

Space group (200) *Pm-3*200
cP8

$\text{W(W}_{0.07}\text{Al}_{0.93})_6\text{Ge}$	<i>cP8</i>	(200) <i>Pm-3</i> – fba
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W(W_{0.07}Al_{0.93})₆Ge [1]

Structural features: W(Al,W)₁₂ and Ge(Al,W)₁₂ icosahedra share faces and edges to form a 3D-framework. Ordering variant of Cr₃Si (A15 type).

Milyan V.V., Kuz'ma Y.B. (1986) [1]

$\text{Al}_{5.58}\text{GeW}_{1.42}$

$a = 0.50293 \text{ nm}$, $V = 0.1272 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	6 <i>f</i>	<i>mm2</i> ..	0.237	0	$\frac{1}{2}$		14-vertex Frank-Kasper Al ₁₀ W ₂ Ge ₂
Ge2	1 <i>b</i>	<i>m-3</i> .	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Al ₁₂
W3	1 <i>a</i>	<i>m-3</i> .	0	0	0		icosahedron Al ₁₂

$M1 = 0.93\text{Al} + 0.07\text{W}$

Experimental: powder, diffractometer, X-rays, $R = 0.157$

References: [1] Milyan V.V., Kuz'ma Y.B. (1986), Russ. Metall. (Engl. Transl.) 1986(6), 158-161.

200
cP11

$\text{RbHg[NO}_2\text{]}_3$	<i>cP11</i>	(200) <i>Pm-3</i> – fdba
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RbHg(NO₂)₃ [1]

Structural features: Hg(NO₂)₆ octahedral units (HgN₆ octahedron, O-N-O linear units perpendicular to the Hg-N bonds) share vertices to form a 3D-framework.

Ferrari A., Colla C. (1935) [1]

$\text{HgN}_3\text{O}_6\text{Rb}$

$a = 0.545 \text{ nm}$, $V = 0.1619 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>f</i>	<i>mm2</i> ..	0.26	0	$\frac{1}{2}$		single atom N
N2	3 <i>d</i>	<i>mmm</i> ..	$\frac{1}{2}$	0	0		colinear O ₂
Rb3	1 <i>b</i>	<i>m-3</i> .	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron O ₁₂
Hg4	1 <i>a</i>	<i>m-3</i> .	0	0	0		octahedron N ₆

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

Experimental: powder, film, X-rays

References: [1] Ferrari A., Colla C. (1935), Gazz. Chim. Ital. 65, 789-797.

200
cP15

$\text{Na}_{0.28}\text{Co}_{0.74}\text{Pt}_6\text{O}_8$	<i>cP15</i>	(200) <i>Pm-3</i> – ifa
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Na_{0.14}Co_{0.37}Pt₃O₄ [1]

Structural features: Mutually perpendicular (Pt,Co)O₄ squares share vertices to form a 3D-framework, (Co,Na) in cubic voids.

Schwartz K.B. et al. (1982) [1]

$\text{Co}_{0.74}\text{Na}_{0.28}\text{O}_8\text{Pt}_{5.58}$

$a = 0.56321 \text{ nm}$, $V = 0.1787 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	8i	.3.	0.242	0.242	0.242		tetrahedron Pt_3Co
M2	6f	$mm2..$	0.253	0	$\frac{1}{2}$		non-coplanar square O_4
M3	1a	$m-3.$	0	0	0	0.6	square prism (cube) O_8

$\text{M2} = 0.93\text{Pt} + 0.07\text{Co}$; $\text{M3} = 0.533\text{Co} + 0.467\text{Na}$

Experimental: powder, diffractometer, neutrons, $R = 0.026$

Remarks: Refinement of the occupancy of Wyckoff position 1b showed no significant deviation from zero.

References: [1] Schwartz K.B., Parise J.B., Prewitt C.T., Shannon R.D. (1982), Acta Crystallogr. B 38, 2109-2116.

200
cP20

$\text{CsCd}[\text{NO}_2]_3$	cP20	(200) $Pm-3$ – jeba
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$\text{CsCd}(\text{NO}_2)_3$ [1]

Structural features: Cd atoms (half of them forming $\text{Cd}(\text{NO}_2)_6$ octahedral units, disorder) and Cs atoms in a CsCl-type arrangement.

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

CdCsN_3O_6

$a = 0.5466 \text{ nm}$, $V = 0.1633 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	$m..$	0	0.191	0.474	0.5	
N2	6e	$mm2..$	0.418	0	0	0.5	
Cs3	1b	$m-3.$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Cd4	1a	$m-3.$	0	0	0		octahedron N_6

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

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

Remarks: Short interatomic distances for partly occupied site(s). Space group (221) $Pm-3m$ was tested and rejected ($R = 0.111$).

References: [1] Barnes J.C., Duncan C.S., Hetherington A., Paton J., Sesay L.J., Smith W.R. (1979), J. Less-Common Met. 63, 287-295.

200
cP26

Cr	cP26	(200) $Pm-3$ – lba
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$\text{Cr } \delta$ [1]

Structural features: Cr forms a distorted unary Cr_3Si -type arrangement (partial disorder).

Kimoto K., Nishida I. (1967) [1]

Cr

$a = 0.4588 \text{ nm}$, $V = 0.0966 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cr1	24l	1	0.01	0.252	0.46	0.25	
Cr2	1b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
Cr3	1a	m-3.	0	0	0		

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

Experimental: polycrystalline sample, electron diffraction

Remarks: Metastable phase (?), may be maintained up to ~723 K. Short interatomic distances for partly occupied site(s).

References: [1] Kimoto K., Nishida I. (1967), J. Phys. Soc. Jpn. 22, 744-756.

200
cP32

$H_{0.99}MoO_3$	cP32	(200) <i>Pm</i> -3 – kji
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$H_{0.99}MoO_3$ [1]

Structural features: $Mo(O,OH)_6$ octahedra share vertices to form a 3D-arrangement (H preferentially bonded to one of the two O sites).

Parise J.B. et al. (1987) [1]

$D_{0.99}MoO_3$

$a = 0.75734$ nm, $V = 0.4344$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	m..	$\frac{1}{2}$	0.28	0.211		non-colinear Mo_2
O2	12j	m..	0	0.201	0.283		non-colinear Mo_2
Mo3	8i	.3.	0.25	0.25	0.25		octahedron O_6
D4	12k	m..	$\frac{1}{2}$	0.37	0.13	0.08	
D5	12k	m..	$\frac{1}{2}$	0.412	0.179	0.08	
D6	12j	m..	0	0.079	0.302	0.28	
D7	12j	m..	0	0.19	0.433	0.22	

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.050$

Remarks: Space group (204) *Im*-3 was tested ($R_B = 0.031$ for X-rays) but rejected based on the presence of additional reflections in the neutron diffraction pattern. 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] Parise J.B., McCarron E.M. III, Sleight A.W. (1987), Mater. Res. Bull. 22, 803-811.

200
cP36

$CaTa_2O_6$	cP36	(200) <i>Pm</i> -3 – kjica
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$CaTa_2O_6$ ht [2]

Structural features: TaO_6 octahedra share vertices to form a 3D-framework; Ca occupies half of the distorted cuboctahedral voids. Ca-deficient derivative of $CaTiO_3$ (perovskite).

Tiedemann P., Müller Buschbaum H. (1984) [1]

CaO_6Ta_2

$a = 0.778$ nm, $V = 0.4709$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	m..	$\frac{1}{2}$	0.28	0.227		non-colinear Ta ₂
O2	12j	m..	0	0.216	0.273		non-colinear Ta ₂
Ta3	8i	.3.	0.2525	0.2525	0.2525		octahedron O ₆
Ca4	3c	mmm..	0	$\frac{1}{2}$	$\frac{1}{2}$		coplanar square O ₄
Ca5	1a	m-3.	0	0	0		icosahedron O ₁₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.067

Remarks: A refinement in space group (221) *Pm-3m* ($\frac{1}{8}$ cell volume) on powder diffraction data gave R = 0.04, but unreasonable anisotropic displacement parameters.

References: [1] Tiedemann P., Müller Buschbaum H. (1984), Z. Anorg. Allg. Chem. 516, 201-206. [2] Propach V. (1977), Z. Anorg. Allg. Chem. 435, 161-171.

200
cP38

CuTa ₂ O ₆	cP38	(200) <i>Pm-3</i> – kjidc
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CuTa₂O₆ [1]

Structural features: TaO₆ octahedra share vertices to form a 3D-framework; Cu in square voids (disorder).

Propach V. (1977) [1]

CuO₆Ta₂

a = 0.7487 nm, *V* = 0.4197 nm³, *Z* = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	m..	$\frac{1}{2}$	0.185	0.3049		non-coplanar triangle Ta ₂ Cu
O2	12j	m..	0	0.2978	0.1812		non-coplanar triangle Ta ₂ Cu
Ta3	8i	.3.	0.25	0.25	0.25		octahedron O ₆
Cu4	3d	mmm..	$\frac{1}{2}$	0	0	0.667	coplanar square O ₄
Cu5	3c	mmm..	0	$\frac{1}{2}$	$\frac{1}{2}$	0.667	coplanar square O ₄

Experimental: powder, diffractometer, neutrons

Remarks: Splitting of some reflections indicate lower symmetry. Space group (47) *Pmmm* was tested and rejected, however, the structure was later refined in this space group [2].

References: [1] Propach V. (1977), Z. Anorg. Allg. Chem. 435, 161-171. [2] Vincent H., Bochu B., Aubert J.J., Joubert J.C., Marezio M. (1978), J. Solid State Chem. 24, 245-253.

200
cP39

Mg ₂ Zn ₁₁	cP39	(200) <i>Pm-3</i> – jihgfa
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Mg₂Zn₁₁ [1], Strukturbericht notation D8_c

Structural features: ZnZn₁₂ icosahedra and empty Zn₆ octahedra in a CsCl-type arrangement, separated by additional Zn and Mg atoms.

Samson S. (1949) [1]

Mg₂Zn₁₁

a = 0.8552 nm, *V* = 0.6255 nm³, *Z* = 3

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	12j	m..	0	0.157	0.257		icosahedron Zn ₉ Mg ₃
Zn2	8i	.3.	0.278	0.278	0.278		icosahedron Zn ₉ Mg ₃
Zn3	6h	mm2..	0.265	1/2	1/2		10-vertex polyhedron Zn ₁₀
Zn4	6g	mm2..	0.340	1/2	0		pseudo Frank-Kasper Zn ₉ Mg ₄
Mg5	6f	mm2..	0.18	0	1/2		7-capped pentagonal prism Zn ₁₆ Mg
Zn6	1a	m-3.	0	0	0		icosahedron Zn ₁₂

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

Experimental: single crystal, Weissenberg photographs, X-rays

References: [1] Samson S. (1949), Acta Chem. Scand. 3, 835-843.

200
cP39

Mg ₂ Cu ₆ Al ₅	cP39	(200) <i>Pm</i> -3 – jihgfa
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Mg₂Cu₆Al₅ [1]

Structural features: AlCu₁₂ icosahedra and empty Cu₆ octahedra in a CsCl-type arrangement, separated by additional Al and Mg atoms. Ordering variant of Mg₂Zn₁₁.

Samson S. (1949) [1]

Al₅Cu₆Mg₂

$a = 0.8311 \text{ nm}$, $V = 0.5741 \text{ nm}^3$, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	12j	m..	0	0.164	0.257		icosahedron Al ₄ Cu ₅ Mg ₃
Al2	8i	.3.	0.285	0.285	0.285		icosahedron Cu ₆ Al ₃ Mg ₃
Cu3	6h	mm2..	0.275	1/2	1/2		10-vertex polyhedron Al ₆ Cu ₄
Al4	6g	mm2..	0.34	1/2	0		pseudo Frank-Kasper Cu ₄ Al ₅ Mg ₄
Mg5	6f	mm2..	0.18	0	1/2		7-capped pentagonal prism Cu ₈ Al ₈ Mg
Al6	1a	m-3.	0	0	0		icosahedron Cu ₁₂

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

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

References: [1] Samson S. (1949), Acta Chem. Scand. 3, 809-834.

200
cP39

K ₆ Na ₁₄ MgTl ₁₈	cP39	(200) <i>Pm</i> -3 – jihgfa
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K₆Na₁₄Tl₁₈Mg [1]

Structural features: MgTl₁₂ icosahedra and empty Tl₆ octahedra in a CsCl-type arrangement, embedded in a matrix of Na and K atoms.

Dong Z.C., Corbett J.D. (1996) [1]

K₆MgNa₁₄Tl₁₈

$a = 1.15914 \text{ nm}$, $V = 1.5574 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	12j	m..	0	0.15475	0.25325		icosahedron MgNa ₃ Tl ₅ K ₃
Na2	8i	.3.	0.2812	0.2812	0.2812		icosahedron Tl ₆ Na ₃ K ₃
Tl3	6h	mm2..	0.2808	1/2	1/2		10-vertex polyhedron Na ₆ Tl ₄

Na4	6g	<i>mm2</i> ..	0.33	$\frac{1}{2}$	0	pseudo Frank-Kasper $\text{Ti}_4\text{Na}_5\text{K}_4$
K5	6f	<i>mm2</i> ..	0.1876	0	$\frac{1}{2}$	7-capped pentagonal prism $\text{Ti}_8\text{Na}_8\text{K}$
Mg6	1a	<i>m-3</i> .	0	0	0	icosahedron Ti_{12}

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

References: [1] Dong Z.C., Corbett J.D. (1996), *Angew. Chem. Int. Ed. Engl.* 35, 1006-1009.

200
cP40

$\text{Ba}_4\text{Cu}_3\text{YO}_9$	<i>cP40</i>	(200) <i>Pm-3</i> – ihgfdcba
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$\text{YBa}_4\text{Cu}_3\text{O}_9$ [1]

Structural features: YO_6 octahedra and mutually perpendicular CuO_4 squares (partial orientational disorder) share vertices to form a 3D-framework, Ba in large voids (O_{12} cuboctahedron with 3 vertices vacant). O-deficient derivative of perovskite.

De Leeuw D.M. et al. (1989) [1]

$\text{Ba}_4\text{Cu}_3\text{O}_9\text{Y}$

$a = 0.81174 \text{ nm}$, $V = 0.5349 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	8i	.3.	0.2445	0.2445	0.2445		cuboctahedron O_{12}
O2	6h	<i>mm2</i> ..	0.227	$\frac{1}{2}$	$\frac{1}{2}$		colinear CuY
O3	6g	<i>mm2</i> ..	0.242	$\frac{1}{2}$	0	0.808	colinear Cu_2
O4	6f	<i>mm2</i> ..	0.26	0	$\frac{1}{2}$	0.192	colinear Cu_2
O5	6e	<i>mm2</i> ..	0.276	0	0		colinear CuY
Cu6	3d	<i>mmm</i> ..	$\frac{1}{2}$	0	0		octahedron O_6
Cu7	3c	<i>mmm</i> ..	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_6
Y8	1b	<i>m-3</i> .	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_6
Y9	1a	<i>m-3</i> .	0	0	0		octahedron O_6

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

Experimental: powder, diffractometer, neutrons, R = 0.036, T = 300 K

Remarks: The description of a related model in space group (200) *Pm-3* in [2] (idealized coordinates, site O3 fully occupied, site O4 vacant) does not take into consideration all symmetry elements of the proposed structure; correct space group is (223) *Pm-3n*.

References: [1] De Leeuw D.M., Mutsaers C.A.H.A., Steeman R.A., Frikkee E., Zandbergen H.W. (1989), *Physica C* (Amsterdam) 158, 391-396. [2] Abbattista F., Vallino M., Mazza D., Lucco Borlera M., Brisi C. (1988), *Mater. Chem. Phys.* 20, 191-199. [3] Vallino M., Mazza D., Abbattista F. (1991), *J. Less-Common Met.* 170, 83-91.

200
cP40

$\text{K}_6\text{Na}_{15}\text{Ti}_{18}\text{H}$	<i>cP40</i>	(200) <i>Pm-3</i> – kigfeba
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$\text{K}_6\text{Na}_{15}\text{Ti}_{18}\text{H}$ [1]

Structural features: NaTi_{12} icosahedra and HTi_6 octahedra in a CsCl-type arrangement, embedded in a matrix of additional Na and K atoms.

Dong Z.C., Corbett J.D. (1995) [1]

$\text{HK}_6\text{Na}_{15}\text{Ti}_{18}$

$a = 1.06405 \text{ nm}$, $V = 1.2047 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	12k	m..	$\frac{1}{2}$	0.24704	0.34498		icosahedron Na ₄ Tl ₅ K ₃
Na2	8i	.3.	0.2198	0.2198	0.2198		13-vertex polyhedron Tl ₆ Na ₃ K ₃ H
Na3	6g	mm2..	0.171	$\frac{1}{2}$	0		pseudo Frank-Kasper Tl ₄ Na ₅ K ₄
K4	6f	mm2..	0.3139	0	$\frac{1}{2}$		7-capped pentagonal prism Tl ₈ Na ₈ K
Tl5	6e	mm2..	0.21767	0	0		single atom H
Na6	1b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Tl ₁₂
H7	1a	m-3.	0	0	0		octahedron Tl ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.023, T = 296 K

References: [1] Dong Z.C., Corbett J.D. (1995), Inorg. Chem. 34, 5709-5710.

200
cP46

Lu ₃ Co _{8.8} In ₇	cP46	(200) <i>Pm</i> -3 – kigfe ² ba
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Lu₆Co_{17.59}In₁₄ [2]

Structural features: Pairs of interpenetrating Lu(LuCo₆In₈) polyhedra share atoms to form a 3D-framework; additional Co atoms form empty Co₆ octahedra or larger CoCo₆ octahedra (disorder).

Zaremba V.I. et al. (1990) [1]

Co_{8.80}In₇Lu₃

$a = 0.8652$ nm, $V = 0.6477$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	12k	m..	$\frac{1}{2}$	0.2598	0.3548		icosahedron Co ₆ In ₃ Lu ₃
In2	8i	.3.	0.2176	0.2176	0.2176		
In3	6g	mm2..	0.179	$\frac{1}{2}$	0		
Lu4	6f	mm2..	0.3158	0	$\frac{1}{2}$		
Co5	6e	mm2..	0.213	0	0	0.45	
Co6	6e	mm2..	0.263	0	0	0.26	
Co7	1b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Co ₁₂
Co8	1a	m-3.	0	0	0	0.33	octahedron Co ₆

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

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

Remarks: The same data are reported in [2]. In the title of [2] the compound is misprinted as Lu₆Co_{26-x}In instead of Lu₆Co_{26-x}In₁₄. Short interatomic distances for partly occupied site(s).

References: [1] Zaremba V.I., Kalychak Y.M., Zavalii P.Y., Zavodnik V.E. (1990), Sov. Phys. Crystallogr. (Engl. Transl.) 35, 286. [2] Kalychak Y.M., Zaremba V.I., Gladyshevsky E.I. (1989), Coll. Abs. Eur. Crystallogr. Meet., 12th, Moscow, Vol. 2, p. 86.

200
cP54

Ni[NH ₂] ₂	cP54	(200) <i>Pm</i> -3 – ljjgfe
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Ni₆(NH₂)₁₂ [1]

Structural features: Single Ni₆(NH₂)₁₂ units consisting of a central Ni₆ octahedron surrounded by a (NH₂)₁₂ cuboctahedron (one non-linear NH₂ unit above each octahedron edge).

Tenten A., Jacobs H. (1991) [1]

 $\text{H}_4\text{N}_2\text{Ni}$ $a = 1.0825 \text{ nm}$, $V = 1.2685 \text{ nm}^3$, $Z = 18$

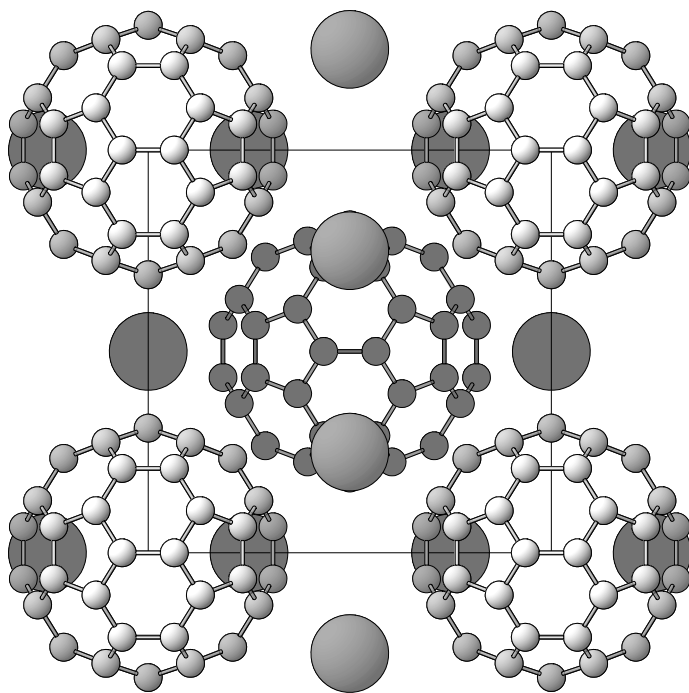
site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24l	1	0.125	0.1741	0.3753		non-colinear Ni_2
Ni2	12j	$m..$	0	0.3675	0.1307		non-coplanar square N_4
Ni3	6g	$mm2..$	0.1868	$\frac{1}{2}$	0		non-coplanar square N_4
N4	6f	$mm2..$	0.245	0	$\frac{1}{2}$		non-colinear Ni_2
N5	6e	$mm2..$	0.246	0	0		non-colinear Ni_2
H6	24l	1	0.111	0.21	0.322		
H7	24l	1	0.18	0.2	0.4		
H8	12k	$m..$	$\frac{1}{2}$	0.32	0.06		
H9	12j	$m..$	0	0.1	0.2		

Experimental: single crystal, diffractometer, X-rays, $R = 0.032$ Remarks: Space group (195) $P23$ was tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Tenten A., Jacobs H. (1991), J. Less-Common Met. 170, 145-159.

200
 $cP126$

$\text{Sr}_3[\text{C}_{60}]$	$cP126$	$(200) Pm-3 - 1^4k\bar{1}f$
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 Sr_3C_{60} [1]Structural features: Pseudo-spherical C_{60} fullerene units (twelve 5- and twenty 6-membered rings) and Sr atoms in a Cr_3Si -type (A15) arrangement. See Fig. II.64.Fig. II.64. Sr_3C_{60} Arrangement of C_{60} cages (C atoms small) and Sr atoms (large).

Kortan A.R. et al. (1994) [1]

 $C_{60}Sr_3$ $a = 1.1140 \text{ nm}$, $V = 1.3825 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24l	1	0.0647	0.2095	0.2343		non-coplanar triangle C_3
C2	24l	1	0.1048	0.2743	0.1294		non-coplanar triangle C_3
C3	24l	1	0.2257	0.3706	0.3952		non-coplanar triangle C_3
C4	24l	1	0.2657	0.4353	0.2905		non-coplanar triangle C_3
C5	12k	$m..$	$\frac{1}{2}$	0.1856	0.4353		non-coplanar triangle C_3
C6	12j	$m..$	0	0.3096	0.0647		non-coplanar triangle C_3
Sr7	6f	$mm2..$	0.25	0	$\frac{1}{2}$		22-vertex polyhedron C_{22}

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

Experimental: powder, diffractometer, X-rays

Remarks: Space group (223) $Pm\bar{3}n$ (orientational disorder) could not be excluded. On page 502 of [1] the x-coordinate of former C4 is misprinted as 0.5547 instead of 0.5647 (equal C-C bond lengths).

References: [1] Kortan A.R., Kopylov N., Özdas E., Ramirez A.P., Fleming R.M., Haddon R.C. (1994), Chem. Phys. Lett. 223, 501-505.

200
cP126 $Mn_{18}Pd_{14.7}Al_{81.2}Si_{8.6}$

cP126

(200) $Pm\bar{3} - Ik^{2^2_3^2}i^2hg^2ba$ **$Mn_{14.7}Pd_{12.0}Al_{66.3}Si_{7.0}$** [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Sugiyama K. et al. (1998) [1]

 $Al_{81.32}Mn_{18}Pd_{14.68}Si_{8.70}$ $a = 1.2281 \text{ nm}$, $V = 1.8523 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24l	1	0.1137	0.3319	0.3793		icosahedron $SiPd_2MnAl_8$
Al2	12k	$m..$	$\frac{1}{2}$	0.2282	0.1798		icosahedron $MnAl_7Pd_3Si$
Al3	12k	$m..$	$\frac{1}{2}$	0.3072	0.3913		icosahedron Pd_3Al_8Si
Al4	12j	$m..$	0	0.123	0.3075		
Mn5	12j	$m..$	0	0.17533	0.10652		icosahedron Al_7Mn_5
Al6	12j	$m..$	0	0.3491	0.1912		icosahedron Mn_2SiAl_9
Al7	8i	.3.	0.1909	0.1909	0.1909		pseudo Frank-Kasper $PdMn_3Al_9$
Pd8	8i	.3.	0.30813	0.30813	0.30813		bicapped square prism Al_{10}
Si9	6h	$mm2..$	0.1037	$\frac{1}{2}$	$\frac{1}{2}$		9-vertex polyhedron Mn_2Al_6Si
Pd10	6g	$mm2..$	0.1963	$\frac{1}{2}$	0		
Si11	6f	$mm2..$	0.0516	0	$\frac{1}{2}$	0.45	
Mn12	6f	$mm2..$	0.3213	0	$\frac{1}{2}$		bicapped square prism Al_8Si_2
M13	1b	$m\bar{3}$.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Al_{12}
Al14	1a	$m\bar{3}$.	0	0	0		icosahedron Mn_{12}

 $M13 = 0.68Pd + 0.32Al$

Transformation from published data: y,x,-z

Experimental: single crystal, diffractometer, X-rays, $R = 0.032$ Remarks: Phase referred to as α -(AlMnPdSi). Short interatomic distances for partly occupied site(s).

References: [1] Sugiyama K., Kaji N., Hiraga K., Ishimasa T. (1998), *Z. Kristallogr.* 213, 168-173.

200
cP138

$\text{Mn}_4\text{Al}_{14}(\text{Al}_{0.5}\text{Si}_{0.5})_4\text{Si}$	<i>cP138</i>	(200) <i>Pm-3</i> – $\text{I}^2\text{k}^3\text{j}^3\text{hfe}$
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Mn₄Al₁₆Si₃ [2]

Structural features: Units consisting of twelve vertex-linked Mn(Al,Si)₁₂ icosahedra or Mn(Al,Si)₁₁ defect icosahedra are interconnected to form a 3D-framework; the centering atoms form large Mn₁₂ icosahedra. Commensurate approximant of icosahedral quasicrystals.

Sugiyama K. et al. (1998) [1]

$\text{Al}_{16.05}\text{Mn}_4\text{Si}_{2.95}$

$a = 1.2643 \text{ nm}$, $V = 2.0209 \text{ nm}^3$, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	24I	1	0.10926	0.30383	0.18709		14-vertex polyhedron Mn ₃ Al ₈ Si ₃
Al2	24I	1	0.20094	0.3114	0.38202		tricapped pentagonal prism Mn ₃ Al ₁₀
Al3	12 <i>k</i>	<i>m..</i>	$\frac{1}{2}$	0.09794	0.16865		pseudo Frank-Kasper Al ₉ SiMn ₃
Mn4	12 <i>k</i>	<i>m..</i>	$\frac{1}{2}$	0.30221	0.17369		icosahedron Al ₁₁ Si
M5	12 <i>k</i>	<i>m..</i>	$\frac{1}{2}$	0.39859	0.33448		11-vertex polyhedron MnAl ₁₀
M6	12 <i>j</i>	<i>m..</i>	0	0.09974	0.16389		11-vertex polyhedron MnSi ₅ Al ₅
Mn7	12 <i>j</i>	<i>m..</i>	0	0.1921	0.32075		11-vertex polyhedron SiAl ₁₀
Al8	12 <i>j</i>	<i>m..</i>	0	0.38232	0.37613		14-vertex Frank-Kasper Mn ₃ SiAl ₁₀
Al9	6 <i>h</i>	<i>mm2..</i>	0.13216	$\frac{1}{2}$	$\frac{1}{2}$		tricapped pentagonal prism Mn ₂ Al ₁₁
M10	6 <i>f</i>	<i>mm2..</i>	0.21034	0	$\frac{1}{2}$		icosahedron Mn ₂ Al ₁₀
Al11	6 <i>e</i>	<i>mm2..</i>	0.37571	0	0		15-vertex polyhedron Mn ₂ Al ₉ Si ₄

M5 = 0.65Al + 0.35Si; M6 = 0.63Si + 0.37Al; M10 = 0.99Si + 0.01Al

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.031$, $T = 297 \text{ K}$

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

References: [1] Sugiyama K., Kaji N., Hiraga K. (1998), *Acta Crystallogr. C* 54, 445-447. [2] Cooper M., Robinson K. (1966), *Acta Crystallogr.* 20, 614-617.

200
cP140

$\text{Sc}_{57}\text{Rh}_{13}$	<i>cP140</i>	(200) <i>Pm-3</i> – $\text{I}^2\text{k}^3\text{j}^3\text{hfeba}$
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Sc₅₇Rh₁₃ [1]

Structural features: Units consisting of a central RhSc₁₂ icosahedron sharing vertices with twelve vertex-linked RhSc₁₂ icosahedra or RhSc₁₁ defect icosahedra are interconnected to form a 3D-framework; the centering atoms form large RhRh₁₂ icosahedra. See Fig. II.65.

Cenzual K. et al. (1985) [1]

$\text{Rh}_{13}\text{Sc}_{57}$

$a = 1.44051 \text{ nm}$, $V = 2.9892 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sc1	24I	1	0.1145	0.1796	0.2920		tricapped pentagonal prism Rh ₃ Sc ₁₀
Sc2	24I	1	0.2022	0.3878	0.3114		14-vertex polyhedron Rh ₃ Sc ₁₁
Sc3	12 <i>k</i>	<i>m..</i>	$\frac{1}{2}$	0.1085	0.1310		14-vertex Frank-Kasper Rh ₃ Sc ₁₁

Rh4	12k	<i>m..</i>	$\frac{1}{2}$	0.1663	0.2977	pseudo Frank-Kasper Sc ₁₁
Sc5	12k	<i>m..</i>	$\frac{1}{2}$	0.3211	0.3924	12-vertex polyhedron Rh ₂ Sc ₁₀
Sc6	12j	<i>m..</i>	0	0.1758	0.1097	12-vertex polyhedron Rh ₂ Sc ₁₀
Sc7	12j	<i>m..</i>	0	0.3257	0.3971	pseudo Frank-Kasper Rh ₃ Sc ₁₀
Rh8	12j	<i>m..</i>	0	0.3338	0.202	icosahedron Sc ₁₂
Sc9	6h	<i>mm2..</i>	0.1254	$\frac{1}{2}$	$\frac{1}{2}$	15-vertex polyhedron Rh ₂ Sc ₁₃
Sc10	6f	<i>mm2..</i>	0.2729	0	$\frac{1}{2}$	icosahedron Rh ₂ Sc ₁₀
Sc11	6e	<i>mm2..</i>	0.3618	0	0	12-vertex polyhedron Rh ₂ Sc ₁₀
Rh12	1b	<i>m-3.</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	icosahedron Sc ₁₂
Rh13	1a	<i>m-3.</i>	0	0	0	icosahedron Sc ₁₂

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.051, T = 293 K

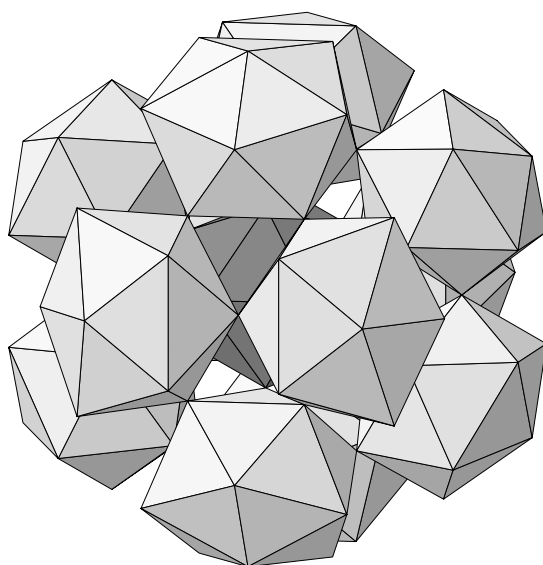


Fig. II.65. **Sc₅₇Rh₁₃**

Icosahedron unit: a central RhSc₁₂ icosahedron (dark) surrounded by twelve other RhSc₁₂ icosahedra (light).

References: [1] Cenxual K., Chabot B., Parthé E. (1985), Acta Crystallogr. C 41, 313-319.

200
cP140

Sc ₂₉ Fe ₆	cP140	(200) <i>Pm-3</i> – <i>I</i> ² <i>k</i> ³ <i>j</i> ³ hfeba
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Sc₂₉Fe₆ [1]

Structural features: Units consisting of a central ScSc₁₂ icosahedron sharing vertices with twelve surrounding FeSc₁₂ icosahedra or twelve FeSc₁₁ defect icosahedra are interconnected to form a 3D-framework; the centering atoms form large ScFe₁₂ icosahedra. Ordering variant of Sc₅₇Rh₁₃.

Kotur B.Y. et al. (1986) [1]

Fe₆Sc₂₉

a = 1.4361 nm, *V* = 2.9618 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sc1	24l	1	0.1138	0.1816	0.2925		tricapped pentagonal prism Fe ₃ Sc ₁₀
Sc2	24l	1	0.2017	0.3842	0.3121		14-vertex polyhedron Fe ₃ Sc ₁₁
Sc3	12k	<i>m..</i>	$\frac{1}{2}$	0.1130	0.1290		14-vertex Frank-Kasper Fe ₃ Sc ₁₁
Fe4	12k	<i>m..</i>	$\frac{1}{2}$	0.1659	0.3000		11-vertex polyhedron Sc ₁₁

Sc5	12 <i>k</i>	<i>m</i> ..	$\frac{1}{2}$	0.3204	0.3895	12-vertex polyhedron FeSc ₁₁
Sc6	12 <i>j</i>	<i>m</i> ..	0	0.1809	0.1113	12-vertex polyhedron FeSc ₁₁
Sc7	12 <i>j</i>	<i>m</i> ..	0	0.3232	0.3989	pseudo Frank-Kasper Fe ₃ Sc ₁₀
Fe8	12 <i>j</i>	<i>m</i> ..	0	0.3352	0.2054	icosahedron Sc ₁₂
Sc9	6 <i>h</i>	<i>mm</i> 2..	0.1274	$\frac{1}{2}$	$\frac{1}{2}$	15-vertex Frank-Kasper Fe ₂ Sc ₁₃
Sc10	6 <i>f</i>	<i>mm</i> 2..	0.2768	0	$\frac{1}{2}$	icosahedron Fe ₂ Sc ₁₀
Sc11	6 <i>e</i>	<i>mm</i> 2..	0.3651	0	0	12-vertex polyhedron Fe ₂ Sc ₁₀
Sc12	1 <i>b</i>	<i>m</i> -3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	icosahedron Sc ₁₂
Sc13	1 <i>a</i>	<i>m</i> -3.	0	0	0	icosahedron Sc ₁₂

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.067$

Remarks: In table 1 of [1] the Wyckoff position of former Sc3 is misprinted as 6*k* instead of 6*h*.

References: [1] Kotur B.Y., Bodak O.I., Andrusyak R.I., Zavodnik V.E., Belsky V.K. (1986), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1986(11), 28-31.

200
cP146

Mg ₃₀ Ag ₁₉ Al ₂₄	cP146	(200) $Pm-3 - I^2k^3j^3hgfeba$
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Mg_{41.1}Ag_{26.0}Al_{32.9} [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Kreiner G., Spiekermann S. (1997) [1]

Ag₁₉Al₂₄Mg₃₀

$a = 1.45 \text{ nm}$, $V = 3.0486 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	24 <i>l</i>	1	0.1146	0.1854	0.3		14-vertex polyhedron Ag ₄ Al ₄ Mg ₆
Al2	24 <i>l</i>	1	0.1931	0.3806	0.309		14-vertex polyhedron Mg ₅ Ag ₄ Al ₅
Al3	12 <i>k</i>	<i>m</i> ..	$\frac{1}{2}$	0.1545	0.0955		icosahedron Ag ₅ Al ₃ Mg ₄
Ag4	12 <i>k</i>	<i>m</i> ..	$\frac{1}{2}$	0.1667	0.294		icosahedron Mg ₄ AgAl ₇
Mg5	12 <i>k</i>	<i>m</i> ..	$\frac{1}{2}$	0.3333	0.397		12-vertex polyhedron Ag ₂ Mg ₆ Al ₄
Mg6	12 <i>j</i>	<i>m</i> ..	0	0.1667	0.103		12-vertex polyhedron Ag ₂ Mg ₁₀
Ag7	12 <i>j</i>	<i>m</i> ..	0	0.3333	0.206		icosahedron Mg ₆ AgAl ₅
Al8	12 <i>j</i>	<i>m</i> ..	0	0.3455	0.4045		icosahedron Ag ₅ Al ₃ Mg ₄
Mg9	6 <i>h</i>	<i>mm</i> 2..	0.1292	$\frac{1}{2}$	$\frac{1}{2}$		15-vertex polyhedron Ag ₄ Al ₈ Mg ₃
Ag10	6 <i>g</i>	<i>mm</i> 2..	0.191	$\frac{1}{2}$	0		icosahedron Al ₄ Ag ₂ Mg ₆
Ag11	6 <i>f</i>	<i>mm</i> 2..	0.309	0	$\frac{1}{2}$		icosahedron Al ₈ Ag ₂ Mg ₂
Mg12	6 <i>e</i>	<i>mm</i> 2..	0.3708	0	0		15-vertex polyhedron Ag ₄ Al ₄ Mg ₇
Ag13	1 <i>b</i>	<i>m</i> -3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Mg ₁₂
Ag14	1 <i>a</i>	<i>m</i> -3.	0	0	0		icosahedron Mg ₁₂

Experimental: single crystal, photographs, X-rays

References: [1] Kreiner G., Spiekermann S. (1997), J. Alloys Compd. 261, 62-82.

200
cP148

Cu _{19.5} Ru ₇ Al _{35.5}	cP148	(200) $Pm-3 - I^2k^3j^3ihfeba$
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Ru_{11.3}Cu_{31.4}Al_{57.3} [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Sugiyama K. et al. (2000) [1]

 $\text{Al}_{35.09}\text{Cu}_{19.35}\text{Ru}_7$ $a = 1.23773 \text{ nm}$, $V = 1.8962 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24l	1	0.1174	0.3159	0.1946		14-vertex Frank-Kasper $\text{Ru}_2\text{Cu}_4\text{Al}_8$
M2	24l	1	0.20394	0.31729	0.3863		tricapped pentagonal prism $\text{Al}_6\text{Cu}_6\text{Ru}$
Al3	12k	m..	$\frac{1}{2}$	0.1003	0.185		pseudo Frank-Kasper $\text{Al}_7\text{Cu}_4\text{Ru}_2$
M4	12k	m..	$\frac{1}{2}$	0.3026	0.1726		icosahedron Al_6Cu_6
Al5	12k	m..	$\frac{1}{2}$	0.404	0.321	0.18	12-vertex polyhedron $\text{Cu}_6\text{Al}_5\text{Ru}$
Ru6	12j	m..	0	0.1932	0.31078		
Al7	12j	m..	0	0.195	0.053	0.2	
Al8	12j	m..	0	0.3872	0.3757		14-vertex Frank-Kasper RuCu_7Al_6
Al9	8i	.3.	0.119	0.119	0.119	0.29	non-coplanar triangle Al_3
M10	6h	mm2..	0.1226	$\frac{1}{2}$	$\frac{1}{2}$		tricapped pentagonal prism Cu_7Al_6
Cu11	6f	mm2..	0.1892	0	$\frac{1}{2}$		icosahedron $\text{Al}_{10}\text{Cu}_2$
Al12	6e	mm2..	0.3914	0	0		
Ru13	1b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Al_{12}
Ru14	1a	m-3.	0	0	0		

M2 = 0.72Cu + 0.28Al; M4 = 0.83Cu + 0.17Al; M10 = 0.91Cu + 0.09Al

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

Experimental: single crystal, diffractometer, X-rays, R = 0.050

Remarks: Phase referred to as α -(AlCuRu). Short interatomic distances for partly occupied site(s).

References: [1] Sugiyama K., Kato T., Ogawa T., Hiraga K., Saito K. (2000), J. Alloys Compd. 299, 169-174.

200
cP152

$\text{Co}[\text{ClO}_4]_3[\text{NH}_3]_3[\text{H}_2\text{O}]_3$	cP152	(200) $Pm-3 - I^{4+3}hgfedcba$
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 $[\text{Co}(\text{NH}_3)_3(\text{H}_2\text{O})_3](\text{ClO}_4)_3$ [1]Structural features: $\text{Co}([\text{OH}_2]_3[\text{NH}_3]_3)$ octahedral units (two kinds of substitutional disorder, OH_2 and NH_3 in partial orientational disorder around the octahedron axes) and ClO_4 tetrahedra (orientational disorder) in a BiF_3 -type arrangement.

Brennan T.F. et al. (1978) [1]

 $\text{Cl}_3\text{CoH}_{14.99}\text{N}_3\text{O}_{15}$ $a = 1.1213 \text{ nm}$, $V = 1.4098 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.0787	0.4319	0.4215	0.5	4-vertex polyhedron ClO_3
O2	24l	1	0.1183	0.244	0.2507	0.42	non-coplanar triangle O_2Cl
O3	24l	1	0.1717	0.1915	0.326	0.39	4-vertex polyhedron O_3Cl
O4	24l	1	0.2669	0.2679	0.3927	0.39	single atom O
O5	8i	.3.	0.0684	0.0684	0.0684	0.5	4-vertex polyhedron ClO_3
Cl6	8i	.3.	0.2492	0.2492	0.2492		tetrahedron O_4
O7	8i	.3.	0.3207	0.3207	0.3207	0.4	4-vertex polyhedron O_3Cl
M8	6h	mm2..	0.3263	$\frac{1}{2}$	$\frac{1}{2}$		single atom Co
M9	6g	mm2..	0.1751	$\frac{1}{2}$	0		single atom Co
N10	6f	mm2..	0.1677	0	$\frac{1}{2}$		single atom Co
O11	6e	mm2..	0.3285	0	0		single atom Co

Co12	3d	mmm..	$\frac{1}{2}$	0	0	octahedron N ₄ O ₂
Cl13	3c	mmm..	0	$\frac{1}{2}$	$\frac{1}{2}$	square prism (cube) O ₈
Co14	1b	m-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	octahedron N ₆
Cl15	1a	m-3.	0	0	0	square prism (cube) O ₈
H16	24l	1	0.0218	0.0811	0.3	0.167
H17	24l	1	0.0218	0.2063	0.4189	0.208
H18	24l	1	0.0218	0.3	0.0811	0.167
H19	24l	1	0.0218	0.4189	0.1992	0.25
H20	24l	1	0.0596	0.0596	0.3008	0.167
H21	24l	1	0.0596	0.2054	0.4404	0.208
H22	24l	1	0.0596	0.4404	0.1983	0.25
H23	24l	1	0.0811	0.2063	0.4782	0.208
H24	24l	1	0.0811	0.4792	0.1992	0.25
H25	24l	1	0.2966	0.4189	0.4782	0.208
H26	24l	1	0.2966	0.4782	0.4189	0.208
H27	24l	1	0.2974	0.4404	0.4404	0.208

M8 = 0.50N + 0.50O; M9 = 0.50N + 0.50O

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.062

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] Brennan T.F., Davies G., Garafalo A.R., Gardner A.P. (1978), Inorg. Chim. Acta 30, 97-101.

200
cP157

K ₄₉ Tl ₁₀₈	cP157	(200) $Pm-3 - I^2k^3j^3i^2gf^2d$
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K₄₉Tl₁₀₈ [1]

Structural features: Empty Tl₁₂ icosahedra and TlTl₁₃ monocapped hexagonal antiprisms are interconnected via exo-bonds. Pseudo-spherical 104-atom Samson polyhedron units consisting of twenty KTl₁₂ truncated tetrahedra with common hexagonal faces (a Tl₁₂ icosahedron surrounded by a K₂₀ pentagonal dodecahedron, a Tl₁₂ icosahedron and a Tl₆₀ truncated icosahedron with pentagonal and hexagonal faces). See Fig. II.66.

Cordier G. et al. (1993) [1]

K₄₉Tl₁₀₈

$a = 1.7287$ nm, $V = 5.1661$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	24l	1	0.0920	0.3374	0.3214		icosahedron Tl ₇ K ₅
Tl2	24l	1	0.1659	0.1690	0.4084		icosahedron Tl ₆ K ₆
K3	12k	m..	$\frac{1}{2}$	0.195	0.377		16-vertex Frank-Kasper Tl ₁₂ K ₄
Tl4	12k	m..	$\frac{1}{2}$	0.3263	0.1817		icosahedron Tl ₇ K ₅
Tl5	12k	m..	$\frac{1}{2}$	0.4081	0.3497		11-vertex polyhedron Tl ₆ K ₅
K6	12j	m..	0	0.134	0.295		15-vertex Frank-Kasper Tl ₁₀ K ₅
Tl7	12j	m..	0	0.1511	0.0903		11-vertex polyhedron Tl ₆ K ₅
Tl8	12j	m..	0	0.3228	0.1595		icosahedron Tl ₆ K ₆
K9	8i	.3.	0.190	0.190	0.190		16-vertex Frank-Kasper K ₄ Tl ₁₂
K10	8i	.3.	0.3126	0.3126	0.3126		16-vertex Frank-Kasper K ₄ Tl ₁₂
K11	6g	mm2..	0.271	$\frac{1}{2}$	0		15-vertex Frank-Kasper Tl ₁₀ K ₅
Tl12	6f	mm2..	0.2241	0	$\frac{1}{2}$		14-vertex Frank-Kasper Tl ₁₃ K

Tl13	6f	mm2..	0.4076	0	$\frac{1}{2}$	14-vertex Frank-Kasper Tl ₈ K ₆
K14	3d	mmm..	$\frac{1}{2}$	0	0	pseudo Frank-Kasper Tl ₁₄ K ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.086, T = 293 K

Remarks: The structure is discussed in [2].

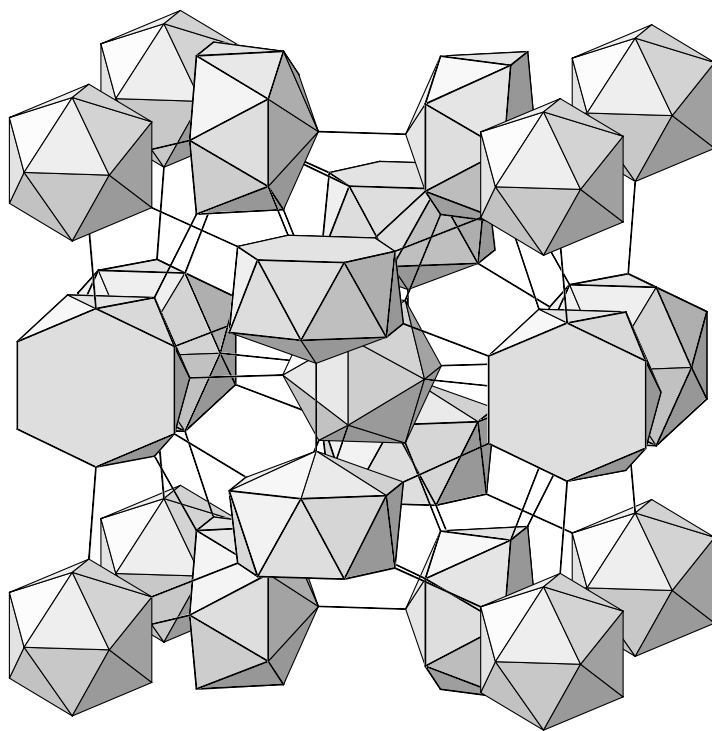


Fig. II.66. **K₄₉Tl₁₀₈**

Arrangement of empty Tl₁₂ icosahedra and TlTl₁₃ monocapped hexagonal antiprisms.

References: [1] Cordier G., Müller V., Fröhlich R. (1993), Z. Kristallogr. 203, 148-149. [2] Cordier G., Müller V. (1993), Z. Naturforsch. B 48, 1035-1040.

200
cP597

Mn_{31.3}Pd_{124.6}Al_{357.1}

cP597

(200) $Pm-3 - 1^{13}k^{11-7-4}2^2c^2e^2a$

Mn₆Pd₂₃Al₇₀Si [1]

Structural features: Commensurate approximant of icosahedral quasicrystals.

Sugiyama K. et al. (1998) [1]

Al_{357.06}Mn_{31.26}Pd_{124.56}

$a = 2.0211$ nm, $V = 8.2559$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24/	1	0.0668	0.1068	0.4276		icosahedron Pd ₂ Al ₉ Mn
Al2	24/	1	0.0754	0.1213	0.1891		pseudo Frank-Kasper Pd ₅ Al ₈
Pd3	24/	1	0.07675	0.30821	0.31297		
Al4	24/	1	0.079	0.2622	0.1916		pseudo Frank-Kasper Pd ₅ Al ₈
Al5	24/	1	0.1154	0.4301	0.3075		14-vertex Frank-Kasper Pd ₄ Al ₁₀
Pd6	24/	1	0.11667	0.38301	0.18749		

Al7	24l	1	0.1183	0.1869	0.3044		
M8	24l	1	0.11979	0.3793	0.4281		
Al9	24l	1	0.1675	0.257	0.3948	0.35	
Al10	24l	1	0.1929	0.3058	0.262		
Al11	24l	1	0.1937	0.266	0.383	0.65	
Al12	24l	1	0.2387	0.3795	0.3859	0.46	single atom Al
Al13	24l	1	0.2646	0.429	0.3071	0.54	single atom Al
Al14	12k	m..	$\frac{1}{2}$	0.0482	0.3092	0.5	
Al15	12k	m..	$\frac{1}{2}$	0.0899	0.2505	0.35	
Al16	12k	m..	$\frac{1}{2}$	0.1849	0.0668		icosahedron Pd ₃ Al ₉
M17	12k	m..	$\frac{1}{2}$	0.1928	0.3091		
Al18	12k	m..	$\frac{1}{2}$	0.1938	0.4536	0.41	single atom Al
M19	12k	m..	$\frac{1}{2}$	0.2314	0.1927		
Pd20	12k	m..	$\frac{1}{2}$	0.3121	0.3831	0.29	
Pd21	12k	m..	$\frac{1}{2}$	0.3774	0.4255	0.6	
M22	12k	m..	$\frac{1}{2}$	0.3818	0.1909		pseudo Frank-Kasper Al ₁₃
Al23	12k	m..	$\frac{1}{2}$	0.4215	0.0705		14-vertex Frank-Kasper Pd ₄ Al ₁₀
Al24	12k	m..	$\frac{1}{2}$	0.4254	0.3083		16-vertex Frank-Kasper Pd ₇ Al ₉
Al25	12j	m..	0	0.0715	0.2982		14-vertex Frank-Kasper MnPd ₃ Al ₁₀
Pd26	12j	m..	0	0.19017	0.26255		11-vertex polyhedron Al ₈ Pd ₃
Pd27	12j	m..	0	0.20384	0.11226		pseudo Frank-Kasper Al ₁₀ Pd ₃
Al28	12j	m..	0	0.2345	0.384		
Al29	12j	m..	0	0.3445	0.1108		icosahedron MnAl ₈ Pd ₃
Al30	12j	m..	0	0.3859	0.2411		pseudo Frank-Kasper Pd ₅ Al ₈
Al31	12j	m..	0	0.3861	0.3791		14-vertex Frank-Kasper Pd ₄ Al ₁₀
M32	8i	.3.	0.07415	0.07415	0.07415		pseudo Frank-Kasper Al ₇ Pd ₆
Pd33	8i	.3.	0.19119	0.19119	0.19119		icosahedron Al ₁₂
M34	8i	.3.	0.3096	0.3096	0.3096		pseudo Frank-Kasper Al ₁₃
Al35	8i	.3.	0.3819	0.3819	0.3819		16-vertex Frank-Kasper Pd ₇ Al ₉
Pd36	6g	mm2..	0.1931	$\frac{1}{2}$	0	0.68	
Pd37	6g	mm2..	0.4255	$\frac{1}{2}$	0		pseudo Frank-Kasper Al ₁₂ Pd
M38	6f	mm2..	0.064	0	$\frac{1}{2}$		9-vertex polyhedron Mn ₂ Al ₇
Pd39	6f	mm2..	0.3052	0	$\frac{1}{2}$		icosahedron Al ₁₂
Al40	6e	mm2..	0.1459	0	0		pseudo Frank-Kasper Pd ₆ Al ₇
Mn41	6e	mm2..	0.3961	0	0		bicapped square prism Al ₁₀
Al42	1a	m-3.	0	0	0		rhombic dodecahedron Pd ₈ Al ₆

M8 = 0.55Al + 0.45Mn; M17 = 0.86Mn + 0.14Al; M19 = 0.67Al + 0.33Mn; M22 = 0.63Pd + 0.37Al;

M32 = 0.66Pd + 0.34Al; M34 = 0.62Pd + 0.38Al; M38 = 0.97Al + 0.03Mn

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

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

Remarks: Phase referred to as β -(AlMnPdSi). Small amounts of Si ignored. Short interatomic distances for partly occupied site(s). In table 1 of [1] the Wyckoff positions of former Pd1, Pd2, Pd8, and Pd13 are misprinted as 6g, 6f, 12g, and 6f instead of 6f, 6g, 12j, and 6g, respectively.

References: [1] Sugiyama K., Kaji N., Hiraga K., Ishimasa T. (1998), Z. Kristallogr. 213, 90-95.