between non-planar 6-rings (C) and at the centers of 8-rings (D), H_2O in the channels (disorder).

Hirano M. et al. (1992) [1]

$Al_{9.50}H_{10.20}K_{9.32}O_{77.10}Si_{26.50}$

$a = 1.8367$, $c = 0.75227$ nm, $c/a = 0.410$, $V = 2.1978$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.103	0.415	0.168		non-colinear Si ₂
M2	24r	1	0.1673	0.4998	0.2861		tetrahedron O ₄
O3	12q	<i>m..</i>	0.146	0.478	$\frac{1}{2}$		non-colinear Si ₂
M4	12p	<i>m..</i>	0.0929	0.3578	0		tetrahedron O ₄
(OH ₂)5	12o	<i>.m.</i>	0.073	0.146	0.26	0.1	non-colinear (OH ₂) ₂
O6	12o	<i>.m.</i>	0.2641	0.5282	0.249		non-colinear Si ₂
O7	12o	<i>.m.</i>	0.5728	0.1456	0.216		non-colinear Si ₂
(OH ₂)8	12n	<i>.m</i>	0.137	0	0.241	0.1	non-colinear (OH ₂) ₂
(OH ₂)9	6m	<i>mm2</i>	0.132	0.264	$\frac{1}{2}$	0.1	non-colinear (OH ₂) ₂
(OH ₂)10	6l	<i>mm2</i>	0.075	0.15	0	0.1	non-colinear (OH ₂) ₂
O11	6l	<i>mm2</i>	0.1615	0.323	0		non-colinear Si ₂
(OH ₂)12	6k	<i>m2m</i>	0.195	0	$\frac{1}{2}$	0.1	trigonal bipyramid K(OH ₂) ₄
K13	6k	<i>m2m</i>	0.298	0	$\frac{1}{2}$	0.72	single atom (OH ₂)
(OH ₂)14	6j	<i>m2m</i>	0.09	0	0	0.1	non-colinear (OH ₂) ₂
O15	6j	<i>m2m</i>	0.274	0	0		non-colinear Si ₂
K16	3f	<i>mmm</i>	$\frac{1}{2}$	0	0		coplanar square O ₄
(OH ₂)17	2e	<i>6mm</i>	0	0	0.349	0.1	7-vertex polyhedron (OH ₂) ₇
K18	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆
(OH ₂)19	1a	<i>6/mmm</i>	0	0	0	0.1	coplanar hexagon (OH ₂) ₆

$M2 = 0.736Si + 0.264Al$; $M4 = 0.736Si + 0.264Al$

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R = 0.034$

Remarks: Refinement of the occupancies of sites M2, M4, K16 and K18 showed no significant deviation from unity. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition and an arbitrary low value to the occupancies of sites (OH₂). 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] Hirano M., Kato M., Asada E., Tsutsumi K., Shiraishi A. (1992), X-sen Bunseki no Shinpo 23, 101-110.

191
hP172

$\text{K}_6\text{Na}_3(\text{Al}_{0.25}\text{Si}_{0.75})_{36}\text{O}_{72}[\text{H}_2\text{O}]_{21}$ *hP172* (191) *P6/mmm* – $\text{r}^2\text{qpo}^3\text{nml}^2\text{k}^2\text{j}^2\text{fedca}$

$\text{K}_6\text{Na}_3\text{Al}_9\text{Si}_{27}\text{O}_{72}\cdot 21\text{H}_2\text{O}$ [1], zeolite LTL-K,Na hydrated

Structural features: (Si,Al) O_4 tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions) and between non-planar 6-rings (C), Na at the centers of 8-rings (D) and at prism centers (A), H_2O in the channels (disorder).

Barrer R.M., Villiger H. (1969) [1]

$\text{Al}_9\text{H}_{41.60}\text{K}_{4.70}\text{Na}_{4.80}\text{O}_{92.80}\text{Si}_{27}$

$a = 1.84$, $c = 0.752$ nm, $c/a = 0.409$, $V = 2.2049$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1004	0.4078	0.17		non-colinear Si ₂
M2	24r	1	0.1662	0.4989	0.2863		tetrahedron O ₄
O3	12q	<i>m..</i>	0.136	0.4691	$\frac{1}{2}$		non-colinear Si ₂
M4	12p	<i>m..</i>	0.0946	0.3595	0		tetrahedron O ₄
(OH ₂)5	12o	<i>.m.</i>	0.092	0.184	0.297	0.25	non-coplanar triangle (OH ₂) ₃
O6	12o	<i>.m.</i>	0.262	0.524	0.24		non-colinear Si ₂
O7	12o	<i>.m.</i>	0.5739	0.1478	0.225		non-colinear Si ₂
(OH ₂)8	12n	<i>..m</i>	0.135	0	0.257	0.25	non-colinear (OH ₂) ₂
(OH ₂)9	6m	<i>mm2</i>	0.116	0.232	$\frac{1}{2}$	0.7	non-coplanar square (OH ₂) ₄
(OH ₂)10	6l	<i>mm2</i>	0.07	0.14	0	0.7	non-colinear (OH ₂) ₂
O11	6l	<i>mm2</i>	0.1646	0.3292	0		non-colinear Si ₂
(OH ₂)12	6k	<i>m2m</i>	0.195	0	$\frac{1}{2}$	0.5	trigonal bipyramid (OH ₂) ₄ Na
Na13	6k	<i>m2m</i>	0.303	0	$\frac{1}{2}$	0.6	single atom (OH ₂)
(OH ₂)14	6j	<i>m2m</i>	0.09	0	0	0.25	non-colinear (OH ₂) ₂
O15	6j	<i>m2m</i>	0.2674	0	0		non-colinear Si ₂
K16	3f	<i>mmm</i>	$\frac{1}{2}$	0	0	0.9	coplanar square O ₄
(OH ₂)17	2e	<i>6mm</i>	0	0	0.311	0.7	single atom (OH ₂)
Na18	2d	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.6	trigonal prism O ₆
K19	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism O ₆
(OH ₂)20	1a	<i>6/mmm</i>	0	0	0	0.5	coplanar hexagon (OH ₂) ₆

M2 = 0.75Si + 0.25Al; M4 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.140$

Remarks: Partial substitution by K on site Na18 could not be excluded. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (194) *P6₃/mmc* was tested and rejected. In table 1 of [1] the Wyckoff position of former O(1) is misprinted as 6j instead of 6k.

References: [1] Barrer R.M., Villiger H. (1969), Z. Kristallogr. 128, 352-370.

191
hP172

$\text{Li}_{13}\text{Ni}_{40}\text{Si}_{31}$ *hP172* (191) *P6/mmm* – $\text{rqpo}^4\text{nm}^2\text{l}^2\text{k}^2\text{j}^2\text{ih}^2\text{e}$

$\text{Li}_{13}\text{Ni}_{40}\text{Si}_{31}$ [2]

Structural features: Intergrowth of ternary CaCu_5 - and MnCu_2Al -type columns; columns of alternating single NiSi_6 and SiNi_6 trigonal prisms in channels. Variant of $\text{Y}_{13}\text{Pd}_{40}\text{Sn}_{31}$ with splitting of the sites centering the trigonal prisms.

Bodak O.I. et al. (1990) [1]

$\text{Li}_{13}\text{Ni}_{40}\text{Si}_{31}$

$a = 1.7092$, $c = 0.7848$ nm, $c/a = 0.459$, $V = 1.9855$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	24r	1	0.1014	0.444	0.2746		pseudo Frank-Kasper $\text{Si}_5\text{Li}_3\text{Ni}_5$
Ni2	12q	$m..$	0.0859	0.3157	$1/2$		pseudo Frank-Kasper $\text{Si}_4\text{Ni}_6\text{Li}_3$
Si3	12p	$m..$	0.1335	0.4189	0		icosahedron $\text{Ni}_6\text{Li}_3\text{Si}_3$
Ni4	12o	$.m.$	0.0938	0.1876	0.2663		pseudo Frank-Kasper $\text{Si}_5\text{Ni}_5\text{Li}_3$
Si5	12o	$.m.$	0.1791	0.3582	0.2622		icosahedron $\text{Ni}_7\text{Li}_3\text{Si}_2$
Ni6	12o	$.m.$	0.265	0.53	0.1628		
Si7	12o	$.m.$	0.6045	0.209	0.326		
Li8	12n	$.m$	0.28	0	0.186		pseudo Frank-Kasper $\text{Ni}_9\text{Si}_8\text{Li}$
Li9	6m	$mm2$	0.234	0.468	$1/2$		
Ni10	6m	$mm2$	0.5424	0.0848	$1/2$		pentacapped trigonal prism Si_6Ni_5
Ni11	6l	$mm2$	0.1424	0.2848	0		icosahedron $\text{Si}_6\text{Ni}_2\text{Li}_4$
Li12	6l	$mm2$	0.574	0.148	0		
Si13	6k	$m2m$	0.1613	0	$1/2$		trigonal prism Ni_6
Si14	6k	$m2m$	0.3831	0	$1/2$		square prism (cube) Ni_8
Si15	6j	$m2m$	0.148	0	0		icosahedron $\text{Ni}_6\text{Si}_2\text{Li}_4$
Ni16	6j	$m2m$	0.4204	0	0		pseudo Frank-Kasper $\text{Si}_4\text{Li}_4\text{Ni}_5$
Si17	6i	$2mm$	$1/2$	0	0.234		8-vertex polyhedron Ni_8
Si18	4h	$3m.$	$1/3$	$2/3$	0.041	0.5	
Ni19	4h	$3m.$	$1/3$	$2/3$	0.436	0.5	
Li20	2e	$6mm$	0	0	0.23		pseudo Frank-Kasper $\text{Ni}_6\text{Si}_{12}\text{Li}$

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s).

References: [1] Bodak O.I., Pavlyuk V.V., Andrusyak R.I., Kotur B.Y., Pecharskii V.K., Bruskov V.A. (1990), Sov. Phys. Crystallogr. 35, 173-175 (Kristallografiya 35, 312-315). [2] Pavlyuk V.V., Bodak O.I., Pecharsky V.K., Gladyshevsky E.I. (1989), Eur. Crystallogr. Meet., 12th, Moscow 1989, Coll. Abstr. vol. 2, p. 126.

191
hP173

$\text{Li}_{27}\text{Cu}_{50}(\text{Cu}_{0.9}\text{Si}_{0.1})_{36}\text{Si}_{50}$	$hP173$	(191) $P6/mmm - \text{rqp}^4\text{nm}^2\text{l}^2\text{k}^2\text{j}^2\text{ih}^2\text{ea}$
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LiCu_3Si_2 [1]

Structural features: Intergrowth of ternary CaCu_5 - and MnCu_2Al -type columns; additional atoms in channels. Variant of $\text{Y}_{13}\text{Pd}_{40}\text{Sn}_{31}$ with splitting of several sites.

Pavlyuk V.V. et al. (1995) [1]

$\text{Cu}_{81.47}\text{Li}_{27}\text{Si}_{54.11}$

$a = 1.7083$, $c = 0.7853$ nm, $c/a = 0.460$, $V = 1.9847$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24r	1	0.10192	0.44442	0.22544		pseudo Frank-Kasper $\text{Si}_4\text{Cu}_6\text{Li}_3$
Si2	12q	$m..$	0.1325	0.4178	$1/2$		icosahedron $\text{Cu}_6\text{Li}_3\text{Si}_3$

Cu3	12p	<i>m.</i>	0.08596	0.31568	0		pseudo Frank-Kasper Si ₄ Cu ₆ Li ₃
M4	12o	<i>.m.</i>	0.09377	0.18754	0.2348		pseudo Frank-Kasper Si ₅ Cu ₅ Li ₃
Si5	12o	<i>.m.</i>	0.17936	0.35872	0.2377		icosahedron Cu ₇ Si ₂ Li ₃
Cu6	12o	<i>.m.</i>	0.2649	0.5298	0.3373		
Cu7	12o	<i>.m.</i>	0.60429	0.20858	0.1748	0.458	
Li8	12n	<i>..m</i>	0.2724	0	0.308		7-capped pentagonal prism Si ₇ Cu ₉ Li
Cu9	6m	<i>mm2</i>	0.14215	0.2843	$\frac{1}{2}$		icosahedron Si ₆ Cu ₂ Li ₄
Li10	6m	<i>mm2</i>	0.5757	0.1514	$\frac{1}{2}$		
Li11	6l	<i>mm2</i>	0.2421	0.4842	0		
Cu12	6l	<i>mm2</i>	0.54255	0.0851	0		pentacapped trigonal prism Cu ₇ Si ₄
Si13	6k	<i>m2m</i>	0.1466	0	$\frac{1}{2}$		icosahedron Cu ₆ Si ₂ Li ₄
Cu14	6k	<i>m2m</i>	0.42064	0	$\frac{1}{2}$		pseudo Frank-Kasper Si ₄ Li ₄ Cu ₅
Si15	6j	<i>m2m</i>	0.1603	0	0		pseudo Frank-Kasper Cu ₆ Si ₂ Li ₃
Si16	6j	<i>m2m</i>	0.3821	0	0		cuboctahedron Cu ₈ Si ₂ Li ₂
Si17	6i	<i>2mm</i>	$\frac{1}{2}$	0	0.2654		14-vertex Frank-Kasper Cu ₁₀ Si ₂ Li ₂
Cu18	4h	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0631	0.501	
Si19	4h	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.4641	0.52	
Li20	2e	<i>6mm</i>	0	0	0.325		14-vertex Frank-Kasper Li ₂ Si ₆ Cu ₆
Li21	1a	<i>6/mmm</i>	0	0	0		8-vertex polyhedron Li ₂ Si ₆

M1 = 0.914Cu + 0.086Si; M4 = 0.836Cu + 0.164Si

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.027

References: [1] Pavlyuk V.V., Kevorkov D.G., Bodak O.I., Pecharskii V.K. (1995), Crystallogr. Rep. 40, 161-162 (Kristallografiya 40, 178-179).

191
hP174

K_{6.8}Ba_{1.1}(Al_{0.25}Si_{0.75})₃₆O₇₂[H₂O]_{18.4} hP174 (191) P6/mmm – r³qpo³nmlkjfca

K_{6.8}Ba_{1.1}Al₉Si₂₇O₇₂·18.4H₂O [1], zeolite LTL-K,Ba hydrated

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions) and between non-planar 6-rings (C), Ba at the centers of 8-rings (D), H₂O and additional Ba in the channels (disorder).

Sato M. et al. (1990) [1]

Al₉Ba_{1.14}H_{36.72}K_{4.86}O_{90.36}Si₂₇

a = 1.8361, *c* = 0.7525 nm, *c/a* = 0.410, *V* = 2.1970 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24r	1	0.1073	0.4213	0.1876		
(OH ₂)2	24r	1	0.114	0.431	0.27	0.16	
M3	24r	1	0.1671	0.5022	0.2824		single atom (OH ₂)
O4	12q	<i>m.</i>	0.1465	0.4793	$\frac{1}{2}$		coplanar square Si ₂ (OH ₂) ₂
M5	12p	<i>m.</i>	0.094	0.361	0		tetrahedron O ₄
(OH ₂)6	12o	<i>.m.</i>	0.07	0.14	0.105	0.34	single atom (OH ₂)
O7	12o	<i>.m.</i>	0.2659	0.5318	0.208		non-colinear Si ₂
O8	12o	<i>.m.</i>	0.5787	0.1574	0.2184		non-colinear Si ₂
(OH ₂)9	12n	<i>..m</i>	0.1345	0	0.396	0.42	single atom (OH ₂)
(OH ₂)10	6m	<i>mm2</i>	0.1405	0.281	$\frac{1}{2}$	0.9	trigonal prism Ba ₂ (OH ₂) ₄
O11	6l	<i>mm2</i>	0.1648	0.3296	0		non-colinear Si ₂

Ba12	6k	m2m	0.298	0	1/2	0.18	trigonal prism (OH ₂) ₆
O13	6j	m2m	0.2752	0	0		non-collinear Si ₂
K14	3f	mmm	1/2	0	0		coplanar square O ₄
K15	2c	-6m2	1/3	2/3	0	0.93	trigonal prism O ₆
Ba16	1a	6/mmm	0	0	0	0.06	hexagonal prism (OH ₂) ₁₂

M3 = 0.75Si + 0.25Al; M5 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 1/2

Experimental: powder, diffractometer, X-rays, R_B = 0.032

Remarks: Approximate composition, we took the amounts of Ba and H₂O from the refinement and adjusted the charge balance in the formula given above by adding K. We set the y-coordinate of former O(2) (framework oxygen) equal to 2x to be in agreement with Wyckoff position 6m (given in [1]). We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. Short interatomic distances: d(O1-(OH₂)₂) = 0.064 nm. 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] Sato M., Morikawa K., Kurosawa S. (1990), Eur. J. Mineral. 2, 851-859.

191
hP174

K ₆ Sr _{1.5} (Al _{0.25} Si _{0.75}) ₃₆ O ₇₂ [H ₂ O] ₂₁	hP174	(191) P6/mmm – r ³ qpo ⁴ mlkjfca
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K₆Sr_{1.5}Al₉Si₂₇O₇₂·xH₂O [1], zeolite LTL-K,Sr hydrated

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at the centers of cancrinite-type cages (B positions) and between non-planar 6-rings (C), Sr at the centers of 8-rings (D), H₂O and additional Sr in the channels (disorder).

Sato M. et al. (1990) [1]

Al₉H_{23.88}K_{4.64}O_{83.94}Si₂₇Sr_{1.46}

a = 1.8358, c = 0.7523 nm, c/a = 0.410, V = 2.1957 nm³, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24r	1	0.09	0.4235	0.404	0.27	non-collinear O(OH ₂)
O2	24r	1	0.1074	0.4244	0.1876		non-coplanar triangle Si ₂ (OH ₂)
M3	24r	1	0.1677	0.5019	0.2864		square pyramid O ₄ (OH ₂)
O4	12q	m..	0.1508	0.4856	1/2		non-collinear (OH ₂) ₂
M5	12p	m..	0.0928	0.3556	0		tetrahedron O ₄
(OH ₂)6	12o	.m.	0.082	0.164	0.166	0.15	single atom (OH ₂)
(OH ₂)7	12o	.m.	0.124	0.248	0.356	0.13	single atom (OH ₂)
O8	12o	.m.	0.2622	0.5244	0.2163		non-collinear Si ₂
O9	12o	.m.	0.5787	0.1575	0.2182		non-collinear Si ₂
(OH ₂)10	6m	mm2	0.1287	0.2575	1/2	0.35	non-collinear (OH ₂) ₂
O11	6l	mm2	0.1593	0.3186	0		non-collinear Si ₂
Sr12	6k	m2m	0.3094	0	1/2	0.16	non-coplanar square (OH ₂) ₄
O13	6j	m2m	0.2814	0	0		non-collinear Si ₂
K14	3f	mmm	1/2	0	0	0.96	hexagonal prism O ₁₂
K15	2c	-6m2	1/3	2/3	0	0.88	trigonal prism O ₆
Sr16	1a	6/mmm	0	0	0	0.5	hexagonal prism (OH ₂) ₁₂

M3 = 0.75Si + 0.25Al; M5 = 0.75Si + 0.25Al

Transformation from published data: origin shift 0 0 1/2

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

Remarks: Part of H_2O not located. Approximate composition, we took the amount of Sr from the refinement and adjusted the charge balance in the formula given above by adding K. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the y -coordinate of former O(2) is misprinted as 0.3196 instead of 0.3186 (agreement with Wyckoff position 6m).

References: [1] Sato M., Morikawa K., Kurosawa S. (1990), Eur. J. Mineral. 2, 851-859.

191
hP175

$K_8Tl_4(Al_{0.33}Si_{0.67})_{36}O_{72}[H_2O]_{20}$ hP175 (191) $P6/mmm - r^2qpo^3nml^2kj^3hgedc$

$K_8Tl_4Al_{12}Si_{24}O_{72} \cdot 20H_2O$ [1], perialite, zeolite LTL-K,Tl hydrated

Structural features: (Si,Al) O_4 tetrahedra share vertices to form an LTL-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 12-rings parallel to [001]; K at and near the centers of cancrinite-type cages (B positions) and hexagonal prisms (A), additional K, Tl and (K,Tl) at the centers of 8-rings (D, E), H_2O in the channels (disorder).

Artioli G., Kvik Å. (1990) [1]

$Al_{11.88}H_{42.76}K_{7.45}O_{93.38}Si_{24.12}Tl_{3.81}$

$a = 1.85548$, $c = 0.75313$ nm, $c/a = 0.406$, $V = 2.2455$ nm³, $Z = 1$

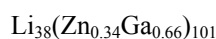
site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1075	0.4149	0.331		non-colinear Si ₂
M2	24r	1	0.1703	0.4976	0.2172		tetrahedron O ₄
M3	12q	$m..$	0.0918	0.3522	$1/2$		tetrahedron O ₄
O4	12p	$m..$	0.16	0.489	0		non-colinear Si ₂
(OH ₂)5	12o	$.m.$	0.137	0.274	0.24	0.42	non-colinear (OH ₂)O
O6	12o	$.m.$	0.265	0.53	0.283		non-colinear Si ₂
O7	12o	$.m.$	0.5819	0.164	0.263		non-colinear Si ₂
(OH ₂)8	12n	$.m$	0.1351	0	0.364	0.83	single atom (OH ₂)
O9	6m	$mm2$	0.1618	0.324	$1/2$		non-colinear Si ₂
(OH ₂)10	6l	$mm2$	0.144	0.288	0	0.53	non-colinear (OH ₂) ₂
(OH ₂)11	6l	$mm2$	0.277	0.554	0	0.31	coplanar triangle KO ₂
O12	6k	$m2m$	0.276	0	$1/2$		non-colinear Si ₂
(OH ₂)13	6j	$m2m$	0.12	0	0	0.1	non-colinear (OH ₂) ₂
K14	6j	$m2m$	0.299	0	0	0.521	
Tl15	6j	$m2m$	0.315	0	0	0.479	
K16	4h	$3m.$	$1/3$	$2/3$	0.443	0.2	
M17	3g	mmm	$1/2$	0	$1/2$		coplanar square O ₄
(OH ₂)18	2e	$6mm$	0	0	0.19	0.37	
K19	2d	$-6m2$	$1/3$	$2/3$	$1/2$	0.6	
K20	2c	$-6m2$	$1/3$	$2/3$	0	0.13	coplanar triangle (OH ₂) ₃

$M2 = 0.67Si + 0.33Al$; $M3 = 0.67Si + 0.33Al$; $M17 = 0.687K + 0.313Tl$

Experimental: powder, diffractometer, X-rays, $R_p = 0.056$

Remarks: Natural specimen from the Murun alkaline massif, Russia. Al/Si ratio ~0.5 from electron microprobe analysis, no Ba detected. 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] Artioli G., Kvik Å. (1990), Eur. J. Mineral. 2, 749-759.

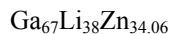
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hP184

hP184

(191) $P6/mmm - \text{rqp}^2\text{o}^4\text{n}^3\text{mlj}^3\text{he}^2\text{c}$ **Li₃₈(Ga,Zn)₁₀₁** [1]

Structural features: (Ga,Zn) forms a 3D-framework with (Ga,Zn)₁₂ icosahedra, (Ga,Zn)₁₆ and (Ga,Zn)₂₉ polyhedra.

Tillard Charbonnel M. et al. (1992) [1]



$a = 1.4174$, $c = 1.3535$ nm, $c/a = 0.955$, $V = 2.3549$ nm³, $Z = 1$

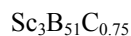
site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24r	1	0.1984	0.4364	0.0961	0.5	
M2	12q	m..	0.1602	0.4898	$\frac{1}{2}$		11-vertex polyhedron Ga ₆ Li ₅
M3	12p	m..	0.1020	0.5150	0	0.18	
M4	12p	m..	0.103	0.461	0	0.33	
M5	12o	.m.	0.1187	0.2374	0.1521		
Li6	12o	.m.	0.209	0.418	0.3		
M7	12o	.m.	0.5522	0.1044	0.3359		11-vertex polyhedron Ga ₆ Li ₅
M8	12o	.m.	0.6020	0.2040	0.176		
M9	12n	..m	0.1843	0	0.3176		icosahedron Ga ₆ Li ₆
M10	12n	..m	0.3440	0	0.3988		11-vertex polyhedron Ga ₆ Li ₅
Li11	12n	..m	0.367	0	0.175		
Li12	6m	mm2	0.128	0.256	$\frac{1}{2}$		16-vertex Frank-Kasper Ga ₁₂ Li ₄
M13	6l	mm2	0.5514	0.1028	0	0.32	
M14	6j	m2m	0.1092	0	0	0.5	
M15	6j	m2m	0.2351	0	0	0.38	
M16	6j	m2m	0.3071	0	0	0.29	
Li17	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.383		16-vertex Frank-Kasper Ga ₁₂ Li ₄
Li18	2e	6mm	0	0	0.185		
M19	2e	6mm	0	0	0.4091		14-vertex Frank-Kasper Ga ₇ Li ₇
Li20	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	0		

M1-M19 = 0.663Ga + 0.337Zn

Experimental: single crystal, diffractometer, X-rays, wR = 0.052

Remarks: Composition Li:0.88Zn:1.73Ga from atomic absorption. We assigned an approximate value to the Ga/Zn ratio of sites M based on the chemical analysis. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Average structure; additional reflections could be indexed with an 18-fold supercell (new axes 3a,3b,2c), space group (189) $P-62m$.

References: [1] Tillard Charbonnel M., Chouaibi N., Belin C., Lapasset J. (1992), Eur. J. Solid State Inorg. Chem. 29, 347-359.

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hP212

hP212

(191) $P6/mmm - \text{r}^2\text{q}^2\text{p}^2\text{o}^4\text{n}^3\text{m}^2\text{l}^2\text{h}^2$ **ScB₁₇C_{0.25}** [1]

Structural features: B₁₂ icosahedra and B₁₂ hexagonal antiprisms are interconnected via exo-bonds to form a 3D-framework; additional B in tubes formed by the directly superposed antiprisms (partial disorder).

Leithe Jasper A. et al. (2000) [1]

$B_{48.10}C_{0.71}Sc_3$

$a = 1.45501$, $c = 0.89543$ nm, $c/a = 0.615$, $V = 1.6417$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	24r	1	0.0726	0.3803	0.1661		pentagonal pyramid B ₆
B2	24r	1	0.1395	0.4015	0.3351		pentagonal pyramid B ₆
B3	12q	m..	0.0663	0.3301	$\frac{1}{2}$		pentagonal pyramid B ₆
B4	12q	m..	0.1329	0.47	$\frac{1}{2}$		pentagonal pyramid B ₆
B5	12p	m..	0.1139	0.3405	0		pentagonal pyramid B ₆
B6	12p	m..	0.1187	0.4625	0		pentagonal pyramid B ₆
B7	12o	.m.	0.0771	0.1542	0.3347		pentagonal pyramid B ₆
B8	12o	.m.	0.1419	0.2838	0.4011		pentagonal pyramid B ₆
B9	12o	.m.	0.2621	0.5242	0.4014		pentagonal pyramid B ₆
Sc10	12o	.m.	0.5749	0.1498	0.2496		16-vertex Frank-Kasper B ₁₆
B11	12n	..m	0.1327	0	0.1664		7-vertex polyhedron B ₇
B12	12n	..m	0.2429	0	0.0995		pentagonal pyramid B ₆
B13	12n	..m	0.4395	0	0.0984		pentagonal pyramid B ₆
B14	6m	mm2	0.0391	0.0782	$\frac{1}{2}$	0.53	coplanar triangle B ₃
M15	6m	mm2	0.5306	0.0612	$\frac{1}{2}$		
B16	6l	mm2	0.0379	0.0758	0	0.67	tetrahedron B ₄
M17	6l	mm2	0.6056	0.2112	0		
B18	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1165		tetrahedron B ₄
B19	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.3288		tetrahedron B ₄

M15 = 0.73B + 0.27C; M17 = 0.80B + 0.20C

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

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

Remarks: Homogeneity range $ScB_{16.5+x}C_{0.2+y}$, $0 < x < 2.2$, $0 < y < 0.44$. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies.

References: [1] Leithe Jasper A., Bourgeois L., Michiue Y., Shi Y., Tanaka T. (2000), J. Solid State Chem. 154, 130-136.

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hP216

SiO ₂	hP216	(191) $P6/mmm - r^2o^7n^4i^2h^4d$
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SiO₂ ITQ-1 [1], zeolite MWW

Structural features: SiO₄ tetrahedra share vertices to form an MWW-type zeolite framework with 2D-systems of channels delimited by 10-rings perpendicular to [001].

Camblor M.A. et al. (1998) [1]

O₂Si

$a = 1.42081$, $c = 2.4945$ nm, $c/a = 1.756$, $V = 4.3610$ nm³, $Z = 72$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.1048	0.3942	0.3652		non-colinear Si ₂
O2	24r	1	0.1063	0.3945	0.1884		non-colinear Si ₂
Si3	12o	.m.	0.1272	0.2544	0.0593		tetrahedron O ₄
O4	12o	.m.	0.1768	0.3536	0.0986		non-colinear Si ₂
Si5	12o	.m.	0.2108	0.4216	0.153		tetrahedron O ₄
Si6	12o	.m.	0.2342	0.4684	0.3644		tetrahedron O ₄

O7	12o	.m.	0.2705	0.541	0.4178	non-colinear Si ₂
O8	12o	.m.	0.2726	0.5453	0.3118	non-colinear Si ₂
O9	12o	.m.	0.2735	0.547	0.1362	non-colinear Si ₂
O10	12n	..m	0.1835	0	0.07	non-colinear Si ₂
O11	12n	..m	0.3763	0	0.2761	non-colinear Si ₂
Si12	12n	..m	0.3895	0	0.2128	tetrahedron O ₄
Si13	12n	..m	0.3904	0	0.3393	tetrahedron O ₄
O14	6l	mm2	0.1508	0.3016	0	non-colinear Si ₂
O15	6i	2mm	$\frac{1}{2}$	0	0.1979	non-colinear Si ₂
O16	6i	2mm	$\frac{1}{2}$	0	0.3551	non-colinear Si ₂
Si17	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1596	tetrahedron O ₄
O18	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2245	colinear Si ₂
Si19	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2892	tetrahedron O ₄
Si20	4h	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.4367	tetrahedron O ₄
O21	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	colinear Si ₂

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, synchrotron, R_B = 0.065

References: [1] Cambor M.A., Corma A., Diaz Cabanas M.J., Baerlocher C. (1998), J. Phys. Chem. B 102, 44-51.

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hP324

K₂₄(Al_{0.22}Si_{0.78})₁₀₈O₂₁₆

hP324

(191) $P6/mmm - r^8 q^3 p^4 o^2 l^2 j^2$

K₂₄Al₂₄Si₈₄O₂₁₆ [1], zeolite ZSM-10

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and two kinds of channel delimited by 12-rings parallel to [001].

Higgins J.B., Schmitt K.D. (1996) [1]

Al_{23.98}O₂₁₆Si_{84.02}

$a = 3.1575$, $c = 0.7525$ nm, $c/a = 0.238$, $V = 6.4972$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24r	1	0.063	0.242	0.174		non-colinear Si ₂
O2	24r	1	0.064	0.402	0.174		non-colinear Si ₂
O3	24r	1	0.089	0.335	0.237		non-colinear Si ₂
M4	24r	1	0.096	0.29	0.295		tetrahedron O ₄
M5	24r	1	0.098	0.388	0.295		tetrahedron O ₄
O6	24r	1	0.155	0.43	0.271		non-colinear Si ₂
O7	24r	1	0.178	0.518	0.173		non-colinear Si ₂
M8	24r	1	0.195	0.487	0.294		tetrahedron O ₄
O9	12q	m..	0.08	0.277	$\frac{1}{2}$		non-colinear Si ₂
O10	12q	m..	0.083	0.386	$\frac{1}{2}$		non-colinear Si ₂
O11	12q	m..	0.196	0.502	$\frac{1}{2}$		non-colinear Si ₂
M12	12p	m..	0.056	0.209	0		tetrahedron O ₄
M13	12p	m..	0.056	0.426	0		tetrahedron O ₄
O14	12p	m..	0.094	0.484	0		non-colinear Si ₂
M15	12p	m..	0.152	0.526	0		tetrahedron O ₄
O16	12o	.m.	0.153	0.306	0.277		non-colinear Si ₂
O17	12o	.m.	0.248	0.496	0.239		non-colinear Si ₂
O18	6l	mm2	0.095	0.19	0		non-colinear Si ₂

O19	<i>6l</i>	<i>mm2</i>	0.579	0.158	0	non-colinear Si ₂
O20	<i>6j</i>	<i>m2m</i>	0.164	0	0	non-colinear Si ₂
O21	<i>6j</i>	<i>m2m</i>	0.415	0	0	non-colinear Si ₂

M4 = 0.778Si + 0.222Al; M5 = 0.778Si + 0.222Al; M8 = 0.778Si + 0.222Al; M12 = 0.778Si + 0.222Al;
M13 = 0.778Si + 0.222Al; M15 = 0.778Si + 0.222Al

Transformation from published data: origin shift 0 0 1/2

Experimental: powder, diffractometer, X-rays, synchrotron

Remarks: K not located. Framework model tested on X-ray synchrotron and electron diffraction data.

References: [1] Higgins J.B., Schmitt K.D. (1996), Zeolites 16, 236-244.