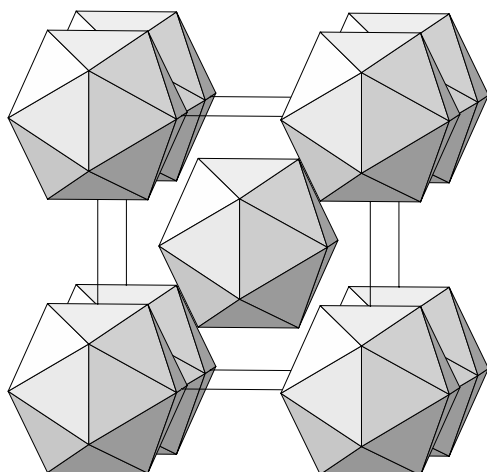


Space group (204) *Im-3*204  
*cI26*

$\text{WAl}_{12}$	<i>cI26</i>	(204) <i>Im-3</i> – ga
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**WAl<sub>12</sub>** [1], G phase; MoAl<sub>12</sub> [1]Structural features: Single WAl<sub>12</sub> icosahedra in a W-type (b.c.c.) arrangement. See Fig. II.51.Fig. II.51. **WAl<sub>12</sub>**Arrangement of WAl<sub>12</sub> icosahedra.

Adam J., Rich J.B. (1954) [1]

Al<sub>12</sub>W $a = 0.75803 \text{ nm}$ ,  $V = 0.4356 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	24g	$m\bar{3}$	0	0.184	0.309		11-vertex polyhedron WAl <sub>10</sub>
W2	2a	$m\bar{3}$	0	0	0		icosahedron Al <sub>12</sub>

Experimental: powder, film, X-rays,  $R = 0.060$ 

References: [1] Adam J., Rich J.B. (1954), Acta Crystallogr. 7, 813-816.

204  
*cI32*

$\text{CoAs}_3$	<i>cI32</i>	(204) <i>Im-3</i> – gc
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**CoAs<sub>3</sub>** [2], skutterudite, Strukturbericht notation D0<sub>2</sub>Structural features: CoAs<sub>6</sub> octahedra share vertices to form a 3D-framework. Single planar As<sub>4</sub> rings. See Fig. II.52.

Kjekshus A., Rakke T. (1974) [1]

As<sub>3</sub>Co $a = 0.82055 \text{ nm}$ ,  $V = 0.5525 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	24g	<i>m.</i>	0	0.1514	0.3442		tetrahedron Co <sub>2</sub> As <sub>2</sub>
Co2	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron As <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays, R = 0.100

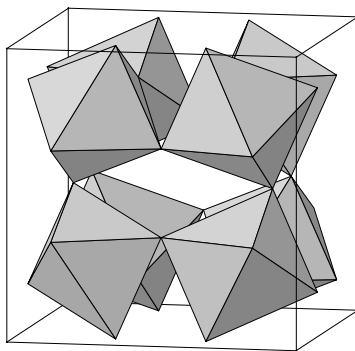


Fig. II.52. **CoAs<sub>3</sub>**

Arrangement of CoAs<sub>6</sub> octahedra.

References: [1] Kjekshus A., Rakke T. (1974), Acta Chem. Scand. A 28, 99-103. [2] (1931), Strukturberichte 1, 232.

204  
cI32

Sc(OH)<sub>3</sub>

cI32

(204) *Im*-3 – gc

**Sc(OH)<sub>3</sub>** [1]

Structural features: Sc(OH)<sub>6</sub> octahedra share vertices to form a 3D-framework.

Schubert K., Seitz A. (1948) [1]

H<sub>3</sub>O<sub>3</sub>Sc

$a = 0.7882 \text{ nm}$ ,  $V = 0.4897 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	24g	<i>m.</i>	0	0.182	0.307		non-colinear Sc <sub>2</sub>
Sc2	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron (OH) <sub>6</sub>

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

Experimental: powder, film, X-rays

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

References: [1] Schubert K., Seitz A. (1948), Z. Anorg. Chem. 256, 226-238.

204  
cI32

H<sub>0.5</sub>WO<sub>3</sub>

cI32

(204) *Im*-3 – gc

**H<sub>0.53</sub>WO<sub>3</sub>** [1]; ReO<sub>3</sub> hp2 [2]

Structural features: WO<sub>6</sub> octahedra share vertices to form a 3D-framework. Distorted derivative of ReO<sub>3</sub>.

Wiseman P.J., Dickens P.G. (1973) [1]

$\text{D}_{0.53}\text{O}_3\text{W}$

$a = 0.7562 \text{ nm}$ ,  $V = 0.4324 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24g	$m..$	0	0.2158	0.2842		non-colinear $\text{W}_2$ octahedron $\text{O}_6$
W2	8c	$..-3.$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
D3	24g	$m..$	0	0.073	0.314	0.088	
D4	24g	$m..$	0	0.186	0.427	0.088	

Experimental: powder, diffractometer, neutrons,  $R_p = 0.017$ ,  $T = 293 \text{ K}$

Remarks:  $\text{ReO}_3$  hp2 is stable at  $p > 0.53 \text{ GPa}$ . Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Wiseman P.J., Dickens P.G. (1973), J. Solid State Chem. 6, 374-377. [2] Jorgensen J.E., Jorgensen J.D., Batlogg B., Remeika J.P., Axe J.D. (1986), Phys. Rev. B: Condens. Matter 33, 4793-4798.

204  
cI34

$\text{LaFe}_4\text{P}_{12}$	$cI34$	(204) $Im-3 - gca$
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**$\text{LaFe}_4\text{P}_{12}$**  [1]

Structural features:  $\text{FeP}_6$  octahedra share vertices to form a 3D-framework; La in icosahedral voids. See Fig. II.53.

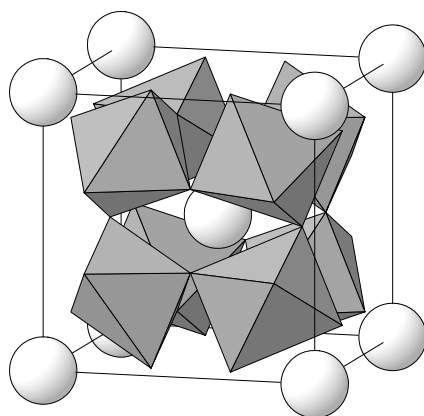


Fig. II.53.  **$\text{LaFe}_4\text{P}_{12}$**

Arrangement of  $\text{FeP}_6$  octahedra and La atoms.

Jeitschko W., Braun D. (1977) [1]

$\text{Fe}_4\text{LaP}_{12}$

$a = 0.78316 \text{ nm}$ ,  $V = 0.4803 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
P1	24g	$m..$	0	0.1504	0.3539		tetrahedron $\text{Fe}_2\text{P}_2$
Fe2	8c	$..-3.$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron $\text{P}_6$
La3	2a	$m-3.$	0	0	0		20-vertex polyhedron $\text{P}_{12}\text{Fe}_8$

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.028$

References: [1] Jeitschko W., Braun D. (1977), Acta Crystallogr. B 33, 3401-3406.

204  
cI36

$N_2O_4$	<i>cI36</i>	(204) <i>Im</i> -3 – gd
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**$N_2O_4$  cubic** [2], Strukturbericht notation C26

Structural features: Mutually perpendicular planar  $O_2N-NO_2$  molecules.

Kvick A. et al. (1982) [1]

$N_2O_4$

$a = 0.76937$  nm,  $V = 0.4554$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.1425	0.32597		single atom N
N2	12 <i>d</i>	<i>mm</i> 2..	0.38587	0	0		non-colinear $O_2$

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

Experimental: single crystal, diffractometer, neutrons,  $wR = 0.027$ ,  $T = 20$  K

Remarks: Only the molecular dimensions and the space group were reported in [2]. The atom coordinates corresponding to a different interpretation (model 3 instead of 1) were preferred in [6]. A structure proposal in space group (199)  $I2_13$  with  $NO_2$  molecules ([3], [5]) is superseded (see [6]). Strukturbericht notation C26a refers to the superseded structure proposal in space group (199)  $I2_13$ , C26b to the superseded structure proposal in space group (204) *Im*-3.

References: [1] Kvick A., McMullan R.K., Newton M.D. (1982), J. Chem. Phys. 76, 3754-3761. [2] Hendricks S.B. (1931), Z. Phys. 70, 699-700. [3] Vegard L. (1931), Z. Phys. 68, 184-203. [4] Broadley J.S., Monteath Robertson J. (1949), Nature (London) 164, 915. [5] Vegard L. (1930), Nature (London) 126, 916. [6] (1937), Strukturberichte 2, 269.

204  
cI36

$N_2O_4$	<i>cI36</i>	(204) <i>Im</i> -3 – ge
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**$N_2O_4$**  (see remark), Strukturbericht notation C26b

Structural features: Mutually perpendicular planar  $O_2N-NO_2$  molecules.

Hendricks S.B. (1931) [1]

$N_2O_4$

$a = 0.777$  nm,  $V = 0.4691$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.37	0.18		single atom N
N2	12 <i>e</i>	<i>mm</i> 2..	0.1	0	$\frac{1}{2}$		coplanar triangle $O_2N$

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

Experimental: powder, film, X-rays

Remarks: Only the molecular dimensions and the space group were reported in [1]. The atom coordinates reported here correspond to the (erroneous) interpretation made in [2] (model 3). The correct interpretation (model 1) was confirmed in [3].

References: [1] Hendricks S.B. (1931), Z. Phys. 70, 699-700. [2] (1937), Strukturberichte 2, 21. [3] Broadley J.S., Monteath Robertson J. (1949), Nature (London) 164, 915.

204  
cI38

$\text{Li}_{1.44}\text{W}_4\text{O}_{12}$	<i>cI38</i>	(204) <i>Im-3</i> – gcb
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**Li<sub>0.36</sub>WO<sub>3</sub>** [2], tungsten bronzeStructural features: WO<sub>6</sub> octahedra share vertices to form a 3D-framework; Li in distorted cuboctahedral voids (partial disorder).

Cava R.J. et al. (1983) [1]

 $\text{Li}_{1.44}\text{O}_{12}\text{W}_4$  $a = 0.74529 \text{ nm}$ ,  $V = 0.4140 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24g	<i>m</i> ..	0	0.2059	0.29		non-coplanar triangle W <sub>2</sub> Li
W2	8c	..-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron O <sub>6</sub>
Li3	6b	<i>mmm</i> ..	0	$\frac{1}{2}$	$\frac{1}{2}$	0.48	coplanar square O <sub>4</sub>

Experimental: powder, diffractometer, neutrons,  $R_p = 0.070$ 

References: [1] Cava R.J., Santoro A., Murphy D.W., Zahurak S.M., Roth R.S. (1983), J. Solid State Chem. 50, 121-128. [2] Wiseman P.J., Dickens P.G. (1976), J. Solid State Chem. 17, 91-100.

204  
cI38

$\text{Sm}_{12}\text{Ni}_6\text{In}$	<i>cI38</i>	(204) <i>Im-3</i> – gea
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**Sm<sub>12</sub>Ni<sub>6</sub>In** [1]Structural features: InSm<sub>12</sub> icosahedra and NiSm<sub>6</sub>Ni monocapped trigonal prisms (tricapped if two additional Sm atoms at longer distances are considered) share atoms to form a 3D-framework.

Kalychak Y.M. et al. (1998) [1]

 $\text{InNi}_6\text{Sm}_{12}$  $a = 0.98 \text{ nm}$ ,  $V = 0.9412 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sm1	24g	<i>m</i> ..	0	0.1966	0.3219		non-coplanar triangle Ni <sub>3</sub>
Ni2	12e	<i>mm2</i> ..	0.1256	0	$\frac{1}{2}$		monocapped trigonal prism NiSm <sub>6</sub>
In3	2a	<i>m-3</i> ..	0	0	0		icosahedron Sm <sub>12</sub>

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

References: [1] Kalychak Y.M., Zaremba V.I., Stepen' Damm A., Galadzhun Y.V., Akselrud L.G. (1998), Kristallografiya 43, 17-20.

204  
cI40

$\text{Na}_{0.54}\text{WO}_3$	<i>cI40</i>	(204) <i>Im-3</i> – gcba
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**Na<sub>0.54</sub>WO<sub>3</sub>** [1], tungsten bronzeStructural features: WO<sub>6</sub> octahedra share vertices to form a 3D-framework; Na in distorted cuboctahedral voids (disorder).

Wiseman P.J., Dickens P.G. (1976) [1]

 $\text{Na}_{0.54}\text{O}_3\text{W}$  $a = 0.7656 \text{ nm}$ ,  $V = 0.4488 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	<i>m.</i>	0	0.2386	0.2614		non-colinear W <sub>2</sub>
W2	8c	<i>.-3.</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron O <sub>6</sub>
Na3	6b	<i>mmm.</i>	0	$\frac{1}{2}$	$\frac{1}{2}$	0.54	cuboctahedron O <sub>12</sub>
Na4	2a	<i>m-3.</i>	0	0	0	0.54	cuboctahedron O <sub>12</sub>

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

References: [1] Wiseman P.J., Dickens P.G. (1976), J. Solid State Chem. 17, 91-100.

204  
cI40

NaMn <sub>7</sub> O <sub>12</sub>	<i>cI40</i>	(204) <i>Im-3</i> – gcba
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**NaMn<sub>7</sub>O<sub>12</sub> rt** [1], perovskite [AB<sub>3</sub>]B<sub>4</sub>O<sub>12</sub>

Structural features: MnO<sub>6</sub> octahedra and MnO<sub>4</sub> squares share atoms to form a 3D-framework, Na in icosahedral voids.

Marezio M. et al. (1973) [1]

Mn<sub>7</sub>NaO<sub>12</sub>

$a = 0.73036$  nm,  $V = 0.3896$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	<i>m.</i>	0	0.1828	0.3132		non-coplanar triangle Mn <sub>3</sub>
M2	8c	<i>.-3.</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron O <sub>6</sub>
(Mn <sup>3+</sup> )3	6b	<i>mmm.</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		coplanar square O <sub>4</sub>
Na4	2a	<i>m-3.</i>	0	0	0		icosahedron O <sub>12</sub>

$M2 = 0.5Mn^{3+} + 0.5Mn^{4+}$

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

Remarks: In [1] the number of formula units  $Z$  is misprinted as 4 instead of 2.

References: [1] Marezio M., Dernier P.D., Chenavas J., Joubert J.C. (1973), J. Solid State Chem. 6, 16-20.

204  
cI40

CaCu <sub>3</sub> Mn <sub>4</sub> O <sub>12</sub>	<i>cI40</i>	(204) <i>Im-3</i> – gcba
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**CaCu<sub>3</sub>Mn<sub>4</sub>O<sub>12</sub> cubic** [1], perovskite A<sub>3</sub>A'B<sub>4</sub>O<sub>12</sub>

Structural features: MnO<sub>6</sub> octahedra share vertices to form a 3D-framework; Ca in icosahedral, Cu in square voids. Single CuO<sub>4</sub> squares. Ordering variant of NaMn<sub>7</sub>O<sub>12</sub>. See Fig. II.54.

Chenavas J. et al. (1975) [1]

CaCu<sub>3</sub>Mn<sub>4</sub>O<sub>12</sub>

$a = 0.7241$  nm,  $V = 0.3797$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	<i>m.</i>	0	0.1822	0.3033		non-coplanar triangle Mn <sub>2</sub> Cu
Mn2	8c	<i>.-3.</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron O <sub>6</sub>
Cu3	6b	<i>mmm.</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		coplanar square O <sub>4</sub>

Ca4      2a    *m*-3.      0          0          0          icosahedron O<sub>12</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.013

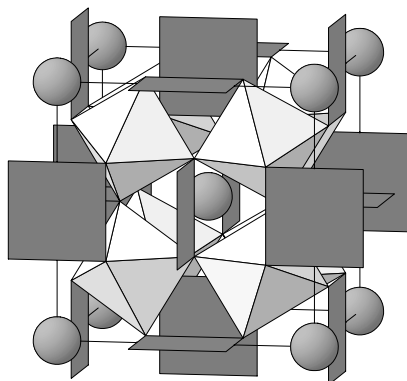


Fig. II.54. **CaCu<sub>3</sub>Mn<sub>4</sub>O<sub>12</sub> cubic**

Arrangement of MnO<sub>6</sub> (light) octahedra, CuO<sub>4</sub> squares (dark) and Ca atoms.

References: [1] Chenavas J., Joubert J.C., Marezio M., Bochu B. (1975), J. Solid State Chem. 14, 25-32.

204  
c/46

Na <sub>4</sub> Ba <sub>0.87</sub> Co <sub>3.13</sub> F <sub>12</sub>	<i>c</i> /46	(204) <i>Im</i> -3 – geca
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**Na<sub>4</sub>Ba<sub>0.87</sub>Co<sub>3.13</sub>F<sub>12</sub>** [1], perovskite family; "Na<sub>2</sub>BaFe<sub>4</sub>F<sub>12</sub>" (see remark)

Structural features: (Co,Na)F<sub>6</sub> octahedra share vertices to form a 3D-framework; (Ba,Na) and Na in distorted cuboctahedral voids (Na displaced towards an edge, split site).

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

Ba<sub>0.87</sub>Co<sub>3.13</sub>F<sub>12</sub>Na<sub>4</sub>

*a* = 0.80185 nm, *V* = 0.5156 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24g	<i>m</i> ..	0	0.3029	0.2129		non-coplanar triangle NaCo <sub>2</sub>
Na2	12e	<i>mm</i> 2..	0.0498	0	1/2	0.5	
M3	8c	.-3.	1/4	1/4	1/4		octahedron F <sub>6</sub>
M4	2a	<i>m</i> -3.	0	0	0		icosahedron F <sub>12</sub>

M3 = 0.782Co + 0.218Na; M4 = 0.869Ba + 0.131Na

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.099

Remarks: Homogeneity range Na<sub>4</sub>(Ba<sub>*x*</sub>Co<sub>1-*x*</sub>)<sub>4</sub>F<sub>12</sub>, 0.2125 < *x* < 0.2325. Short interatomic distances for partly occupied site(s). A similar structure proposal for so-called Na<sub>2</sub>BaFe<sub>4</sub>F<sub>12</sub> [2] (idealized composition) was later superseded by in part the same authors [3].

We assume that in table III of [1] the occupation of the site in Wyckoff position 8c is misprinted as 0.782Co + 0.217Na instead of 0.782Co + 0.218Na.

References: [1] Ducau M., Roisnel T., Darriet J. (1993), J. Solid State Chem. 107, 387-396. [2] Darriet J., Mayorga S.G., Tressaud A. (1990), Eur. J. Solid State Inorg. Chem. 27, 783-790. [3] Darriet J., Ducau M., Tressaud A. (1992), Eur. J. Solid State Inorg. Chem. 29, 395-398.

204  
cI46

$K_6(K_{0.75}Na_{0.25})_4Tl_{13}$	<i>cI46</i>	(204) <i>Im-3</i> – geca
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**K<sub>9</sub>NaTl<sub>13</sub>** [1]Structural features: Single TlTl<sub>12</sub> icosahedra in a W-type (b.c.c.) arrangement, separated by K and (K,Na).

Cordier G., Müller V. (1994) [1]

K<sub>9</sub>NaTl<sub>13</sub> $a = 1.152 \text{ nm}$ ,  $V = 1.5288 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	24g	<i>m.</i>	0	0.14152	0.24176		icosahedron K <sub>6</sub> Tl <sub>6</sub>
K2	12e	<i>mm2.</i>	0.1709	0	$\frac{1}{2}$		7-capped pentagonal prism Tl <sub>8</sub> K <sub>9</sub>
M3	8c	<i>.-3.</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron Tl <sub>6</sub>
Tl4	2a	<i>m-3.</i>	0	0	0		icosahedron Tl <sub>12</sub>

M3 = 0.75K + 0.25Na

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

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

Remarks: In the abstract of [1] the number of formula units per unit cell Z is misprinted as 1 instead of 2 (given in table 1). An ordered structure is reported for composition K<sub>6</sub>Na<sub>4</sub>Tl<sub>13</sub> in [2].

References: [1] Cordier G., Müller V. (1994), Z. Naturforsch. B 49, 935-938. [2] Dong Z.C., Corbett J.D. (1995), J. Am. Chem. Soc. 117, 6447-6455.

204  
cI46

$K_6(Na_{0.5}Cd_{0.5})_4Tl_{12}Cd$	<i>cI46</i>	(204) <i>Im-3</i> – geca
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**K<sub>6</sub>Na<sub>2</sub>Cd<sub>3</sub>Tl<sub>12</sub>** [1]Structural features: Single CdTl<sub>12</sub> icosahedra in a W-type (b.c.c.) arrangement, separated by K and (Na,Cd). Ordering variant of K<sub>9</sub>NaTl<sub>13</sub>.

Tillard Charbonnel M.M. et al. (1996) [1]

Cd<sub>2.92</sub>K<sub>6</sub>Na<sub>2.08</sub>Tl<sub>12</sub> $a = 1.1321 \text{ nm}$ ,  $V = 1.4510 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	24g	<i>m.</i>	0	0.14086	0.24322		icosahedron Na <sub>2</sub> CdTl <sub>5</sub> K <sub>4</sub>
K2	12e	<i>mm2.</i>	0.1721	0	$\frac{1}{2}$		7-capped pentagonal prism Tl <sub>8</sub> K <sub>5</sub> Na <sub>4</sub>
M3	8c	<i>.-3.</i>	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron Tl <sub>6</sub> K <sub>6</sub>
Cd4	2a	<i>m-3.</i>	0	0	0		icosahedron Tl <sub>12</sub>

M3 = 0.52Na + 0.48Cd

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

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

References: [1] Tillard Charbonnel M.M., Belin C.H.E., Manteghetti A.P., Flot D.M. (1996), Inorg. Chem. 35, 2583-2589.



$\text{Li}(\text{Li}_{0.11}\text{Cu}_{0.89})_3(\text{Ti}_{0.67}\text{Nb}_{0.33})_4\text{O}_{12}$	<i>cI62</i>	(204) <i>Im-3</i> – $g^2cb$
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**Li(Cu<sub>2.67</sub>Li<sub>0.33</sub>)(Ti<sub>2.67</sub>Nb<sub>1.33</sub>)O<sub>12</sub>** [1], perovskite family

Structural features: (Ti,Nb)O<sub>6</sub> octahedra share vertices to form a 3D-framework; (Cu,Li) in square voids, Li in icosahedral voids (displaced towards one O, disorder). Single (Cu,Li)O<sub>4</sub> squares.

Mouron P., Choisnet J. (1987) [1]

$\text{Cu}_{2.67}\text{Li}_{1.33}\text{Nb}_{1.33}\text{O}_{12}\text{Ti}_{2.67}$

$a = 0.74314 \text{ nm}$ ,  $V = 0.4104 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	24 <i>g</i>	<i>m</i> ..	0	0.06	0.11	0.083	
O2	24 <i>g</i>	<i>m</i> ..	0	0.18	0.31		tetrahedron LiCuTi <sub>2</sub>
M3	8 <i>c</i>	..3.	1/4	1/4	1/4		octahedron O <sub>6</sub>
M4	6 <i>b</i>	<i>mmm</i> ..	0	1/2	1/2		coplanar square O <sub>4</sub>

M3 = 0.668Ti + 0.332Nb; M4 = 0.89Cu + 0.11Li

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

Experimental: powder, diffractometer, X-rays,  $R_B = 0.036$

Remarks: Homogeneity range Li[Cu<sub>3-x</sub>Li<sub>x</sub>][Ti<sub>3-x</sub>Nb<sub>1+x</sub>]O<sub>12</sub>, 0.12 < *x* < 0.33. Short interatomic distances for partly occupied site(s).

References: [1] Mouron P., Choisnet J. (1987), J. Solid State Chem. 66, 311-317.

$\text{Sr}_{1.2}\text{Re}_3\text{O}_9$	<i>cI64</i>	(204) <i>Im-3</i> – <i>gfd</i>
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**Sr<sub>x</sub>ReO<sub>3</sub>** [1]

Structural features: Pairs of edge-linked ReO<sub>6</sub> octahedra share vertices to form a 3D-framework; Sr in voids (disorder).

Baud G. et al. (1979) [1]

$\text{O}_9\text{Re}_3\text{Sr}_{1.20}$

$a = 0.9192 \text{ nm}$ ,  $V = 0.7767 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.3508	0.2885		non-colinear Re <sub>2</sub>
Sr2	16 <i>f</i>	.3.	0.1832	0.1832	0.1832	0.3	
Re3	12 <i>e</i>	<i>mm2</i> ..	0.1321	0	1/2		octahedron O <sub>6</sub>
O4	12 <i>d</i>	<i>mm2</i> ..	0.3301	0	0		non-colinear Re <sub>2</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). Space group (197) *I23* was tested and rejected ( $R = 0.069$ ).

References: [1] Baud G., Besse J.P., Chevalier R., Chamberland B.L. (1979), J. Solid State Chem. 28, 157-162.

204  
cI70

$\text{Na}_4\text{Ba}_{0.84}\text{Fe}_{3.16}\text{F}_{12}$	<i>cI70</i>	(204) <i>Im</i> -3 – <i>g</i> <sup>2</sup> <i>eca</i>
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**Na<sub>4</sub>Ba<sub>0.84</sub>Fe<sub>3.16</sub>F<sub>12</sub>** [1], perovskite familyStructural features: (Fe,Na)F<sub>6</sub> octahedra share vertices to form a 3D-framework (split F site); (Ba,Na) and Na in distorted cuboctahedral voids (Na displaced towards an edge, split site).

Darriet J. et al. (1992) [1]

 $\text{Ba}_{0.84}\text{F}_{12}\text{Fe}_{3.16}\text{Na}_4$  $a = 0.8075 \text{ nm}$ ,  $V = 0.5265 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24 <i>g</i>	<i>m</i> ..	0	0.1912	0.2937	0.9	single atom F
F2	24 <i>g</i>	<i>m</i> ..	0	0.302	0.195	0.1	single atom F
Na3	12 <i>e</i>	<i>mm</i> 2..	0.0409	0	$\frac{1}{2}$	0.5	
M4	8 <i>c</i>	..-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		12-vertex polyhedron F <sub>12</sub>
M5	2 <i>a</i>	<i>m</i> -3.	0	0	0		24-vertex polyhedron F <sub>24</sub>

M4 = 0.79Fe + 0.21Na; M5 = 0.84Ba + 0.16Na

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

Remarks: Short interatomic distances for partly occupied site(s). Supersedes a structure proposal with one single F site by in part the same authors [2] (cell parameter from the same reference).

References: [1] Darriet J., Ducau M., Tressaud A. (1992), Eur. J. Solid State Inorg. Chem. 29, 395-398.

[2] Darriet J., Mayorga S.G., Tressaud A. (1990), Eur. J. Solid State Inorg. Chem. 27, 783-790.

204  
cI72

$\text{NaSbO}_3$	<i>cI72</i>	(204) <i>Im</i> -3 – <i>g</i> <i>fedc</i>
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**NaSbO<sub>3</sub>** [1]Structural features: Pairs of edge-linked SbO<sub>6</sub> octahedra share vertices to form a 3D-framework; Na in channels along <111> (partial disorder).

Hong H.Y.P. et al. (1974) [1]

 $\text{Na}_{1.29}\text{O}_3\text{Sb}$  $a = 0.9378 \text{ nm}$ ,  $V = 0.8248 \text{ nm}^3$ ,  $Z = 12$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.334	0.287		non-colinear Sb <sub>2</sub>
Na2	16 <i>f</i>	..3.	0.1229	0.1229	0.1229	0.82	bicapped square prism Na <sub>4</sub> O <sub>6</sub>
Sb3	12 <i>e</i>	<i>mm</i> 2..	0.1616	0	$\frac{1}{2}$		octahedron O <sub>6</sub>
O4	12 <i>d</i>	<i>mm</i> 2..	0.356	0	0		non-colinear Sb <sub>2</sub>
Na5	8 <i>c</i>	..-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.29	square prism (cube) Na <sub>2</sub> O <sub>6</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). Space groups (197) *I*23 and (199) *I*2<sub>1</sub>3 were tested and rejected.

References: [1] Hong H.Y.P., Kafalas J.A., Goodenough J.B. (1974), J. Solid State Chem. 9, 345-351.

KBiO <sub>3</sub>	cI74	(204) <i>Im</i> -3 – gfedca
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**KBiO<sub>3</sub>** [1]

Structural features: Pairs of edge-linked BiO<sub>6</sub> octahedra share vertices to form a 3D-framework; K in channels along <111> (disorder).

Nguyen Tu N. et al. (1993) [1]

BiKO<sub>3</sub>

$a = 1.00194$  nm,  $V = 1.0058$  nm<sup>3</sup>,  $Z = 12$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24g	$m..$	0	0.3387	0.2874		non-colinear Bi <sub>2</sub>
K2	16f	.3.	0.1571	0.1571	0.1571	0.6	
Bi3	12e	$mm2..$	0.16004	0	$\frac{1}{2}$		octahedron O <sub>6</sub>
O4	12d	$mm2..$	0.363	0	0		non-colinear Bi <sub>2</sub>
K5	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.22	
K6	2a	$m-3.$	0	0	0	0.34	square prism (cube) K <sub>8</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.021

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

References: [1] Nguyen Tu N., Giaquinta D.M., Davis W.M., Zur Loye H.C. (1993), Chem. Mater. 5, 1273-1276.

K <sub>7</sub> Sb <sub>6</sub> O <sub>18</sub> F	cI74	(204) <i>Im</i> -3 – gfedca
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**KSbO<sub>3</sub>· $\frac{1}{6}$ KF** [1]; KBiO<sub>3</sub>·xH<sub>2</sub>O [2]

Structural features: Pairs of edge-linked SbO<sub>6</sub> octahedra share vertices to form a 3D-framework; K and F in channels along <111> (disorder).

Goodenough J.B. et al. (1976) [1]

FK<sub>6,56</sub>O<sub>18</sub>Sb<sub>6</sub>

$a = 0.9606$  nm,  $V = 0.8864$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24g	$m..$	0	0.346	0.292		non-colinear Sb <sub>2</sub>
K2	16f	.3.	0.1582	0.1582	0.1582	0.66	
Sb3	12e	$mm2..$	0.1579	0	$\frac{1}{2}$		octahedron O <sub>6</sub>
O4	12d	$mm2..$	0.363	0	0		non-colinear Sb <sub>2</sub>
K5	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.32	
F6	2a	$m-3.$	0	0	0		square prism (cube) K <sub>8</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.077

Remarks: Short interatomic distances for partly occupied site(s). We assume that the second K site mentioned in the text of [2] was omitted unintentionally in table 1; we further assume that the y-coordinate of former O(1) (also omitted) is equal 0.

References: [1] Goodenough J.B., Hong H.Y., Kafalas J.A. (1976), Mater. Res. Bull. 11, 203-220. [2] Kodialam S., Korthius V.C., Hoffmann R.D., Sleight A.W. (1992), Mater. Res. Bull. 27, 1379-1384.

204  
cI76

$\text{Na}_{0.38}\text{Li}_{0.62}\text{Ba}_{0.62}\text{Co}_{0.38}\text{F}_3$	<i>cI76</i>	(204) <i>Im-3</i> – <i>g</i> <sup>2</sup> <i>ecba</i>
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**(Li<sub>1-x</sub>Na<sub>x</sub>)(Ba<sub>1-x</sub>Co<sub>x</sub>)F<sub>3</sub>** [1], perovskite family

Structural features: (Co,Li)F<sub>6</sub> octahedra share vertices to form a 3D-framework (split F site); Ba and Na in distorted cuboctahedral voids (disorder).

Welsch M. et al. (1999) [1]

$\text{Ba}_{0.62}\text{Co}_{0.38}\text{F}_3\text{Li}_{0.62}\text{Na}_{0.38}$

$a = 0.8018 \text{ nm}$ ,  $V = 0.5155 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24 <i>g</i>	<i>m</i> ..	0	0.1947	0.29	0.5	
F2	24 <i>g</i>	<i>m</i> ..	0	0.25	0.25	0.5	
Na3	12 <i>e</i>	<i>mm</i> 2..	0.073	0	$\frac{1}{2}$	0.127	
M4	8 <i>c</i>	..-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
M5	6 <i>b</i>	<i>mmm</i> ..	0	$\frac{1}{2}$	$\frac{1}{2}$	0.745	
Ba6	2 <i>a</i>	<i>m</i> -3.	0	0	0		

M4 = 0.618Li + 0.382Co; M5 = 0.659Ba + 0.341Na

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

Remarks: Short interatomic distances for partly occupied site(s). Refinement of a simple perovskite model  $\text{BaCo}_{0.5}\text{F}_3$  gave R = 0.025.

References: [1] Welsch M., Kummer Dörner S., Peschel B., Babel D. (1999), Z. Anorg. Allg. Chem. 625, 1255-1260.

204  
cI80

$\text{AgSbO}_3$	<i>cI80</i>	(204) <i>Im-3</i> – <i>gf</i> <sup>2</sup> <i>ed</i>
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**AgSbO<sub>3</sub>** [1]; HSbO<sub>3</sub>·H<sub>2</sub>O [2]

Structural features: Pairs of edge-linked SbO<sub>6</sub> octahedra share vertices to form a 3D-framework; Ag in channels along <111> (partial disorder).

Hong H.Y.P. et al. (1974) [1]

$\text{Ag}_{1.03}\text{O}_3\text{Sb}$

$a = 0.9404 \text{ nm}$ ,  $V = 0.8316 \text{ nm}^3$ ,  $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.296	0.291		tetrahedron Sb <sub>2</sub> Ag <sub>2</sub>
Ag2	16 <i>f</i>	.3.	0.111	0.111	0.111	0.33	
Ag3	16 <i>f</i>	.3.	0.184	0.184	0.184	0.44	
Sb4	12 <i>e</i>	<i>mm</i> 2..	0.1607	0	$\frac{1}{2}$		octahedron O <sub>6</sub>
O5	12 <i>d</i>	<i>mm</i> 2..	0.371	0	0		non-colinear Sb <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.080

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

References: [1] Hong H.Y.P., Kafalas J.A., Goodenough J.B. (1974), J. Solid State Chem. 9, 345-351. [2] Watelet H., Picard J.P., Baud G., Besse J.P., Chevalier R. (1981), Mater. Res. Bull. 16, 1131-1137.

204  
cI82

$\text{Gd}_4(\text{Gd}_{0.5}\text{Sn}_{0.5})\text{Ni}_{12}\text{Sn}_{24}$	<i>cI82</i>	(204) <i>Im-3</i> – $\text{g}^3\text{ca}$
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**GdNi<sub>2.67</sub>Sn<sub>5.44</sub>** [1]

Structural features: NiSn<sub>6</sub> trigonal prisms share edges and single vertices to form a 3D-framework; Gd in cuboctahedral, (Gd,Sn) in distorted icosahedral voids.

Akselrud L.G. et al. (1983) [1]

$\text{Gd}_{4.50}\text{Ni}_{12}\text{Sn}_{24.50}$

$a = 1.18548 \text{ nm}$ ,  $V = 1.6660 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	24g	<i>m</i> ..	0	0.1562	0.3242		trigonal prism Sn <sub>6</sub>
Sn2	24g	<i>m</i> ..	0	0.2524	0.1329		non-coplanar triangle Ni <sub>3</sub>
Sn3	24g	<i>m</i> ..	0	0.3718	0.3734		non-coplanar triangle Ni <sub>3</sub>
Gd4	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		18-vertex polyhedron Sn <sub>12</sub> Ni <sub>6</sub>
M5	2a	<i>m</i> -3.	0	0	0		icosahedron Sn <sub>12</sub>

$\text{M5} = 0.5\text{Gd} + 0.5\text{Sn}$

Experimental: powder, diffractometer, X-rays,  $R = 0.075$

References: [1] Akselrud L.G., Komarovskaya L.P., Skolozdra R.V. (1983), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1983(5), 33-35.

204  
cI82

$\text{Ce}_4\text{Pt}_{12}\text{Sn}_{25}$	<i>cI82</i>	(204) <i>Im-3</i> – $\text{g}^3\text{ca}$
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**Ce<sub>4</sub>Pt<sub>12</sub>Sn<sub>25</sub>** [1]

Structural features: PtSn<sub>6</sub> trigonal prisms share edges and single vertices to form a 3D-framework; Ce in cuboctahedral, additional Sn in distorted icosahedral voids. Ordering variant of GdNi<sub>2.67</sub>Sn<sub>5.44</sub>.

Chafik El Idrissi B. et al. (1990) [1]

$\text{Ce}_4\text{Pt}_{12}\text{Sn}_{25}$

$a = 1.2281 \text{ nm}$ ,  $V = 1.8523 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Pt1	24g	<i>m</i> ..	0	0.1671	0.3183		square antiprism Sn <sub>6</sub> Ce <sub>2</sub>
Sn2	24g	<i>m</i> ..	0	0.2505	0.123		14-vertex Frank-Kasper Pt <sub>3</sub> Sn <sub>9</sub> Ce <sub>2</sub>
Sn3	24g	<i>m</i> ..	0	0.3738	0.3793		14-vertex Frank-Kasper Pt <sub>3</sub> Sn <sub>9</sub> Ce <sub>2</sub>
Ce4	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		18-vertex polyhedron Pt <sub>6</sub> Sn <sub>12</sub>
Sn5	2a	<i>m</i> -3.	0	0	0		icosahedron Sn <sub>12</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.033$

Remarks: Large displacement parameters were observed for site Sn5; a model considering splitting of this site (Pearson symbol cI106) is also proposed.

References: [1] Chafik El Idrissi B., Venturini G., Malaman B. (1990), Mater. Res. Bull. 25, 807-814.

204  
c/90

SrIrO <sub>3</sub>	<i>c/90</i>	(204) <i>Im-3</i> – g <sup>2</sup> edca
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**SrIrO<sub>3</sub>** [1]

Structural features: Pairs of edge-linked IrO<sub>6</sub> octahedra share vertices to form a 3D-framework; Sr in channels along <111> (disorder).

Schmalle H. et al. (1990) [1]

IrO<sub>3</sub>Sr<sub>0.85</sub> $a = 0.934 \text{ nm}$ ,  $V = 0.8148 \text{ nm}^3$ ,  $Z = 12$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	<i>m</i> ..	0	0.3353	0.2902		non-collinear Ir <sub>2</sub>
Sr2	16 <i>f</i>	.3.	0.1427	0.1427	0.1427	0.234	
Sr3	16 <i>f</i>	.3.	0.2028	0.2028	0.2028	0.3	
Ir4	12 <i>e</i>	<i>mm</i> 2..	0.15671	0	<sup>1</sup> / <sub>2</sub>		octahedron O <sub>6</sub>
O5	12 <i>d</i>	<i>mm</i> 2..	0.3574	0	0		non-collinear Ir <sub>2</sub>
Sr6	8 <i>c</i>	.-3.	<sup>1</sup> / <sub>4</sub>	<sup>1</sup> / <sub>4</sub>	<sup>1</sup> / <sub>4</sub>	0.12	
Sr7	2 <i>a</i>	<i>m</i> -3.	0	0	0	0.336	square prism (cube) Sr <sub>8</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.018

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

References: [1] Schmalle H., Gurtner C., Oswald H.R., Reller A. (1990), Z. Kristallogr. 191, 239-247.

204  
c/106

Ce <sub>4</sub> Pt <sub>12</sub> Sn <sub>25</sub>	<i>c/106</i>	(204) <i>Im-3</i> – g <sup>4</sup> ca
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**Ce<sub>4</sub>Pt<sub>12</sub>Sn<sub>25</sub>** [1]

Structural features: PtSn<sub>6</sub> trigonal prisms share edges and single vertices to form a 3D-framework (split Sn site); Ce in cuboctahedral, additional Sn in distorted icosahedral voids.

Chafik El Idrissi B. et al. (1990) [1]

Ce<sub>4</sub>Pt<sub>12</sub>Sn<sub>25</sub> $a = 1.2281 \text{ nm}$ ,  $V = 1.8523 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sn1	24 <i>g</i>	<i>m</i> ..	0	0.1145	0.2287	0.45	
Sn2	24 <i>g</i>	<i>m</i> ..	0	0.1289	0.2657	0.55	
Pt3	24 <i>g</i>	<i>m</i> ..	0	0.3183	0.1671		
Sn4	24 <i>g</i>	<i>m</i> ..	0	0.3792	0.3738		
Ce5	8 <i>c</i>	.-3.	<sup>1</sup> / <sub>4</sub>	<sup>1</sup> / <sub>4</sub>	<sup>1</sup> / <sub>4</sub>		
Sn6	2 <i>a</i>	<i>m</i> -3.	0	0	0		icosahedron Sn <sub>12</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). A model without site splitting (Pearson symbol cI82) gave a similar agreement but large displacement parameters.

References: [1] Chafik El Idrissi B., Venturini G., Malaman B. (1990), Mater. Res. Bull. 25, 807-814.

204  
cI108

$\text{Rb}_{7.3}\text{Ni}_3[\text{NH}_2]_{12.3}[\text{CN}]$	<i>cI108</i>	(204) <i>Im-3</i> – $\text{g}^3\text{f}^2\text{d}$
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**Rb<sub>7.3</sub>Ni<sub>3</sub>(NH<sub>2</sub>)<sub>12.3</sub>(CN) [1]**

Structural features: Ni(NH<sub>2</sub>)<sub>4</sub> square units (mutually perpendicular non-linear NH<sub>2</sub> units) and CN units embedded in a Rb matrix.

Bock J., Jacobs H. (1988) [1]

$\text{CNH}_{24}\text{N}_{13}\text{Ni}_3\text{Rb}_{7.35}$

$a = 1.3872 \text{ nm}$ ,  $V = 2.6694 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24 <i>g</i>	<i>m</i> ..	0	0.138	0.335		single atom Ni
N2	24 <i>g</i>	<i>m</i> ..	0	0.335	0.139		single atom Ni
Rb3	24 <i>g</i>	<i>m</i> ..	0	0.3635	0.3635		trigonal prism N <sub>6</sub>
Rb4	16 <i>f</i>	.3.	0.103	0.103	0.103	0.338	non-coplanar triangle Rb <sub>3</sub>
Ni5	12 <i>d</i>	<i>mm2</i> ..	0.3293	0	0		non-coplanar square N <sub>4</sub>
CN6	8 <i>c</i>	..3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.5	colinear Rb <sub>2</sub>
H7	48 <i>h</i>	1	0.05	0.13	0.28		
H8	48 <i>h</i>	1	0.05	0.29	0.15		

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

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

Remarks:  $\text{Rb}_6\text{Ni}_3(\text{NH}_2)_{12} \cdot (\text{RbCN})_{1.0} \cdot (\text{RbNH}_2)_{0.3}$ . Part of NH<sub>2</sub> not located. The atom coordinates correspond to the positions of Rb, Ni and N atoms belonging to NH<sub>2</sub> units and the centers of CN dumbbells. Distinct positions for the atoms of the cyanide units were refined for the K-analogue. 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] Bock J., Jacobs H. (1988), *J. Less-Common Met.* 137, 105-122.

204  
cI116

$\text{K}_{7.2}\text{Ni}_3[\text{NH}_2]_{12.2}[\text{CN}]$	<i>cI116</i>	(204) <i>Im-3</i> – $\text{g}^3\text{f}^2\text{d}$
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**K<sub>7.2</sub>Ni<sub>3</sub>(NH<sub>2</sub>)<sub>12.2</sub>(CN) [1]**

Structural features: Ni(NH<sub>2</sub>)<sub>4</sub> square units (mutually perpendicular non-linear NH<sub>2</sub> units) and CN units embedded in a K matrix.

Bock J., Jacobs H. (1988) [1]

$\text{C}_{0.99}\text{H}_{24}\text{K}_{7.26}\text{N}_{12.99}\text{Ni}_3$

$a = 1.3454 \text{ nm}$ ,  $V = 2.4353 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24 <i>g</i>	<i>m</i> ..	0	0.1432	0.3363		single atom Ni
N2	24 <i>g</i>	<i>m</i> ..	0	0.3362	0.1433		single atom Ni
K3	24 <i>g</i>	<i>m</i> ..	0	0.3653	0.3653		trigonal prism N <sub>6</sub>
K4	16 <i>f</i>	.3.	0.1056	0.1056	0.1056	0.315	tetrahedron CK <sub>3</sub>
M5	16 <i>f</i>	.3.	0.227	0.227	0.227	0.494	single atom C
Ni6	12 <i>d</i>	<i>mm2</i> ..	0.3321	0	0		non-coplanar square N <sub>4</sub>
H7	48 <i>h</i>	1	0.051	0.303	0.164		

H8	48h	1	0.054	0.165	0.305
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$$M5 = 0.5C + 0.5N$$

Experimental: single crystal, diffractometer, X-rays, R = 0.021

Remarks:  $\text{K}_6\text{Ni}_3(\text{NH}_2)_{12} \cdot (\text{KCN})_{1.0} \cdot (\text{KNH}_2)_{0.2}$  Part of  $\text{NH}_2$  not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bock J., Jacobs H. (1988), J. Less-Common Met. 137, 105-122.

204  
c/122

$\text{Cs}_4\text{KCu}_3[\text{NO}_2]_{111}[\text{H}_2\text{O}]$	<i>cI122</i>	(204) <i>Im-3</i> – $\text{g}^2\text{e}^2\text{d}^3\text{cb}$
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$$\text{Cs}_4\text{KCu}_3(\text{NO}_2)_{11-x}(\text{OH})_x \cdot \text{H}_2\text{O} \text{ [1]}$$

Structural features:  $\text{Cu}(\text{NO}_2)_4$  square units (mutually perpendicular non-linear  $\text{NO}_2$  units); disorder caused by flipping of  $\text{NO}_2$  units (bonded to Cu via one N or two O, respectively).

Ozarowski A. et al. (1991) [1]

$$\text{Cs}_4\text{Cu}_3\text{KN}_{11}\text{O}_{22}$$
 $a = 1.101 \text{ nm}, V = 1.3346 \text{ nm}^3, Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24g	$m..$	0	0.096	0.266		
O2	24g	$m..$	0	0.404	0.266	0.833	non-collinear N <sub>2</sub>
N3	12e	$mm2..$	0.183	0	$\frac{1}{2}$	0.2	non-coplanar triangle O <sub>2</sub> N
N4	12e	$mm2..$	0.317	0	$\frac{1}{2}$	0.633	non-coplanar triangle O <sub>2</sub> N
K5	12d	$mm2..$	0.04	0	0	0.167	
N6	12d	$mm2..$	0.241	0	0	0.2	
N7	12d	$mm2..$	0.317	0	0	0.8	
Cs8	8c	$.-3.$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron O <sub>12</sub>
Cu9	6b	$mmm..$	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N <sub>6</sub>

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

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

Remarks: H<sub>2</sub>O not located, partial substitution by OH for NO<sub>2</sub> is ignored. 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] Ozarowski A., Allmann R., Pour Ibrahim A., Reinen R. (1991), Z. Anorg. Allg. Chem. 592, 187-201.

204  
c/128

$\text{La}_5\text{Ti}_6(\text{S}_{0.5}\text{Cl}_{0.5})_6\text{O}_{15}$	<i>cI128</i>	(204) <i>Im-3</i> – hg <sup>2</sup> edc
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$$\text{La}_5\text{Ti}_6\text{S}_3\text{O}_{15}\text{Cl}_3$$
 [1]

Structural features:  $\text{Ti}(\text{O}_5(\text{S},\text{Cl}))$  octahedra share vertices to form a 3D-framework.

Palvadeau P. et al. (1998) [1]

$$\text{Cl}_3\text{La}_5\text{O}_{15}\text{S}_3\text{Ti}_6$$
$$a = 1.24156 \text{ nm}, V = 1.9138 \text{ nm}^3, Z = 4$$



site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.11	0.185	0.3882		non-colinear Ti <sub>2</sub>
M2	24g	<i>m..</i>	0	0.2038	0.1824		single atom Ti
Ti3	24g	<i>m..</i>	0	0.30107	0.35953		octahedron O <sub>5</sub> Cl
O4	12e	<i>mm2..</i>	0.131	0	1/2		non-colinear Ti <sub>2</sub>
La5	12d	<i>mm2..</i>	0.34044	0	0		10-vertex polyhedron O <sub>6</sub> Cl <sub>4</sub>
La6	8c	<i>.-3.</i>	1/4	1/4	1/4		octahedron O <sub>6</sub>

$$M2 = 0.5Cl + 0.5S$$

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

Experimental: single crystal, diffractometer, X-rays, R = 0.069, T = 293 K

References: [1] Palvadeau P., Boyer M.C., Meerschaut A., Rouxel J. (1998), J. Solid State Chem. 139, 220-224.

204  
cI132

Cs <sub>6</sub> [C <sub>60</sub> ]	<i>cI132</i>	(204) <i>Im-3</i> – h <sup>2</sup> ge
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**Cs<sub>6</sub>C<sub>60</sub>** [1], fulleride-Cs<sub>6</sub>

Structural features: Pseudo-spherical C<sub>60</sub> fullerene units (twelve 5- and twenty 6-membered rings) in a W-type (b.c.c.) arrangement; Cs in "tetrahedral" voids. See Fig. II.55.

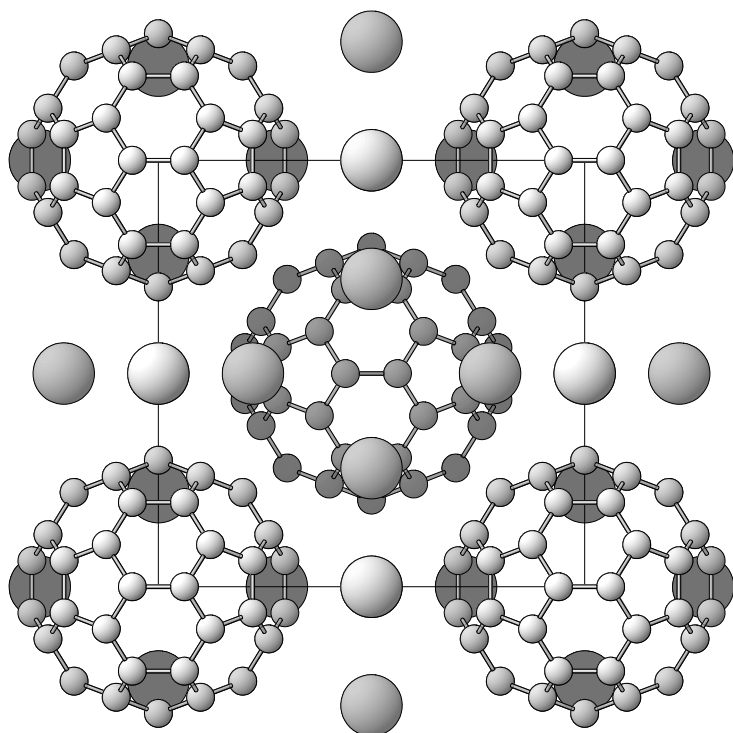


Fig. II.55. Cs<sub>6</sub>C<sub>60</sub>

Arrangement of C<sub>60</sub> cages (C atoms small) and Cs atoms (large).

Zhou O. et al. (1991) [1]

C<sub>60</sub>Cs<sub>6</sub>

$$a = 1.179 \text{ nm}, V = 1.6389 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	48h	1	0.0611	0.2212	0.1978		non-coplanar triangle C <sub>3</sub>
C2	48h	1	0.0989	0.1222	0.259		non-coplanar triangle C <sub>3</sub>
C3	24g	m..	0	0.0611	0.2968		non-coplanar triangle C <sub>3</sub>
Cs4	12e	mm2..	0.2219	0	1/2		22-vertex polyhedron C <sub>22</sub>

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

Experimental: powder, diffractometer, X-rays,  $R_B = 0.043$ ,  $T = 300$  K

References: [1] Zhou O., Fischer J.E., Coustel N., Kycia S., Zhu Q., McGhie A.R., Romanow W.J., McCauley J.P. Jr., Smith A.B. III., Cox D.E. (1991), Nature (London) 351, 462-464.

204  
cI144

<b>K<sub>3</sub>Ba<sub>3</sub>[C<sub>60</sub>]</b>	<i>cI144</i>	(204) <i>Im-3</i> – h <sup>2</sup> ge <sup>2</sup>
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**K<sub>3</sub>Ba<sub>3</sub>C<sub>60</sub>** [1], fulleride-K<sub>3</sub>Ba<sub>3</sub>

Structural features: Pseudo-spherical C<sub>60</sub> fullerene units (twelve 5- and twenty 6-membered rings) in a W-type (b.c.c.) arrangement; (K,Ba) in "tetrahedral" voids (different positions for K and Ba).

Margadonna S. et al. (2000) [1]

Ba<sub>2.90</sub>C<sub>60</sub>K<sub>3.07</sub>

$a = 1.12166$  nm,  $V = 1.4112$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	48h	1	0.06407	0.23303	0.20736		non-coplanar triangle C <sub>3</sub>
C2	48h	1	0.1036	0.12792	0.27151		non-coplanar triangle C <sub>3</sub>
C3	24g	m..	0	0.06407	0.31118		non-coplanar triangle C <sub>3</sub>
K4	12e	mm2..	0.2157	0	1/2	0.512	
Ba5	12e	mm2..	0.2235	0	1/2	0.484	

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

Experimental: powder, diffractometer, X-rays,  $R_B = 0.058$ ,  $T = 10$  K

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

References: [1] Margadonna S., Aslanis E., Li W.Z., Prassides K., Fitch A.N., Hansen T.C. (2000), Chem. Mater. 12, 2736-2740.

204  
cI160

<b>Cs<sub>3</sub>(Re<sub>0.83</sub>Os<sub>0.17</sub>)<sub>6</sub>S<sub>11</sub></b>	<i>cI160</i>	(204) <i>Im-3</i> – h <sup>2</sup> gfed
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**Cs<sub>3</sub>Re<sub>5</sub>OsS<sub>11</sub>** [1]

Structural features: (Re,Os)<sub>6</sub>S<sub>14</sub> clusters (a (Re,Os)<sub>6</sub> octahedron surrounded by a S<sub>8</sub> cube and a S<sub>6</sub> octahedron) share vertices of the S<sub>6</sub> octahedron to form a 3D-framework.

Bronger W. et al. (1997) [1]

Cs<sub>3</sub>OsRe<sub>5</sub>S<sub>11</sub>

$a = 1.6222$  nm,  $V = 4.2689$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	48h	1	0.1128	0.1828	0.3481		non-coplanar triangle Re <sub>3</sub>
M2	48h	1	0.13911	0.26733	0.22973		tricapped trigonal prism S <sub>5</sub> Re <sub>4</sub>

S3	24g	<i>m..</i>	0	0.3003	0.1921	non-colinear Re <sub>2</sub>
S4	16f	.3.	0.1447	0.1447	0.1447	non-coplanar triangle Re <sub>3</sub>
Cs5	12e	<i>mm2..</i>	0.1819	0	<sup>1</sup> / <sub>2</sub>	non-colinear S <sub>2</sub>
Cs6	12d	<i>mm2..</i>	0.2335	0	0	non-colinear S <sub>2</sub>

M2 = 0.833Re + 0.167Os

Experimental: twinned crystal, diffractometer, X-rays, R = 0.031

References: [1] Bronger W., Koppe C., Loevenich M., Schmitz D., Schuster T. (1997), Z. Anorg. Allg. Chem. 623, 695-698.

204  
cI160

Li <sub>13</sub> (Cu <sub>0.53</sub> Si <sub>0.47</sub> ) <sub>27</sub>	cI160	(204) <i>Im</i> -3 – hg <sup>3</sup> fe <sup>2</sup>
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**LiCuSi** [1]; Li<sub>3</sub>CuAl<sub>5</sub> form R [2]; Li<sub>5</sub>Ni<sub>4</sub>Si<sub>7</sub> [1]; (Mg,Na,Al)<sub>2</sub>(Al,Zn)<sub>3</sub> [3]

Structural features: Units of twelve edge-sharing (Cu,Si)((Cu,Si)<sub>6</sub>Li<sub>5</sub>) defect icosahedra (monocapped pentagonal antiprism) share atoms to form a 3D-framework where the centering (Cu,Si) atoms form large icosahedra around the points of the b.c.c. lattice.

Döring W. et al. (1979) [1]

Cu<sub>14.22</sub>Li<sub>13</sub>Si<sub>12.78</sub>

*a* = 1.2933 nm, *V* = 2.1632 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	48h	1	0.093	0.309	0.345		icosahedron Cu <sub>6</sub> Li <sub>6</sub>
Li2	24g	<i>m..</i>	0	0.116	0.300		16-vertex Frank-Kasper Cu <sub>12</sub> Li <sub>4</sub>
M3	24g	<i>m..</i>	0	0.154	0.093		11-vertex polyhedron Cu <sub>6</sub> Li <sub>5</sub>
M4	24g	<i>m..</i>	0	0.307	0.179		icosahedron Cu <sub>6</sub> Li <sub>6</sub>
Li5	16f	.3.	0.184	0.184	0.184		16-vertex Frank-Kasper Cu <sub>12</sub> Li <sub>4</sub>
M6	12e	<i>mm2..</i>	0.093	0	<sup>1</sup> / <sub>2</sub>		14-vertex Frank-Kasper Cu <sub>7</sub> Li <sub>7</sub>
Li7	12e	<i>mm2..</i>	0.307	0	<sup>1</sup> / <sub>2</sub>		15-vertex Frank-Kasper Cu <sub>13</sub> Li <sub>2</sub>

M1 = 0.50Cu + 0.50Si; M3 = 0.55Cu + 0.45Si; M4 = 0.56Cu + 0.44Si; M6 = 0.52Cu + 0.48Si

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

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

Remarks: For Li<sub>5</sub>Ni<sub>4</sub>Si<sub>7</sub>, R-Li<sub>3</sub>CuAl<sub>5</sub> and (Mg,Na,Al)<sub>2</sub>(Al,Zn)<sub>3</sub> site M6 was found to be occupied exclusively by Si or Al. According to [2], a report on R-Li<sub>3</sub>CuAl<sub>5</sub> with Mg<sub>32</sub>(Zn,Al)<sub>49</sub>-type structure (Wyckoff position 2*a* occupied) in [4] is superseded, however, 80% Al occupation in Wyckoff position 2*a* is reported for Li<sub>2.9</sub>CuAl<sub>5.6</sub> in [5].

References: [1] Döring W., Seelentag W., Buchholz W., Schuster H.U. (1979), Z. Naturforsch. B 34, 1715-1718. [2] Audier M., Pannetier J., Leblanc M., Janot C., Lang J., Dubost B. (1988), Physica B+C (Amsterdam) 153, 136-142. [3] Elding Pontén M., Lidin S. (1995), J. Solid State Chem. 115, 270-273. [4] Guryan C.A., Stephens P.W., Goldman A.I., Gayle F.W. (1988), Phys. Rev. B: Condens. Matter 37, 8495-8498. [5] Cherkashin E.E., Kripyakevich P.I., Oleksiv G.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 8, 681-685.

204  
cI160

Li <sub>13</sub> Cu <sub>6</sub> Ga <sub>21</sub>	cI160	(204) <i>Im</i> -3 – hg <sup>3</sup> fe <sup>2</sup>
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**Li<sub>13</sub>Cu<sub>6</sub>Ga<sub>21</sub>** [1]; Na<sub>13</sub>Cd<sub>20</sub>Pb<sub>7</sub> [2]

Structural features: Pseudo-spherical 104-atom Samson polyhedron units formed by twenty  $\text{Li}(\text{Ga}_9\text{Cu}_3)$  truncated tetrahedra with common hexagonal faces (a central  $\text{Ga}_{12}$  icosahedron surrounded by a  $\text{Li}_{20}$  pentagonal dodecahedron, a  $\text{Cu}_{12}$  icosahedron and a  $\text{Ga}_{60}$  truncated icosahedron with pentagonal and hexagonal faces) share atoms to form a 3D-framework. Ordering variant of "LiCuSi".

Tillard Charbonnel M., Belin C. (1991) [1]

$\text{Cu}_6\text{Ga}_{21}\text{Li}_{13}$

$a = 1.3568 \text{ nm}$ ,  $V = 2.4977 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	48h	1	0.0945	0.3097	0.3419		icosahedron $\text{Cu}_2\text{Ga}_4\text{Li}_6$
Li2	24g	m..	0	0.116	0.303		16-vertex Frank-Kasper $\text{Ga}_9\text{Cu}_3\text{Li}_4$
Ga3	24g	m..	0	0.1565	0.0956		pseudo Frank-Kasper $\text{CuGa}_5\text{Li}_5$
Cu4	24g	m..	0	0.3144	0.1779		icosahedron $\text{Ga}_6\text{Li}_6$
Li5	16f	.3.	0.186	0.186	0.186		16-vertex Frank-Kasper $\text{Ga}_9\text{Li}_4\text{Cu}_3$
Ga6	12e	mm2..	0.0932	0	$\frac{1}{2}$		14-vertex Frank-Kasper $\text{Ga}_5\text{Li}_7\text{Cu}_2$
Li7	12e	mm2..	0.294	0	$\frac{1}{2}$		15-vertex Frank-Kasper $\text{Ga}_{11}\text{Li}_2\text{Cu}_2$

Transformation from published data: y,x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.033

Remarks: Site occupation  $\text{Na}_{13}\text{Cd}_6(\text{Cd,Pb})_{21}$  was reported for  $\text{Na}_{13}\text{Cd}_{20}\text{Pb}_7$ .

References: [1] Tillard Charbonnel M., Belin C. (1991), J. Solid State Chem. 90, 270-278. [2] Todorov E., Sevov S.C. (1997), Inorg. Chem. 36, 4298-4302.

204  
cI160

$\text{Be}_{17}\text{Ru}_3$	cI160	(204) $Im\bar{3} - hg^3fed$
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**$\text{Ru}_3\text{Be}_{17}$**  [1]

Structural features:  $\text{RuBe}_{16}$  polyhedra (~ monocapped double pentagonal antiprism) share atoms to form a 3D-framework where the centering Ru atoms form large icosahedra around the points of the b.c.c. lattice.

Sands D.E. et al. (1962) [1]

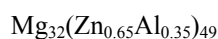
$\text{Be}_{17}\text{Ru}_3$

$a = 1.1337 \text{ nm}$ ,  $V = 1.4571 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Be1	48h	1	0.114	0.3434	0.201		15-vertex Frank-Kasper $\text{Be}_{12}\text{Ru}_3$
Ru2	24g	m..	0	0.1879	0.3014		16-vertex Frank-Kasper $\text{Be}_{16}$
Be3	24g	m..	0	0.2305	0.0914		tricapped trigonal prism $\text{Be}_6\text{Ru}_3$
Be4	24g	m..	0	0.4055	0.3488		icosahedron $\text{Be}_9\text{Ru}_3$
Be5	16f	.3.	0.1645	0.1645	0.1645		tricapped trigonal prism $\text{Be}_6\text{Ru}_3$
Be6	12e	mm2..	0.1956	0	$\frac{1}{2}$		icosahedron $\text{Be}_{10}\text{Ru}_2$
Be7	12d	mm2..	0.4065	0	0		15-vertex Frank-Kasper $\text{Be}_{13}\text{Ru}_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.052

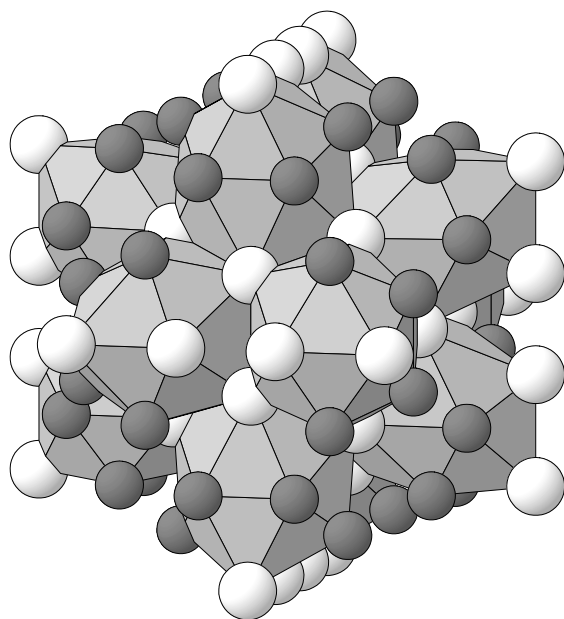
References: [1] Sands D.E., Johnson Q.C., Krikorian O.H., Kromholtz K.L. (1962), Acta Crystallogr. 15, 1191-1195.



cI162

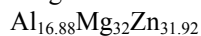
(204)  $Im\bar{3} - \text{hg}^3\text{fe}^2\text{a}$ **Mg<sub>32</sub>(Al,Zn)<sub>49</sub>** [2],  $\lambda$  phase, T phase, Bergman phase, Strukturbericht notation D8<sub>e</sub>

Structural features: Tetrahedrally close-packed structure (Frank-Kasper phase) with interconnected icosahedron units consisting of a central  $\text{MM}_{12}$  icosahedron sharing vertices with twelve edge-linked  $\text{MM}_{12}$  icosahedra, the centering atoms forming a large  $\text{MM}_{12}$  icosahedron (pseudo-spherical 105-atom Samson unit: a central atom + a  $\text{M}_{12}$  icosahedron + a  $\text{M}_{20}$  pentagonal dodecahedron + a  $\text{M}_{12}$  icosahedron + a  $\text{M}_{60}$  polyhedron). See Fig. II.56.

Fig. II.56. **Mg<sub>32</sub>(Al,Zn)<sub>49</sub>**

Arrangement of  $(\text{Zn,Al})_{12}$   $(\text{Mg}_7(\text{Zn,Al})_5)$  icosahedra (Mg atoms light, (Zn,Al) atoms dark) around a central  $\text{Al}(\text{Zn,Al})_{12}$  icosahedron.

Bergman G. et al. (1957) [1]

 $a = 1.416 \text{ nm}$ ,  $V = 2.8392 \text{ nm}^3$ ,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	48h	1	0.0969	0.3140	0.3320		icosahedron $\text{Zn}_5\text{Mg}_7$
Mg2	24g	$m..$	0	0.1194	0.2942		16-vertex Frank-Kasper $\text{Zn}_{10}\text{Mg}_6$
M3	24g	$m..$	0	0.1501	0.0908		icosahedron $\text{Zn}_6\text{AlMg}_5$
M4	24g	$m..$	0	0.3007	0.1748		icosahedron $\text{Zn}_5\text{Mg}_7$
Mg5	16f	.3.	0.1836	0.1836	0.1836		16-vertex Frank-Kasper $\text{Zn}_{12}\text{Mg}_4$
Mg6	12e	$mm2..$	0.0998	0	$\frac{1}{2}$		14-vertex Frank-Kasper $\text{Mg}_8\text{Zn}_6$
Mg7	12e	$mm2..$	0.3203	0	$\frac{1}{2}$		15-vertex Frank-Kasper $\text{Mg}_5\text{Zn}_{10}$
Al8	2a	$m\bar{3}..$	0	0	0	0.80	icosahedron $\text{Zn}_{12}$

 $\text{M1} = 0.64\text{Zn} + 0.36\text{Al}$ ;  $\text{M3} = 0.81\text{Zn} + 0.19\text{Al}$ ;  $\text{M4} = 0.57\text{Zn} + 0.43\text{Al}$ Transformation from published data:  $y, x, -z$ Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.211$ 

Remarks: There is doubt on whether Wyckoff position 2a is occupied or not; this site is stated to be vacant in the Na-substituted phase (see  $\text{LiCuSi}$  type). According to [3] a report on  $\text{R-Li}_3\text{CuAl}_5$  with this

type in [4] is superseded (Wyckoff position  $2a$  vacant), however, 80% Al occupation in Wyckoff position  $2a$  is reported in [5].

References: [1] Bergman G., Waugh J.L.T., Pauling L. (1957), Acta Crystallogr. 10, 254-259. [2] Berman G., Waugh J.L.T., Pauling L. (1952), Nature (London) 169, 1057-1058. [3] Audier M., Pannetier J., Leblanc M., Janot C., Lang J., Dubost B. (1988), Physica B+C (Amsterdam) 153, 136-142. [4] Cherkashin E.E., Kripyakevich P.I., Oleksiv G.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 8, 681-685. [5] Guryan C.A., Stephens P.W., Goldman A.I., Gayle F.W. (1988), Phys. Rev. B: Condens. Matter 37, 8495-8498.

204  
c/I162

$\text{Mg}_{32}\text{Ag}_{13}\text{Al}_{36}$	<i>cI162</i>	(204) <i>Im</i> -3 – $\text{hg}^3\text{fe}^2\text{a}$
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#### **$\text{Mg}_{39.5}\text{Ag}_{16.1}\text{Al}_{44.4}$ [1]**

Structural features: Pseudo-spherical 105-atom Samson polyhedron units consisting of twenty  $\text{Mg}(\text{Al},\text{Ag})_{12}$  truncated tetrahedra with common hexagonal faces (a central Ag atom surrounded by a  $\text{Al}_{12}$  icosahedron, a  $\text{Mg}_{20}$  pentagonal dodecahedron + a  $\text{Ag}_{12}$  icosahedron and a  $(\text{Al},\text{Mg})_{60}$  truncated icosahedron) share atoms to form a 3D-framework; additional Mg in voids. Ordering variant of  $\text{Mg}_{32}(\text{Zn},\text{Al})_{49}$ .

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

$\text{Ag}_{13}\text{Al}_{36}\text{Mg}_{32}$

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

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	48h	1	0.0955	0.309	0.3455		icosahedron $\text{Ag}_2\text{Al}_3\text{Mg}_7$
Mg2	24g	<i>m</i> ..	0	0.1297	0.3018		16-vertex Frank-Kasper $\text{Al}_7\text{Mg}_6\text{Ag}_3$
Al3	24g	<i>m</i> ..	0	0.1545	0.0955		icosahedron $\text{Ag}_2\text{Al}_5\text{Mg}_5$
Ag4	24g	<i>m</i> ..	0	0.309	0.191		icosahedron $\text{Al}_5\text{Mg}_7$
Mg5	16f	.3.	0.1836	0.1836	0.1836		16-vertex Frank-Kasper $\text{Al}_9\text{Ag}_3\text{Mg}_4$
Mg6	12e	<i>mm</i> 2..	0.1308	0	$\frac{1}{2}$		14-vertex Frank-Kasper $\text{Mg}_8\text{Al}_4\text{Ag}_2$
Mg7	12e	<i>mm</i> 2..	0.3022	0	$\frac{1}{2}$		15-vertex Frank-Kasper $\text{Mg}_5\text{Al}_8\text{Ag}_2$
Ag8	2a	<i>m</i> -3.	0	0	0		icosahedron $\text{Al}_{12}$

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

Experimental: single crystal, photographs, X-rays

Remarks: Commensurate approximant of icosahedral quasicrystals.

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

204  
c/I162

$\text{Na}_{26}(\text{Na}_{0.67}\text{Au}_{0.33})_6\text{Au}_{37}\text{Sn}_{12}$	<i>cI162</i>	(204) <i>Im</i> -3 – $\text{hg}^3\text{fe}^2\text{a}$
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#### **$\text{Na}_2\text{Au}_3\text{Sn}$ [1]**

Structural features: Pseudo-spherical 105-atom Samson polyhedron units consisting of twenty  $\text{Na}(\text{Au},\text{Sn},\text{Na})_{12}$  truncated tetrahedra with common hexagonal faces (a central Au atom surrounded by an  $\text{Au}_{12}$  icosahedron, a  $\text{Na}_{20}$  pentagonal dodecahedron, a  $\text{Sn}_{12}$  icosahedron and a  $(\text{Na},\text{Au})_{60}$  truncated icosahedron) share atoms to form a 3D-framework. Ordering variant of  $\text{Mg}_{32}(\text{Zn},\text{Al})_{49}$ .

Döring W. et al. (1979) [1]

$\text{Au}_{38.98}\text{Na}_{30.02}\text{Sn}_{12}$

$a = 1.4989 \text{ nm}$ ,  $V = 3.3676 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Au1	48h	1	0.1552	0.4044	0.1864		icosahedron Sn <sub>2</sub> Au <sub>3</sub> Na <sub>7</sub>
Na2	24g	m..	0	0.121	0.298		16-vertex Frank-Kasper Au <sub>7</sub> Na <sub>6</sub> Sn <sub>3</sub>
Au3	24g	m..	0	0.1596	0.0965		icosahedron SnAu <sub>6</sub> Na <sub>5</sub>
Sn4	24g	m..	0	0.3123	0.1856		icosahedron Au <sub>5</sub> Na <sub>7</sub>
Na5	16f	.3.	0.191	0.191	0.191		16-vertex Frank-Kasper Na <sub>4</sub> Au <sub>9</sub> Sn <sub>3</sub>
M6	12e	mm2..	0.106	0	<sup>1</sup> / <sub>2</sub>		14-vertex Frank-Kasper Na <sub>8</sub> Au <sub>4</sub> Sn <sub>2</sub>
Na7	12e	mm2..	0.301	0	<sup>1</sup> / <sub>2</sub>		15-vertex Frank-Kasper Na <sub>5</sub> Au <sub>8</sub> Sn <sub>2</sub>
Au8	2a	m-3.	0	0	0		icosahedron Au <sub>12</sub>

M6 = 0.67Na + 0.33Au

Transformation from published data: y,x,-z

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

References: [1] Döring W., Seelentag W., Buchholz W., Schuster H.U. (1979), Z. Naturforsch. B 34, 1715-1718.

204  
cI162

Mg <sub>8</sub> Yb <sub>19</sub> H <sub>54</sub>	cI162	(204) Im-3 – hg <sup>3</sup> feda
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### Yb<sub>19</sub>Mg<sub>8</sub>H<sub>54</sub> [1]

Structural features: Mg and Yb form a W-type (b.c.c.) framework; H in tetrahedral (Yb<sub>4</sub>, Yb<sub>3</sub>Mg, Yb<sub>2</sub>Mg<sub>2</sub>) voids.

Huang B. et al. (1995) [1]

D<sub>54</sub>Mg<sub>8</sub>Yb<sub>19</sub>

a = 1.20666 nm, V = 1.7569 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	48h	1	0.1142	0.3137	0.171		single atom Mg
D2	24g	m..	0	0.108	0.168		non-colinear Mg <sub>2</sub>
D3	24g	m..	0	0.186	0.4		non-coplanar triangle Yb <sub>3</sub>
Yb4	24g	m..	0	0.3456	0.3134		square antiprism D <sub>8</sub>
Mg5	16f	.3.	0.154	0.154	0.154		octahedron D <sub>6</sub>
D6	12e	mm2..	0.121	0	<sup>1</sup> / <sub>2</sub>		non-colinear Yb <sub>2</sub>
Yb7	12d	mm2..	0.3343	0	0		10-vertex polyhedron D <sub>10</sub>
Yb8	2a	m-3.	0	0	0		icosahedron D <sub>12</sub>

Transformation from published data: y,x,-z

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.046, T = 50 K

References: [1] Huang B., Gingl F., Yvon K., Rodriguez Carvajal J. (1995), J. Alloys Compd. 227, 131-134.

204  
cI168

(Mn <sub>0.2</sub> Fe <sub>0.8</sub> ) <sub>4</sub> (Al <sub>0.9</sub> Si <sub>0.1</sub> ) <sub>19</sub>	cI168	(204) Im-3 – hg <sup>4</sup> ed
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### MnFe<sub>4</sub>Al<sub>9</sub>Si<sub>2</sub> [1]

Structural features: (Fe,Mn)(Al,Si)<sub>12</sub> icosahedra share atoms to form a 3D-framework (one split (Al,Si) site). 55-atom Mackay icosahedron units (a central atom surrounded by an icosahedron, a larger icosahedron and a 30-vertex polyhedron) are interconnected via additional atoms.

Cooper M. (1967) [1]

$\text{Al}_{19}\text{Fe}_{3.2}\text{Mn}_{0.8}$

$a = 1.256 \text{ nm}$ ,  $V = 1.9814 \text{ nm}^3$ ,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	48h	1	0.1146	0.3003	0.1872		11-vertex polyhedron $\text{FeAl}_{10}$
Al2	24g	m..	0	0.1006	0.1651		
M3	24g	m..	0	0.1981	0.3243		
Al4	24g	m..	0	0.383	0.3725	0.5	
Al5	24g	m..	0	0.403	0.3266	0.5	tetrahedron $\text{Al}_4$
Al6	12e	mm2..	0.201	0	$\frac{1}{2}$	0.5	
Al7	12d	mm2..	0.3777	0	0		

$\text{M3} = 0.8\text{Fe} + 0.2\text{Mn}$

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

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.100$

Remarks: Phase referred to as  $\alpha$ -(AlFeSi). Composition  $\text{MnFe}_4\text{Al}_{19}\text{Si}_2$  from electron microprobe analysis. No attempt was made to distinguish Al and Si. Average structure given as the sum of two primitive cells. Short interatomic distances for partly occupied site(s).

References: [1] Cooper M. (1967), Acta Crystallogr. 23, 1106-1107.

204  
cI172

$\text{Mg}_4\text{W}_6\text{O}_{21}[(\text{OH})_{0.33}[\text{H}_2\text{O}]_{0.67}]_6$	cI172	(204) $Im\bar{3} - \text{hg}^4\text{dcba}$
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**$\text{Mg}_7[\text{MgW}_{12}\text{O}_{42}](\text{OH})_4 \cdot 8\text{H}_2\text{O}$**  [1]

Structural features:  $\text{MgW}_{12}\text{O}_{42}$  units (a central Mg atom surrounded by twelve face- and vertex-linked  $\text{WO}_6$  octahedra) in a W-type (b.c.c.) arrangement; additional Mg and  $(\text{H}_2\text{O}, \text{OH})$  between the units.

Günter J.R. et al. (1990) [1]

$\text{H}_{10}\text{Mg}_4\text{O}_{27}\text{W}_6$

$a = 1.2862 \text{ nm}$ ,  $V = 2.1278 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.1075	0.1878	0.2923		non-colinear WMg
W2	24g	m..	0	0.1191	0.23987		octahedron $\text{O}_6$
O3	24g	m..	0	0.1719	0.1025		non-coplanar triangle $\text{W}_3$
M4	24g	m..	0	0.37	0.4022	0.5	coplanar triangle $\text{W}_2\text{Mg}$
M5	24g	m..	0	0.4026	0.3655	0.5	
O6	12d	mm2..	0.3396	0	0		
Mg7	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		octahedron $\text{O}_6$
Mg8	6b	mmm..	0	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron $\text{O}_{12}$
Mg9	2a	m-3.	0	0	0		

$\text{M4} = 0.667\text{OH}_2 + 0.333\text{OH}$ ;  $\text{M5} = 0.667\text{OH}_2 + 0.333\text{OH}$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.028$

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] Günter J.R., Schmalle H.W., Dubler E. (1990), Solid State Ionics 43, 85-92.



$\text{Ti}_{44}\text{Cr}_{17}\text{Si}_{12}\text{O}_{11.6}$	<i>cI178</i>	(204) <i>Im</i> -3 – hg <sup>4</sup> edca
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**Ti<sub>60</sub>Cr<sub>25</sub>Si<sub>15</sub>O<sub>x</sub> [1]**

Structural features: 55-atom Mackay icosahedron units (a central (Si,Cr) atom surrounded by a Ti<sub>12</sub> icosahedron, a larger (Si,Cr)<sub>12</sub> icosahedron and a Ti<sub>30</sub> polyhedron) are interconnected via additional atoms to form a 3D-framework; O in octahedral voids.

Libbert J.L. et al. (1994) [1]

$\text{Cr}_{17.07}\text{O}_{11.64}\text{Si}_{11.77}\text{Ti}_{44.16}$

$a = 1.3139 \text{ nm}$ ,  $V = 2.2682 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ti1	48 <i>h</i>	1	0.1135	0.3047	0.1831		non-colinear O <sub>2</sub>
Ti2	24 <i>g</i>	<i>m</i> ..	0	0.1082	0.1761		non-coplanar triangle O <sub>3</sub>
M3	24 <i>g</i>	<i>m</i> ..	0	0.2168	0.3416		icosahedron Cr <sub>4</sub> Ti <sub>8</sub>
O4	24 <i>g</i>	<i>m</i> ..	0	0.2433	0.0952	0.67	7-vertex polyhedron Ti <sub>6</sub> O
M5	24 <i>g</i>	<i>m</i> ..	0	0.4026	0.3399		icosahedron Cr <sub>3</sub> Si <sub>3</sub> Ti <sub>6</sub>
M6	12 <i>e</i>	<i>mm</i> 2..	0.1742	0	$\frac{1}{2}$		icosahedron Cr <sub>4</sub> Si <sub>2</sub> Ti <sub>6</sub>
Ti7	12 <i>d</i>	<i>mm</i> 2..	0.381	0	0		non-colinear O <sub>2</sub>
O8	8 <i>c</i>	..3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.9	octahedron Ti <sub>6</sub>
M9	2 <i>a</i>	<i>m</i> -3.	0	0	0		icosahedron Ti <sub>12</sub>

M3 = 0.55Si + 0.45Cr; M5 = 0.66Cr + 0.18Ti + 0.16Si; M6 = 0.58Cr + 0.42Si; M9 = 0.73Si + 0.27Cr

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

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.054$

Remarks: Commensurate approximant of icosahedral quasicrystals.

References: [1] Libbert J.L., Kelton K.F., Goldman A.I., Yelon W.B. (1994), Phys. Rev. B: Condens. Matter 49, 11675-11681.

$\text{Sc}_{56.8}\text{Rh}_{13.6}$	<i>cI182</i>	(204) <i>Im</i> -3 – hg <sup>4</sup> e <sup>2</sup> da
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**Sc<sub>56.8</sub>Rh<sub>13.6</sub> [1]**

Structural features: Units consisting of a central RhSc<sub>12</sub> icosahedron sharing vertices with twelve surrounding RhSc<sub>12</sub> icosahedra (in part replaced by Rh(Sc<sub>11</sub>Rh) and Rh(Sc<sub>11</sub>□) defect icosahedra, disorder) are interconnected to form a 3D-framework; the centering Rh atoms form large RhRh<sub>12</sub> icosahedra. Mackay icosahedron units interconnected via additional atoms.

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

$\text{Rh}_{13.59}\text{Sc}_{56.81}$

$a = 1.4414 \text{ nm}$ ,  $V = 2.9947 \text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sc1	48 <i>h</i>	1	0.1135	0.2952	0.1844		12-vertex polyhedron Rh <sub>2</sub> Sc <sub>10</sub>
Sc2	24 <i>g</i>	<i>m</i> ..	0	0.1084	0.1770		
Rh3	24 <i>g</i>	<i>m</i> ..	0	0.2028	0.3339		
Sc4	24 <i>g</i>	<i>m</i> ..	0	0.3711	0.3921	0.453	
Sc5	24 <i>g</i>	<i>m</i> ..	0	0.3972	0.325	0.550	
Rh6	12 <i>e</i>	<i>mm</i> 2..	0.1551	0	$\frac{1}{2}$	0.099	
Sc7	12 <i>e</i>	<i>mm</i> 2..	0.2255	0	$\frac{1}{2}$	0.463	

Sc8	12d	mm2..	0.3687	0	0	
Rh9	2a	m-3.	0	0	0	icosahedron Sc <sub>12</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.025

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

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

204  
cI184

Cd <sub>6</sub> Y	cI184	(204) <i>Im</i> -3 – hg <sup>4</sup> fed
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### YCd<sub>6</sub> [1]

Structural features: YCd<sub>17</sub> polyhedra (bicapped double pentagonal antiprisms) are interconnected to form a 3D-framework; the centering atoms form large Y<sub>12</sub> icosahedra.

Larson A.C., Cromer D.T. (1971) [1]

Cd<sub>6</sub>Y

$a = 1.5482$  nm,  $V = 3.7109$  nm<sup>3</sup>,  $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	48h	1	0.11835	0.34049	0.20031		15-vertex Frank-Kasper Cd <sub>12</sub> Y <sub>3</sub>
Cd2	24g	m..	0	0.0741	0.0832	0.331	non-coplanar square Cd <sub>4</sub>
Y3	24g	m..	0	0.18985	0.29966		7-capped pentagonal prism Cd <sub>17</sub>
Cd4	24g	m..	0	0.24069	0.09227		icosahedron Cd <sub>9</sub> Y <sub>3</sub>
Cd5	24g	m..	0	0.40438	0.34603		icosahedron Cd <sub>9</sub> Y <sub>3</sub>
Cd6	16f	.3.	0.16081	0.16081	0.16081		icosahedron Cd <sub>9</sub> Y <sub>3</sub>
Cd7	12e	mm2..	0.19018	0	1/2		icosahedron Cd <sub>10</sub> Y <sub>2</sub>
Cd8	12d	mm2..	0.40551	0	0		15-vertex Frank-Kasper Cd <sub>13</sub> Y <sub>2</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.028

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

References: [1] Larson A.C., Cromer D.T. (1971), Acta Crystallogr. B 27, 1875-1879.

204  
cI248

Ag <sub>2</sub> YbIn <sub>4</sub>	cI248	(204) <i>Im</i> -3 – h <sup>2</sup> g <sup>4</sup> f <sup>2</sup> ed
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### YbAg<sub>2</sub>In<sub>4</sub> [1]

Structural features: Ordering variant of YCd<sub>6</sub> with splitting of the three Cd sites occupied by Ag.

Sysa L.V. et al. (1998) [1]

Ag<sub>2.13</sub>In<sub>4</sub>Yb

$a = 1.5362$  nm,  $V = 3.6253$  nm<sup>3</sup>,  $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	48h	1	0.023	0.0664	0.085	0.16	
In2	48h	1	0.1153	0.3392	0.2012		
Yb3	24g	m..	0	0.1851	0.3016		
Ag4	24g	m..	0	0.2164	0.084	0.32	
Ag5	24g	m..	0	0.2478	0.094	0.76	

In6	24g	<i>m.</i>	0	0.4038	0.3497		icosahedron In <sub>9</sub> Yb <sub>3</sub>
Ag7	16f	.3.	0.1448	0.1448	0.1448	0.35	
Ag8	16f	.3.	0.1617	0.1617	0.1617	0.74	
In9	12e	<i>mm2.</i>	0.1966	0	$\frac{1}{2}$		icosahedron In <sub>10</sub> Yb <sub>2</sub>
In10	12d	<i>mm2.</i>	0.4089	0	0		

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

Remarks: Short interatomic distances for partly occupied site(s); impossibly short distances occur for the published occupation factors.

References: [1] Sysa L.V., Kalychak Y.M., Galadzhun Y.V., Zarembo V.I., Akselrud L.G., Skolozdra R.V. (1998), J. Alloys Compd. 266, 17-21.

204  
cI318

[H <sub>3</sub> O] <sub>0.5</sub> Ba <sub>8</sub> V <sub>15</sub> O <sub>45</sub>	cI318	(204) <i>Im</i> -3 – h <sup>4</sup> g <sup>2</sup> fe <sup>4</sup> cb
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### Ba<sub>5.33</sub>(H<sub>3</sub>O)<sub>0.33</sub>[V<sub>10</sub>O<sub>30</sub>] [1]

Structural features: V<sub>10</sub>O<sub>30</sub> units formed by four V<sup>5+</sup><sub>2</sub>O<sub>7</sub> units (two vertex-linked VO<sub>4</sub> tetrahedra) sharing vertices with a central V<sup>4+</sup>V<sup>5+</sup>O<sub>10</sub> unit (two VO<sub>5</sub> square pyramids, two-fold orientational disorder); Ba and H<sub>3</sub>O between the units (partial disorder for the latter).

Zhang Y. et al. (1998) [1]

Ba<sub>8</sub>H<sub>1.50</sub>O<sub>45.50</sub>V<sub>15</sub>

*a* = 1.69439 nm, *V* = 4.8645 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48h	1	0.0802	0.4193	0.1205		
O2	48h	1	0.0969	0.2622	0.1647		single atom V
V3	48h	1	0.0976	0.1229	0.3291		tetrahedron O <sub>4</sub>
O4	48h	1	0.107	0.2209	0.3426		single atom V
O5	24g	<i>m.</i>	0	0.0995	0.2943		non-collinear V <sub>2</sub>
Ba6	24g	<i>m.</i>	0	0.3312	0.2773		
(OH <sub>3</sub> )7	16f	.3.	0.0978	0.0978	0.0978	0.125	non-coplanar triangle O <sub>3</sub>
V8	12e	<i>mm2.</i>	0.0918	0	$\frac{1}{2}$	0.5	
V9	12e	<i>mm2.</i>	0.1376	0	$\frac{1}{2}$	0.5	
O10	12e	<i>mm2.</i>	0.2344	0	$\frac{1}{2}$	0.25	
O11	12e	<i>mm2.</i>	0.2942	0	$\frac{1}{2}$	0.25	
Ba12	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron O <sub>12</sub>
O13	6b	<i>mmm.</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		collinear V <sub>2</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.025, T = 293 K

Remarks: We deduced idealized partial occupancies of former V2, V2A, O6, O6A, and O7 from the description of the structure. 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] Zhang Y., Haushalter R.C., Zubieta J. (1998), Inorg. Chim. Acta 277, 263-267.

204  
cI374

Ba <sub>9</sub> V <sub>15</sub> O <sub>45</sub> [H <sub>2</sub> O] <sub>5.25</sub>	cI374	(204) <i>Im</i> -3 – h <sup>5</sup> g <sup>3</sup> e <sup>4</sup> cb
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### Ba<sub>6</sub>[V<sub>10</sub>O<sub>30</sub>(H<sub>2</sub>O)]·2.5H<sub>2</sub>O [1]

Structural features:  $V_{10}O_{30}(H_2O)$  units formed by two vertex-linked  $V^{4+}(O_5[OH_2])$  octahedra (two-fold orientational disorder, common O or  $H_2O$ ) sharing vertices with four  $V_2O_7$  units (two vertex-linked  $V^{5+}O_4$  tetrahedra); Ba and additional  $H_2O$  between the units (partial disorder).

Kanke Y. et al. (2000) [1]

$Ba_9H_{10.48}O_{50.24}V_{15}$

$a = 1.68323 \text{ nm}$ ,  $V = 4.7690 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH <sub>2</sub> )1	48h	1	0.0337	0.1244	0.1036	0.312	
O2	48h	1	0.08025	0.41911	0.1195		
O3	48h	1	0.09592	0.2617	0.16492		single atom V
V4	48h	1	0.09737	0.12256	0.3282		tetrahedron O <sub>4</sub>
O5	48h	1	0.10656	0.22076	0.34165		single atom V
O6	24g	m..	0	0.09807	0.29186		non-colinear V <sub>2</sub>
Ba7	24g	m..	0	0.15438	0.06097	0.166	
Ba8	24g	m..	0	0.33216	0.27784		
V9	12e	mm2..	0.09125	0	$\frac{1}{2}$	0.36	
V10	12e	mm2..	0.13763	0	$\frac{1}{2}$	0.639	
O11	12e	mm2..	0.2339	0	$\frac{1}{2}$	0.639	
(OH <sub>2</sub> )12	12e	mm2..	0.2927	0	$\frac{1}{2}$	0.36	
Ba13	8c	.-3.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron O <sub>12</sub>
M14	6b	mmm..	0	$\frac{1}{2}$	$\frac{1}{2}$		colinear V <sub>2</sub>

$M14 = 0.721O + 0.279OH_2$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.038$

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] Kanke Y., Oka Y., Yao T. (2000), J. Solid State Chem. 151, 130-138.