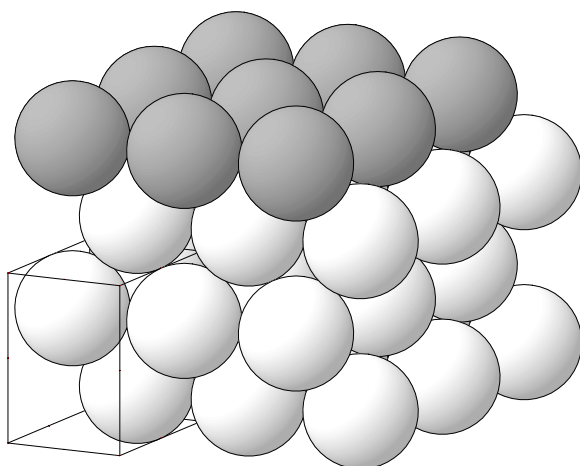


Space group (194)  $P6_3/mmc$ 194  
 $hP2$ 

Mg	$hP2$	(194) $P6_3/mmc - c$
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**Mg** [2], h.c.p. (hexagonal close-packed), Strukturbericht notation A3; Zn [3]

Structural features: Close-packed layers in h stacking, i.e. consecutive layers are shifted in opposite directions. See Fig. III.1.

Fig. III.1. **Mg**

Arrangement of Mg atoms emphasizing a close-packed layer perpendicular to [001].

Predel B., Hülse K. (1978) [1]

Mg

$a = 0.32092$ ,  $c = 0.52121$  nm,  $c/a = 1.624$ ,  $V = 0.0465$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	2c	-6m2	$1/3$	$2/3$	$1/4$		anticoctahedron Mg <sub>12</sub>

Experimental: powder, film, X-rays

Remarks: Zn with  $c/a = 1.86$  and lower coordination number (6+6) is sometimes considered as a branch.

References: [1] Predel B., Hülse K. (1978), Z. Metallkd. 69, 690-696. [2] (1931), Strukturberichte 1, 16,40. [3] (1931), Strukturberichte 1, 16,41.

194  
 $hP4$ 

Nd	$hP4$	(194) $P6_3/mmc - ca$
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**Nd α** [1], d.h.c.p. (double hexagonal close-packed), Strukturbericht notation A3'; La α [2]

Structural features: Close-packed layers in hc stacking. See Fig. III.2.

Ellinger F.H. (1955) [1]

Nd

$a = 0.3655$ ,  $c = 1.1796$  nm,  $c/a = 3.227$ ,  $V = 0.1365$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Nd1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Nd <sub>12</sub>
Nd2	2a	-3m.	0	0	0		cuboctahedron Nd <sub>12</sub>

Experimental: powder, film, X-rays

Remarks: Phase stable at T < 1136 K. Supersedes reports on Nd with a Mg-type close-packed structure in [3] and [4].

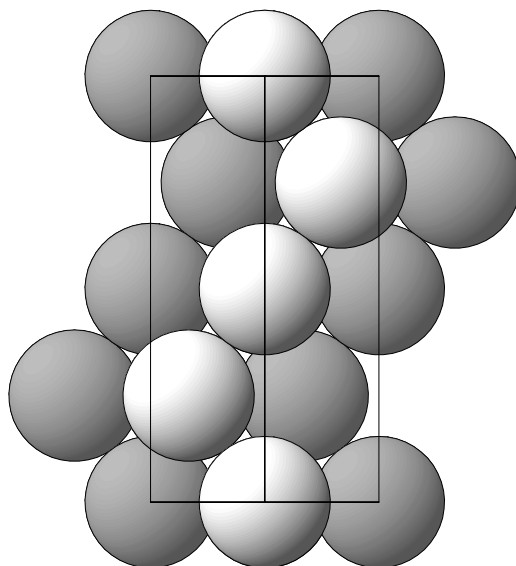


Fig. III.2. **Nd  $\alpha$**

Arrangement of Nd atoms viewed along [110].

References: [1] Ellinger F.H. (1955), J. Met. 7, 411. [2] Spedding F.H., Daane A.H., Herrmann K.W. (1956), Acta Crystallogr. 9, 559-563. [3] Quill L.L. (1932), Z. Anorg. Allg. Chem. 208, 273-281. [4] Klemm W., Bommer H. (1939), Z. Anorg. Allg. Chem. 241, 264-267.

194  
hP4

NiAs	hP4	(194) $P6_3/mmc$ – ca
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**NiAs** [2], nickeline, Strukturbericht notation B8<sub>1</sub>; Fe<sub>2</sub>N  $\epsilon$  disordered [3]; PtB [4]

Structural features: Close-packed As layers in h stacking; Ni occupies all octahedral voids. AsNi<sub>6</sub> trigonal prisms share edges to form a 3D-framework. See Fig. III.3.

Brand P., Briest J. (1965) [1]

AsNi

$a = 0.3619$ ,  $c = 0.5044$  nm,  $c/a = 1.394$ ,  $V = 0.0572$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Ni <sub>6</sub>
Ni2	2a	-3m.	0	0	0		8-vertex polyhedron As <sub>6</sub> Ni <sub>2</sub>

Experimental: powder, film, X-rays, T = 298 K

Remarks: Strukturbericht notation L'3 was defined on a partly disordered structure proposal for Fe<sub>2</sub>N. Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [5], maximum 50% occupation of the N site is expected for nitrides.

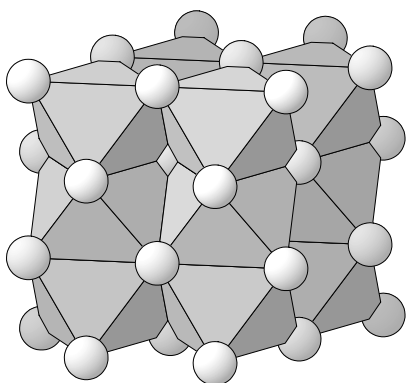


Fig. III.3. NiAs

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

References: [1] Brand P., Briest J. (1965), Z. Anorg. Allg. Chem. 337, 209-213. [2] (1931), Strukturberichte 1, 84, 143. [3] Inokuti Y., Nishida N., Ohashi N. (1975), Metall. Trans. A 6, 773-784. [4] Aronsson B., Stenberg E., Bselius J. (1960), Acta Chem. Scand. 14, 733-741. [5] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163.

194  
hP4

C-a	hP4	(194) $P6_3/mmc - cb$
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**C graphite** [2], graphite, Strukturbericht notation A9

Structural features: Planar hexagon-mesh layers, consecutive layers being shifted. See Fig. III.4.

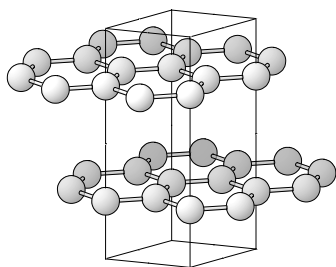


Fig. III.4. C graphite

Arrangement of C atoms.

Trucano P., Chen R. (1975) [1]

C

$a = 0.2464$ ,  $c = 0.6711$  nm,  $c/a = 2.724$ ,  $V = 0.0353$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
C1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle C <sub>3</sub>
C2	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle C <sub>3</sub>

Experimental: single crystal, diffractometer, neutrons, R = 0.042

Remarks: Natural specimen. Space groups (2)  $P-1$  and (11)  $P2_1/m$  were tested and rejected (R = 0.046 and 0.049, respectively). The orthorhombic model proposed in [3] is also rejected in [1]. The pressure dependence up to 20 GPa is studied in [4].

References: [1] Trucano P., Chen R. (1975), Nature (London) 258, 136-137. [2] (1931), Strukturberichte 1, 28,47. [3] Pauling L. (1964), Proc. Nat. Acad. Sci. U.S.A. 56, 1646-1652. [4] Zhao Y.X., Spain I.L. (1989), Phys. Rev. B: Condens. Matter 40, 993-997.

194  
hP4

BN-a	hP4	(194) $P6_3/mmc - cb$
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**BN hexagonal [1]**

Structural features: Planar hexagon-mesh BN layers, consecutive layers being shifted. Ordering variant of graphite.

Hassel O. (1926) [1]

BN

$a = 0.251$ ,  $c = 0.669$  nm,  $c/a = 2.665$ ,  $V = 0.0365$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle N <sub>3</sub>
N2	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle B <sub>3</sub>

Transformation from published data ( $P6_3/mmc$  \*): origin shift 0 0  $\frac{3}{4}$

Experimental: powder, film, X-rays

Remarks: The data in [1] refer to a non-conventional setting with the origin of the cell shifted by 0 0  $\frac{1}{4}$  from the description in the International Tables for Crystallography. Space group (186)  $P6_3mc$  could not be rejected. The structure was redetermined in [2], where different Wyckoff positions were found.

References: [1] Hassel O. (1926), Nor. Geol. Tidsskr. 9, 266-270. [2] Pease R.S. (1950), Nature (London) 166, 722-723.

194  
hP4

BN-b	hP4	(194) $P6_3/mmc - dc$
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**BN hexagonal [2], Strukturbericht notation B<sub>k</sub>**

Structural features: Directly superposed hexagon-mesh BN layers, B and N atoms alternating along [001]. BN<sub>3</sub> trigonal units share vertices to form infinite planar layers of fused B<sub>3</sub>N<sub>3</sub> rings.

Pease R.S. (1952) [1]

BN

$a = 0.2504$ ,  $c = 0.66612$  nm,  $c/a = 2.660$ ,  $V = 0.0362$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
N1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle B <sub>3</sub>
B2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle N <sub>3</sub>

Transformation from published data ( $P6_3/mmc$  \*): origin shift  $\frac{2}{3}$   $\frac{1}{3}$   $\frac{1}{4}$

Experimental: powder, film, X-rays, T = 308 K

Remarks: Transformed from a non-conventional setting with the origin shifted by  $\frac{2}{3}$   $\frac{1}{3}$   $\frac{1}{4}$  with respect to the International Tables for Crystallography. Supersedes a structure proposal with the atoms in Wyckoff positions 2c and 2b ([3];ordered graphite).

References: [1] Pease R.S. (1952), Acta Crystallogr. 5, 356-361. [2] Pease R.S. (1950), Nature (London) 166, 722-723. [3] (1931), Strukturberichte 1, 95, 139.

194  
hP4

C-b	hP4	(194) $P6_3/mmc - f$
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**C hexagonal diamond** [1], lonsdaleite, diamond hexagonal; Si wurtzite [2]

Structural features: Tetrahedral structure.  $CC_4$  tetrahedra share single vertices to form a 3D-framework.

Bundy F.P., Kasper J.S. (1967) [1]

C

$a = 0.252$ ,  $c = 0.412$  nm,  $c/a = 1.635$ ,  $V = 0.0227$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
C1	$4f$	$3m.$	$1/3$	$2/3$	0.0625		tetrahedron $C_4$

Experimental: twinned crystal, precession photographs, X-rays

Remarks: High-temperature high-pressure phase.

References: [1] Bundy F.P., Kasper J.S. (1967), J. Chem. Phys. 46, 3437-3446. [2] Wentorf R.H. Jr., Kasper J.S. (1963), Science (Washington D.C.) 139, 338-339.

194  
hP6

$LiB_{0.9}$	$hP6$	(194) $P6_3/mmc - cba$
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**LiB<sub>x</sub>** [1]

Structural features: Close-packed Li layers in h stacking; infinite linear -B- (borynide) chains (double or alternatively triple and single bonds) parallel to [001].

Wörle M., Nesper R. (2000) [1]

$B_{0.95}Li$

$a = 0.4019$ ,  $c = 0.2792$  nm,  $c/a = 0.695$ ,  $V = 0.0391$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Li1	$2c$	$-6m2$	$1/3$	$2/3$	$1/4$		
B2	$2b$	$-6m2$	0	0	$1/4$	0.47	
B3	$2a$	$-3m.$	0	0	0	0.48	

Experimental: powder, diffractometer, neutrons,  $R_p = 0.082$

Remarks: Homogeneity range  $LiB_x$ ,  $0.82 < x < 1.0$ . A refinement restraining the composition to  $LiB_{0.88}$  gave  $occ(B2) = occ(B3) = 0.44$  ( $wR_p = 0.160$ ). Compositions  $Li_5B_4$  and  $Li_7B_6$ , reported in [2] and [3], respectively, are stated to be doubtful. Short interatomic distances for partly occupied site(s).

References: [1] Wörle M., Nesper R. (2000), Angew. Chem. Int. Ed. 39, 2349-2353. [2] Wang F.E., Mitchell M.A., Sutula R.A., Holden J.R., Bennett L.H. (1978), J. Less-Common Met. 61, 237-251. [3] Dallek S., Ernst D.W., Larrick B.F. (1979), J. Electrochem. Soc. 126, 866-870.

194  
hP6

$Co_{1.75}Ge$	$hP6$	(194) $P6_3/mmc - dca$
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**Co<sub>2</sub>Ge ht** [2], Strukturbericht notation B8<sub>2</sub>; Ni<sub>2</sub>Ge ht [3]; Ni<sub>2</sub>Si θ [7]; Ni<sub>2</sub>In [6]

Structural features: Close-packed Ge layers in h stacking; Co in octahedral and trigonal bipyramidal voids. 3D-framework of fused Co<sub>6</sub> prisms centered alternatively by additional Co (partial vacancies) and Ge. See Fig. III.5.

Ellner M. (1976) [1]

$Co_{1.70}Ge$

$a = 0.3914$ ,  $c = 0.5004$  nm,  $c/a = 1.278$ ,  $V = 0.0664$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.7	pentacapped trigonal prism $\text{Ge}_5\text{Co}_6$
Ge2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		pentacapped trigonal prism $\text{Co}_{11}$
Co3	2a	-3m.	0	0	0		bicapped hexagonal prism $\text{Co}_8\text{Ge}_6$

Experimental: powder, film, X-rays

Remarks: Phase stable at  $T > 473$ -673 depending on the composition; the stoichiometric composition is included in the homogeneity range only at high temperature. We assigned site occupancies in agreement with the nominal composition. The descriptions of  $\theta$ - $\text{Ni}_2\text{Si}$  in space groups (182)  $P6_322$  or (176)  $P6_3/m$  in [7] do not consider all symmetry elements of the proposed structure (see [4]). The same is true for the description of  $\text{ht-Ni}_2\text{Ge}$  in space group (187)  $P-6m2$  in [3] (structure type identified in [5] and [9]). In [6] the cell parameters are expressed in kX instead of Å as indicated (see [8]).

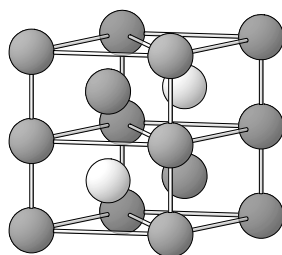


Fig. III.5.  $\text{Co}_2\text{Ge ht}$

Arrangement of  $\text{Co}_6$  trigonal prisms centered by Co (all Co atoms dark) and Ge (light) atoms.

References: [1] Ellner M. (1976), J. Less-Common Met. 48, 21-52. [2] Laves F., Wallbaum H.J. (1942), Z. Angew. Mineral. 4, 17-46. [3] Ellner M., Gödecke T., Schubert K. (1971), J. Less-Common Met. 24, 23-40. [4] Cenxual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439. [5] Lecocq P. (1963), Ann. Chim. (Paris) 8, 85-116. [6] Makarov E.S. (1944), Izv. Akad. Nauk SSSR, Ser. Khim. 1944(1), 29-34. [7] Toman K. (1952), Acta Crystallogr. 5, 329-331. [8] (1955), Structure Reports 9, 90. [9] (1975), Structure Reports 38A, 88.

194  
hP6

BeZrSi

hP6

(194)  $P6_3/mmc - dca$

**ZrBeSi** [2];  $\text{CaCuSb}$  [3];  $\text{CePdAs}$  [11];  $\text{CePdP}$  [8];  $\text{KAuTe}$  [9];  $\text{MnCoGe ht}$  [4];  $\text{NaBeSb}$  [5];  $\text{SrPtAs}$  [7];  $\text{SrZnSi}$  [6];  $\text{CeSeH}$  [12]

Structural features: 3D-framework of fused  $\text{Zr}_6$  trigonal prisms centered alternatively by Be and Si.  $\text{SiZr}_6$  trigonal prisms share edges to form a 3D-framework (the same is true for the  $\text{BeZr}_6$  prisms). Infinite planar hexagon-mesh BeSi layers. Substitution derivative of  $\text{AlB}_2$ . See Fig. III.6.

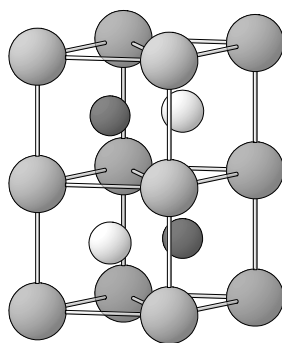


Fig. III.6. **ZrBeSi**

Arrangement of  $\text{Zr}_6$  trigonal prisms (Zr atoms large) centered by Be (dark) and Si (light) atoms.

Nielsen J.W., Baenziger N.C. (1954) [1]

BeSiZr

$a = 0.371$ ,  $c = 0.719$  nm,  $c/a = 1.938$ ,  $V = 0.0857$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Si1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		tricapped trigonal prism Be <sub>3</sub> Zr <sub>6</sub>
Be2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Si <sub>3</sub> Zr <sub>6</sub>
Zr3	2a	-3m.	0	0	0		pseudo Frank-Kasper Be <sub>6</sub> Si <sub>6</sub> Zr <sub>8</sub>

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: We deduced the space group from the coordinates of all atoms in the unit cell. The same data are reported in [2]. H could not be located with certainty in [12] (CeSeH).

References: [1] Nielsen J.W., Baenziger N.C. (1954), Acta Crystallogr. 7, 132-133. [2] Nielsen J.W., Baenziger N.C. (1953), U. S. At. En. Comm. 1953, Publ. AECU-2728. [3] Eisenmann B., Cordier G., Schäfer H. (1974), Z. Naturforsch. B 29, 457-459. [4] Jeitschko W. (1975), Acta Crystallogr. B 31, 1187-1190. [5] Tiburtius C., Schuster H.U. (1977), Z. Naturforsch. B 32, 1133-1138. [6] Dörrscheidt W., Schäfer H. (1981), J. Less-Common Met. 78, 69-79. [7] Wenski G., Mewis A. (1986), Z. Anorg. Allg. Chem. 535, 110-122. [8] Johrendt D., Mewis A. (1990), Z. Naturforsch. B 45, 1262-1266. [9] Bronger W., Kathage H.U. (1990), J. Less-Common Met. 160, 181-184. [10] Rudy E., Benesovsky F., Nowotny H., Toth L.E. (1961), Monatsh. Chem. 92, 692-700. [11] Johrendt D., Mewis A. (1992), J. Alloys Compd. 183, 210-223. [12] Schleid T., Folchmann M. (1996), Z. Anorg. Allg. Chem. 622, 455-461.

194  
hP6

Cu <sub>2</sub> S	hP6	(194) P6 <sub>3</sub> /mmc – dcb
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**Cu<sub>2</sub>S chalcocite ht** [1], chalcocite high

Structural features: Close-packed S layers in h stacking; Cu in trigonal voids.

Belov N.V., Butuzov V.P. (1946) [1]

Cu<sub>2</sub>S

$a = 0.389$ ,  $c = 0.668$  nm,  $c/a = 1.717$ ,  $V = 0.0875$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar hexagon Cu <sub>3</sub> S <sub>3</sub>
S2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar hexagon Cu <sub>6</sub>
Cu3	2b	-6m2	0	0	$\frac{1}{4}$		coplanar hexagon S <sub>3</sub> Cu <sub>3</sub>

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

Remarks: Phase stable at  $T > 377$  K. Diffraction data and cell parameters from [2].

References: [1] Belov N.V., Butuzov V.P. (1946), Sov. Phys. Dokl. 54, 717-720 (Dokl. Akad. Nauk SSSR 54, 721-724). [2] Buerger M.I., Buerger N.W. (1944), Am. Mineral. 20, 55.

194  
hP6

(Na <sub>0.5</sub> Tl <sub>0.5</sub> ) <sub>2</sub> O	hP6	(194) P6 <sub>3</sub> /mmc – fa
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**NaTlO** [1]

Structural features: Directly superposed triangle-mesh O layers; (Na,Tl)<sub>2</sub> dumbbells (parallel to [001]) in trigonal prismatic voids. (Na,Tl) layers in BBCC stacking; O in octahedral voids.

Sabrowsky H. et al. (1985) [1]

NaOTl

$a = 0.3436$ ,  $c = 1.151$  nm,  $c/a = 3.35$ ,  $V = 0.1177$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.122		tetrahedron O <sub>3</sub> Na
O2	$2a$	$-3m.$	0	0	0		octahedron Na <sub>6</sub>

M1 = 0.5Na + 0.5Tl

Remarks: The description in space group (176)  $P6_3/m$  in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Sabrowsky H., Mertens P., Dönhoff F.O. (1985), Z. Naturforsch. B 40, 122-123.

194  
hP6

Tb	<i>hP6</i>	(194) $P6_3/mmc - fb$
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**Tb t.h.c.p.** [1], t.h.c.p. (triple hexagonal close-packed)

Structural features: Close-packed layers in hc<sub>2</sub> stacking.

Staun Olsen J. et al. (1985) [1]

Tb

$a = 0.3068$ ,  $c = 1.487$  nm,  $c/a = 4.847$ ,  $V = 0.1212$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Tb1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.08333		cuboctahedron Tb <sub>12</sub>
Tb2	$2b$	$-6m2$	0	0	$\frac{1}{4}$		anticuboctahedron Tb <sub>12</sub>

Experimental: powder, diffractometer, X-rays, synchrotron,  $p = 28.8$  GPa

Remarks: Phase stable at  $28 < p < 32$  GPa. Idealized coordinates.

References: [1] Staun Olsen J., Steenstrup S., Gerward L. (1985), Phys. Lett. A 109, 235-237.

194  
hP6

NbS <sub>2</sub>	<i>hP6</i>	(194) $P6_3/mmc - fb$
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**NbS<sub>2</sub> 2H** [1]; NbSe<sub>2</sub> 2H rt [2]; TaS<sub>2</sub> 2H [3]; Hf<sub>2</sub>S [4]

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic voids (stacking sequence BaB CaC). NbS<sub>6</sub> trigonal prisms share edges to form infinite layers. See Fig. III.7.

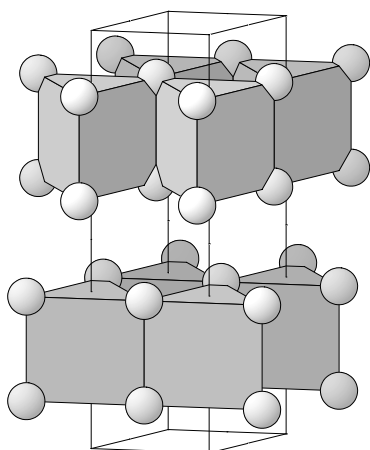
Jellinek F. et al. (1960) [1]

NbS<sub>2</sub>

$a = 0.331$ ,  $c = 1.189$  nm,  $c/a = 3.592$ ,  $V = 0.1128$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.125		non-coplanar triangle Nb <sub>3</sub>
Nb2	$2b$	$-6m2$	0	0	$\frac{1}{4}$		trigonal prism S <sub>6</sub>

Remarks: Phase stable at  $T < 1323$  K. Idealized coordinates.

Fig. III.7. **NbS<sub>2</sub> 2H**Arrangement of NbS<sub>6</sub> trigonal prisms.

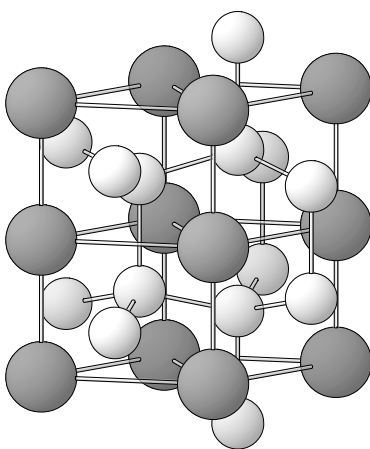
References: [1] Jellinek F., Brauer G., Müller H. (1960), Nature (London) 185, 376-377. [2] Selte K., Kjekshus A. (1964), Acta Chem. Scand. 18, 697-706. [3] Meetsma A., Wiegers G.A., Haange R.J., De Boer J.L. (1990), Acta Crystallogr. C 46, 1598-1599. [4] Franzen H.F., Graham J. (1966), Z. Kristallogr. 123, 133-138.

194  
*hP6*

CaIn <sub>2</sub>	<i>hP6</i>	(194) <i>P6<sub>3</sub>/mmc</i> – fb
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**CaIn<sub>2</sub>** [1]; BaTl<sub>2</sub> [1]

Structural features: 3D-framework of fused Ca<sub>6</sub> trigonal prisms centered by In (displaced from the prism centers). In forms a tetrahedral framework. Derivative of AlB<sub>2</sub>. See Fig. III.8.

Fig. III.8. **CaIn<sub>2</sub>**

Arrangement of Ca<sub>6</sub> trigonal prisms (Ca atoms dark) and tetrahedral framework formed by In atoms (light).

Iandelli A. (1964) [1]

CaIn<sub>2</sub>
 $a = 0.4895$ ,  $c = 0.775$  nm,  $c/a = 1.583$ ,  $V = 0.1608$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
In1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.045		bicapped square prism In <sub>4</sub> Ca <sub>6</sub>
Ca2	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		rhombic dodecahedron In <sub>12</sub> Ca <sub>2</sub>

Experimental: powder, film, X-rays

Remarks: In [2] it is not indicated that  $\frac{1}{4}$  must be added to the  $z$ -coordinate of the In site to be in agreement with Wyckoff position  $4f$ .

References: [1] Iandelli A. (1964), Z. Anorg. Allg. Chem. 330, 221-232. [2] (1972), Structure Reports 29, 3.

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hP6

MoS <sub>2</sub>	hP6	(194) $P6_3/mmc - fc$
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**MoS<sub>2</sub> 2H** [2], molybdenite-2H, Strukturbericht notation C7; Pt<sub>2</sub>B [3]

Structural features: Close-packed S layers in BBCC stacking; Mo in trigonal prismatic voids (stacking sequence BcB CbC). MoS<sub>6</sub> trigonal prisms share edges to form infinite layers. Layer structure with sandwiches consisting of three sublayers in h stacking (S-Mo-S). See Fig. III.9.

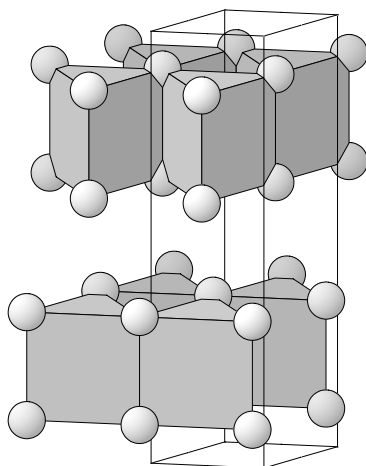


Fig. III.9. **MoS<sub>2</sub> 2H**

Arrangement of MoS<sub>6</sub> trigonal prisms.

Petkov V. et al. (2002) [1]

MoS<sub>2</sub>

$a = 0.3168$ ,  $c = 1.2322$  nm,  $c/a = 3.890$ ,  $V = 0.1071$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	$4f$	$3m$	$\frac{1}{3}$	$\frac{2}{3}$	0.625		non-coplanar triangle Mo <sub>3</sub>
Mo2	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism S <sub>6</sub>

Experimental: powder, diffractometer, X-rays, synchrotron

Remarks: In [5] the  $z$ -coordinate of the S site is misprinted as 0.621 instead of 0.629 (see [4]).

References: [1] Petkov V., Billinge S.J.L., Larson P., Mahanti S.D., Vogt T., Rangan K.K., Kanatzidis M.G. (2002), Phys. Rev. B: Condens. Matter 65, 092105: 1-4. [2] Dickinson R.G., Pauling L. (1923), J. Am. Chem. Soc. 45, 1466-1471. [3] Hassler E., Lundström T., Tergenius L.E. (1979), J. Less-Common Met. 67, 567-572. [4] Bronsema K.D., De Boer J.L., Jellinek F. (1986), Z. Anorg. Allg. Chem. 540/541, 15-17. [5] (1931), Strukturberichte 1, 164.

194  
hP6

ReB <sub>2</sub>	hP6	(194) $P6_3/mmc - fc$
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**ReB<sub>2</sub>** [1]

Structural features: Close-packed Re layers (h stacking) alternate with puckered triangle-mesh B layers along [001].

La Placa S., Post B. (1962) [1]

B<sub>2</sub>Re

$a = 0.2900$ ,  $c = 0.7478$  nm,  $c/a = 2.579$ ,  $V = 0.0545$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.548		non-coplanar triangle B <sub>3</sub>
Re2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		14-vertex polyhedron B <sub>8</sub> Re <sub>6</sub>

Experimental: powder, diffractometer, X-rays, R = 0.019

Remarks: No significant electron density was detected in Wyckoff position 2a. Supersedes a structure proposal for so-called ReB<sub>3</sub> in [2]. In [1] the Hermann-Mauguin symbol for the space group is misprinted as *P6/mmc* instead of *P6<sub>3</sub>/mmc*.

References: [1] La Placa S., Post B. (1962), Acta Crystallogr. 15, 97-99. [2] Aronsson B., Stenberg E., Bselius J. (1960), Acta Chem. Scand. 14, 733-741.

194  
hP6

ScH <sub>0.33</sub>	hP6	(194) <i>P6<sub>3</sub>/mmc</i> – fc
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**ScH<sub>0.33</sub>** [1]

Structural features: Close-packed Sc layers in h stacking; H in tetrahedral voids (disorder).

Saw C.K. et al. (1983) [1]

D<sub>0.34</sub>Sc

$a = 0.3338$ ,  $c = 0.5299$  nm,  $c/a = 1.587$ ,  $V = 0.0511$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.653	0.17	single atom D
Sc2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron D <sub>8</sub>

Experimental: single crystal, diffractometer, neutrons, R = 0.036

Remarks: Homogeneity range ScH<sub>x</sub>, 0 < x < 0.43. We deduced the space group from the coordinates of all atoms in the unit cell. A similar model with H in Wyckoff position 2a was tested and rejected.

References: [1] Saw C.K., Beaudry B.J., Stassis C. (1983), Phys. Rev. B: Condens. Matter 27, 7013-7017.

194  
hP8

TaSnS <sub>2</sub>	hP8	(194) <i>P6<sub>3</sub>/mmc</i> – eca
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**SnTaS<sub>2</sub> 2s** [2]

Structural features: Directly superposed close-packed S and Sn layers; Ta in trigonal prismatic voids between S layers (stacking sequence AbAA'AcAA' where A' = Sn). TaS<sub>6</sub> trigonal prisms share edges to form infinite slabs.

Van Der Lee A., Wiegers G.A. (1990) [1]

S<sub>2</sub>SnTa

$a = 0.33053$ ,  $c = 1.7434$  nm,  $c/a = 5.275$ ,  $V = 0.1649$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	4e	3 <i>m</i> .	0	0	0.1606		non-coplanar triangle Ta <sub>3</sub>
Ta2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism S <sub>6</sub>
Sn3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		8-vertex polyhedron S <sub>2</sub> Sn <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, *R* = 0.023, *T* = 295 K

References: [1] Van Der Lee A., Wiegers G.A. (1990), Mater. Res. Bull. 25, 1011-1018. [2] Eppinga R., Wiegers G.A. (1977), Mater. Res. Bull. 12, 1057-1062.

194  
hP8

GaS-a	<i>hP</i> 8	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – <i>f</i> <sup>2</sup>
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**GaS β** [2]; Li<sub>2</sub>O<sub>2</sub> (see remark)

Structural features: Close-packed S layers in BBCC stacking; Ga<sub>2</sub> dumbbells in trigonal prismatic voids (stacking sequence BccB CbbC). S<sub>3</sub>Ga-GaS<sub>3</sub> units share vertices to form infinite slabs. Layer structure with sandwiches consisting of four sublayers (S-Ga-Ga-S). See Fig. III.10.

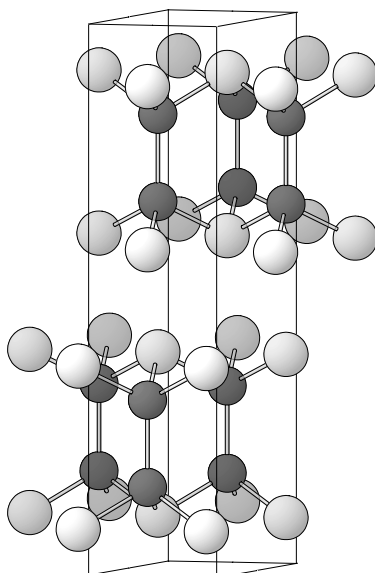


Fig. III.10. **GaS β**

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

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

GaS

*a* = 0.3592, *c* = 1.5465 nm, *c/a* = 4.305, *V* = 0.1728 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.17082		tetrahedron S <sub>3</sub> Ga
S2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.60191		non-coplanar triangle Ga <sub>3</sub>

Experimental: single crystal, diffractometer, X-rays, *wR* = 0.018, *T* = 293 K

Remarks: A similar structure proposal for Li<sub>2</sub>O<sub>2</sub> [3] (antitype) is superseded (see [4]). The description in space group (174) *P*-6 with 4-fold cell volume in [3] (Li<sub>2</sub>O<sub>2</sub>) does not take into consideration all symmetry elements of the proposed structure.



References: [1] Kuhn A., Bourdon A., Rigoult J., Rimsky A. (1982), Phys. Rev. B: Condens. Matter 25, 4081-4088. [2] Hahn H., Frank G. (1955), Z. Anorg. Allg. Chem. 278, 340-348. [3] Fehér F., Von Wilucki I., Dost G. (1953), Chem. Ber. 86, 1429-1437. [4] Föpl H. (1957), Z. Anorg. Allg. Chem. 291, 12-50.

194  
hP8

$\text{Nb}_{1.35}\text{S}_2$	hP8	(194) $P6_3/mmc - fba$
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**$\text{Nb}_{1+x}\text{S}_2$  2s [2];  $\text{WN}_x \delta \text{III}_\text{H}$  [3]**

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic and octahedral voids (partial vacancies in the latter; stacking sequence BaBaCaCa).  $\delta$ -(WN) (antitype) contains directly superposed close-packed W layers; N in trigonal prismatic voids.

Kadijk F., Jellinek F. (1969) [1]

$\text{Nb}_{1.39}\text{S}_2$

$a = 0.3308$ ,  $c = 1.271$  nm,  $c/a = 3.842$ ,  $V = 0.1205$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.123		trigonal prism Nb <sub>6</sub>
Nb2	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism S <sub>6</sub>
Nb3	2a	-3m.	0	0	0	0.39	octahedron S <sub>6</sub>

Remarks: In [4] ( $\delta$ -WN<sub>x</sub> III<sub>H</sub>) the  $z$ -coordinates of the positions of the defect W site are misprinted as  $\frac{1}{4}$  and  $\frac{3}{4}$  instead of 0 and  $\frac{1}{2}$ , respectively (from the description of the structure).

References: [1] Kadijk F., Jellinek F. (1969), J. Less-Common Met. 19, 421-430. [2] Jellinek F., Brauer G., Müller H. (1960), Nature (London) 185, 376-377. [3] Khitrova V.I., Pinsker Z.G. (1962), Sov. Phys. Crystallogr. 6, 712-719 (Kristallografiya 6, 882-891). [4] Khitrova V.I. (1963), Sov. Phys. Crystallogr. 8, 28-33 (Kristallografiya 8, 39-46).

194  
hP8

$\text{Li}_{0.67}\text{NbS}_2$	hP8	(194) $P6_3/mmc - fba$
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**$\text{Li}_{0.67}\text{NbS}_2 \alpha$  [2];  $\text{NiMoP}_2$  [4];  $(\text{Cr,Ni})_{0.33}\text{TaS}_2$  [3]**

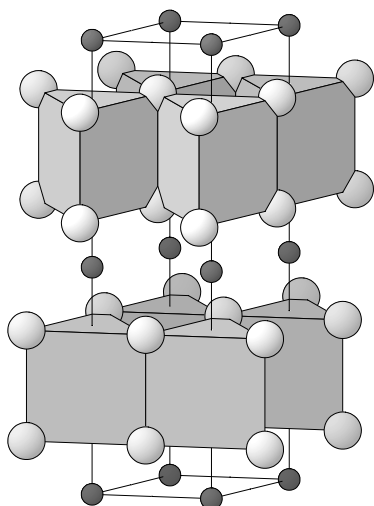


Fig. III.11.  **$\text{Li}_{0.67}\text{NbS}_2 \alpha$**

Arrangement of NbS<sub>6</sub> trigonal prisms (S atoms light) and Li atoms (dark).

Structural features: Close-packed S layers in BBCC stacking; Nb in trigonal prismatic, Li in octahedral voids (stacking sequence BaBa'CaCa' where a' = Li). NbS<sub>6</sub> trigonal prisms share edges to form infinite layers. See Fig. III.11.

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

Li<sub>0.63</sub>NbS<sub>2</sub>

$a = 0.33477$ ,  $c = 1.2875$  nm,  $c/a = 3.846$ ,  $V = 0.1250$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.12824		trigonal prism Nb <sub>3</sub> Li <sub>3</sub>
Nb2	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism S <sub>6</sub>
Li3	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.63	octahedron S <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.018$ ,  $T = 150$  K

References: [1] Salyer P.A., Barker M.G., Blake A.J., Gregory D.H., Wilson C. (2003), Acta Crystallogr. C 59, i4-i6. [2] Omloo W.P.F.A.M., Jellinek F. (1970), J. Less-Common Met. 20, 121-129. [3] Kulikov L.M., Semjonov Kobzar A.A., Akselrud L.G., Romaka L.P., Takzei G.A., Sych I.I. (1995), Int. Conf. Crystal Chem. Internet. Compd., 6th, L'vov 1995, Coll. Abstr. p. 80. [4] Guérin R., Sergent M. (1976), J. Solid State Chem. 18, 317-323.

194  
hP8

TiP	hP8	(194) $P6_3/mmc - fca$
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**TiP** [2], Strukturbericht notation B<sub>i</sub>; MoC  $\gamma'$  [5]; NbN  $\epsilon$  [4]; TiAs [6]; Ti<sub>3</sub>S<sub>4</sub> [3]

Structural features: Close-packed P layers in hc stacking; Ti in octahedral voids.

Snell P.O. (1967) [1]

PTi

$a = 0.3499$ ,  $c = 1.1700$  nm,  $c/a = 3.344$ ,  $V = 0.1241$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ti1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6170		octahedron P <sub>6</sub>
P2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Ti <sub>6</sub>
P3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron Ti <sub>6</sub>

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

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

Remarks: C was not located in [5] (MoC  $\gamma'$ ). The data from [6] are also reported in [7].

References: [1] Snell P.O. (1967), Acta Chem. Scand. 21, 1773-1776. [2] Schönberg N. (1954), Acta Chem. Scand. 8, 226-239. [3] Hahn H., Harder B. (1953), Angew. Chem. 65, 325-326. [4] Schönberg N. (1954), Acta Chem. Scand. 8, 208-212. [5] Kuo K., Hägg G. (1952), Nature (London) 170, 245-246. [6] Lukaszewicz K., Trzebiatowski W. (1954), Bull. Acad. Pol. Sci., Cl. 3, 2, 277-279. [7] Trzebiatowski W., Lukaszewicz K. (1954), Roczn. Chem. 28, 150-151.

194  
hP8

ReB <sub>3</sub>	hP8	(194) $P6_3/mmc - fca$
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**ReB<sub>3</sub>** [1]

Structural features: Close-packed Re layers and puckered triangle-mesh B layers alternate along [001].

Aronsson B. et al. (1960) [1]

 $B_3Re$  $a = 0.2900$ ,  $c = 0.7475$  nm,  $c/a = 2.578$ ,  $V = 0.0544$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.55		bicapped square prism $B_6Re_4$
Re2	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		pseudo Frank-Kasper $B_{14}Re_6$
B3	$2a$	$-3m.$	0	0	0		octahedron $B_6$

Experimental: powder, film, X-rays

Remarks: A model in space group (190)  $P-62c$  with a different arrangement of B atoms was tested and rejected. The composition was later corrected to  $ReB_2$  (see [2]).

References: [1] Aronsson B., Stenberg E., Bselius J. (1960), Acta Chem. Scand. 14, 733-741. [2] La Placa S., Post B. (1962), Acta Crystallogr. 15, 97-99.

194  
*hP8*

$YH_{0.18}$	<i>hP8</i>	(194) $P6_3/mmc - fca$
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 **$YH_{0.18}$**  [2]

Structural features: Close-packed Y layers in h stacking; H in tetrahedral and octahedral voids.

Khatamian D. (1987) [1]

 $D_{0.17}Y$  $a = 0.3665$ ,  $c = 0.5779$  nm,  $c/a = 1.577$ ,  $V = 0.0672$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.658	0.076	single atom D
Y2	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $D_6$
D3	$2a$	$-3m.$	0	0	0	0.018	octahedron $D_6$

Experimental: single crystal, diffractometer, neutrons, T = 573 K

References: [1] Khatamian D. (1987), J. Less-Common Met. 129, 153-158. [2] Khatamian D., Stassis C., Beaudry B.J. (1981), Phys. Rev. B: Condens. Matter 23, 624-627.

194  
*hP8*

$Li_2[O_2]-b$	<i>hP8</i>	(194) $P6_3/mmc - fca$
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 **$Li_2O_2$**  [1];  $Na_2S_2 \beta$  [2]Structural features: Li atoms and  $O_2$  dumbbells (parallel to [001]) in a  $Ni_2In$ -type ( $ht-Co_2Ge$ ) arrangement.

Föppl H. (1957) [1]

 $Li_2O_2$  $a = 0.3142$ ,  $c = 0.7650$  nm,  $c/a = 2.435$ ,  $V = 0.0654$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.651		single atom O
Li2	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $O_6$
Li3	$2a$	$-3m.$	0	0	0		octahedron $O_6$

Transformation from published data (*P*-6): origin shift  $\frac{2}{3} \frac{1}{3} 0.75$

Experimental: powder, film, X-rays

Remarks: The description in space group (174) *P*-6 in [1] does not take into consideration all symmetry elements (see [2]). Supersedes a structure proposal with a different arrangement of Li atoms and  $d(\text{O-O}) = 0.128 \text{ nm}$  in [3]. The description of the superseded structure proposal in space group (174) *P*-6 with 32 atoms in the unit cell [3] does also not take into consideration all symmetry elements of the proposed structure; correct space group is (194) *P*<sub>63</sub>/*mmc* with  $\frac{1}{4}$  cell volume (new axes  $a/2, b/2, c$ ; origin shift  $\frac{1}{3} \frac{2}{3} \frac{1}{4}$ ). On page 40 of [1] the *x*-coordinate of Wyckoff position *2h* is misprinted as  $\frac{1}{2}$  instead of  $\frac{1}{3}$ . In [4] the Wyckoff position of Li(II) is misprinted as *1i* instead of *2i*.

References: [1] Föppl H. (1957), Z. Anorg. Allg. Chem. 291, 12-50. [2] Föppl H., Busmann E., Frorath F.K. (1962), Z. Anorg. Allg. Chem. 314, 12-20. [3] Fehér F., Von Wilucki I., Dost G. (1953), Chem. Ber. 86, 1429-1437. [4] (1964), Structure Reports 21, 233.

194  
hP8

EuPtP	hP8	(194) <i>P</i> <sub>63</sub> / <i>mmc</i> – fca
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#### EuPtP α [1]

Structural features: 3D-framework of fused Eu<sub>6</sub> trigonal prisms centered alternatively by P (displaced from the prism centers) and Pt. Variant of ZrBeSi with site splitting.

Lux C. et al. (1991) [1]

EuPPt

$a = 0.4086, c = 0.863 \text{ nm}, c/a = 2.112, V = 0.1248 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7408	0.5	
Pt2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Eu3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

Experimental: single crystal, diffractometer, X-rays,  $R = 0.019, T = 295 \text{ K}$

Remarks: Phase stable at  $T > 235 \text{ K}$ . Short interatomic distances for partly occupied site(s). Supersedes a structure proposal with P in Wyckoff position *2d* ([2]; ZrBeSi type). Average structure; the authors state that true symmetry is probably trigonal, space group (164) *P*-3*m*1.

References: [1] Lux C., Mewis A., Lossau N., Michels G., Schlabit W. (1991), Z. Anorg. Allg. Chem. 593, 169-180. [2] Wenski G., Mewis A. (1986), Z. Anorg. Allg. Chem. 543, 49-62.

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hP8

AgFeO <sub>2</sub>	hP8	(194) <i>P</i> <sub>63</sub> / <i>mmc</i> – fca
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#### AgFeO<sub>2</sub> δ [1]; CuFeO<sub>2</sub> 2H [2]

Structural features: Close-packed O layers in BBCC stacking; Fe in octahedral voids, Ag in linear coordination between directly superposed O layers (stacking sequence BbBaCcCa). Single O-Ag-O linear units.

Okamoto S. et al. (1972) [1]

AgFeO<sub>2</sub>

$a = 0.3039, c = 1.2395 \text{ nm}, c/a = 4.079, V = 0.0991 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0833		tetrahedron Fe <sub>3</sub> Ag

Ag <sub>2</sub>	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	colinear O <sub>2</sub>
Fe <sub>3</sub>	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

References: [1] Okamoto S., Okamoto S.I., Ito T. (1972), Acta Crystallogr. B 28, 1774-1777. [2] Effenberger H. (1991), Acta Crystallogr. C 47, 2644-2646.

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hP8

Ta(Ta <sub>0.5</sub> Mn <sub>0.5</sub> )N <sub>2</sub>	hP8	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – fca
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**Ta<sub>3</sub>MnN<sub>4</sub>** [1]; TlInS<sub>2</sub> form III [4]; RbScO<sub>2</sub> β [5]; BaCeN<sub>2</sub> [7]; ScTaN [6]

Structural features: Close-packed Ta and (Mn,Ta) layers in hc stacking; N occupies all octahedral voids.

Schönberg N. (1954) [1]

Mn<sub>0.50</sub>N<sub>2</sub>Ta<sub>1.50</sub>

*a* = 0.3023, *c* = 1.049 nm, *c/a* = 3.470, *V* = 0.0830 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.625		octahedron Ta <sub>3</sub> Mn <sub>3</sub>
Ta2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism N <sub>6</sub>
M3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron N <sub>6</sub>

M3 = 0.50Mn + 0.50Ta

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

Experimental: powder, film, X-rays

Remarks: Idealized coordinates. Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [2], maximum 50% occupation of the N site is expected. The description of TlInS<sub>2</sub> (thin film) in space group (187) *P*-6*m*2 in [3] does not take into consideration all symmetry elements of the proposed structure (origin shift  $\frac{2}{3}$   $\frac{1}{3}$   $\frac{3}{4}$ ). The same is true for the description of β-RbScO<sub>2</sub> in [8] (see [5]). In [6] (ScTaN) the arrangement of metal atoms is erroneously stated to be identical to the arrangement of Ti instead of As atoms in TiAs.

References: [1] Schönberg N. (1954), Acta Chem. Scand. 8, 213-220. [2] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163. [3] Agaev K.A., Gasymov V.A., Chiragov M.I. (1973), Sov. Phys. Crystallogr. 18, 226-227 (Kristallografiya 18, 366-368). [4] Range K.J., Engert G., Müller W., Weiss A. (1974), Z. Naturforsch. B 29, 181-185. [5] Wiench H., Brachtel G., Hoppe R. (1977), Z. Anorg. Allg. Chem. 436, 169-172. [6] Lengauer W., Ettmayer P. (1988), J. Less-Common Met. 141, 157-162. [7] Seeger O., Strähle J. (1994), Z. Naturforsch. B 49, 1169-1174. [8] Hoppe R., Sabrowsky H. (1965), Z. Anorg. Allg. Chem. 339, 144-154.

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hP8

Cr <sub>2</sub> AlC	hP8	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – fca
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**Cr<sub>2</sub>AlC** [1], H phase; Ti<sub>2</sub>CS [2]

Structural features: Close-packed Cr and Al layers in h stacking; C in octahedral voids between Cr layers. See Fig. III.12.

Jeitschko W. et al. (1963) [1]

AlCCr<sub>2</sub>

*a* = 0.286, *c* = 1.282 nm, *c/a* = 4.483, *V* = 0.0908 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cr1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.586		non-coplanar triangle C <sub>3</sub>
Al2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Cr <sub>6</sub> Al <sub>6</sub>
C3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron Cr <sub>6</sub>

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

Experimental: single crystal, photographs, X-rays

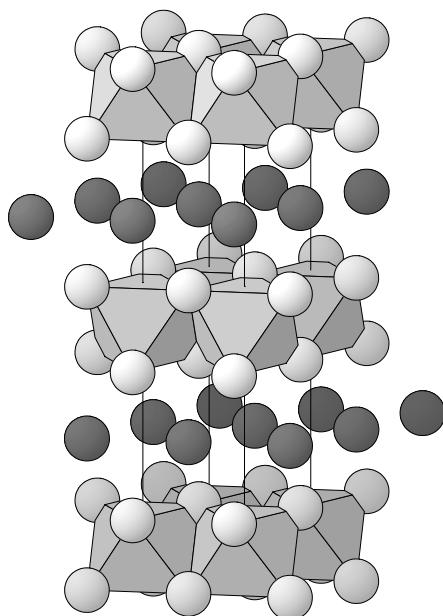


Fig. III.12. **Cr<sub>2</sub>AlC**

Arrangement of CCr<sub>6</sub> octahedra (Cr atoms light) and Al atoms (dark).

References: [1] Jeitschko W., Nowotny H., Benesovsky F. (1963), Monatsh. Chem. 94, 672-676. [2] Kudielka H., Rohde H. (1960), Z. Kristallogr. 114, 447-456.

194  
hP8

LiCu <sub>2</sub> Sn	<i>hP8</i>	(194) <i>P6<sub>3</sub>/mmc</i> – <i>fca</i>
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**LiCu<sub>2</sub>Sn** [1]; GdPt<sub>2</sub>Sn [3]; YPt<sub>2</sub>In [4]; Li<sub>2</sub>CeGe [2]

Structural features: Close-packed Sn layers in h stacking; Li occupies all octahedral, Cu all tetrahedral voids.

Krypyakevich P.I., Oleksiv H.I. (1970) [1]

Cu<sub>2</sub>LiSn

*a* = 0.4303, *c* = 0.7637 nm, *c/a* = 1.775, *V* = 0.1225 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.583		pentacapped trigonal prism Sn <sub>4</sub> Cu <sub>4</sub> Li <sub>3</sub>
Sn2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		rhombic dodecahedron Cu <sub>8</sub> Li <sub>6</sub>
Li3	2 <i>a</i>	-3 <i>m</i> .	0	0	0		cuboctahedron Cu <sub>6</sub> Sn <sub>6</sub>

Experimental: powder, film, X-rays

References: [1] Krypyakevich P.I., Oleksiv H.I. (1970), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1970, 63-65. [2] Pavlyuk V.V., Pechars'kii V.K., Bodak O.I. (1989), Dopov. Akad. Nauk Ukr. RSR, Ser. B

1989(2), 50-53. [3] De Mooij D.B., Buschow K.H.J. (1984), J. Less-Common Met. 102, 113-117. [4] Dwight A.E. (1987), Mater. Res. Bull. 22, 201-204.

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hP8

ScCrC <sub>2</sub>	hP8	(194) $P6_3/mmc - fca$
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### ScCrC<sub>2</sub> β [1]

Structural features: 3D-framework of fused Sc<sub>6</sub> prisms centered alternatively by Cr atoms and C<sub>2</sub> dumbbells (d(C-C)=0.160 nm).

Pöttgen R. et al. (1995) [1]

C<sub>2</sub>CrSc

$a = 0.3237$ ,  $c = 0.9149$  nm,  $c/a = 2.826$ ,  $V = 0.0830$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
C1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6627		7-vertex polyhedron CCr <sub>3</sub> Sc <sub>3</sub>
Cr2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism C <sub>6</sub>
Sc3	2a	-3m.	0	0	0		octahedron C <sub>6</sub>

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

Remarks: Phase stable at high temperature. Refinement of the site occupancies showed no significant deviation from unity.

References: [1] Pöttgen R., Witte A.M., Jeitschko W., Ebel T. (1995), J. Solid State Chem. 119, 324-330.

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hP8

Ti <sub>0.79</sub> Fe <sub>0.25</sub> Sb <sub>0.67</sub>	hP8	(194) $P6_3/mmc - fca$
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### Ti<sub>1.18</sub>Fe<sub>0.56</sub>Sb [1]

Structural features: 3D-framework of (Ti,Fe) trigonal prisms centered alternatively by Sb and additional Fe (the latter displaced from the prism centers, partial vacancies).

Skolozdra R.V. et al. (1995) [1]

Fe<sub>0.38</sub>Sb<sub>0.66</sub>Ti<sub>0.78</sub>

$a = 0.41649$ ,  $c = 0.62589$  nm,  $c/a = 1.503$ ,  $V = 0.0940$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Fe1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.624	0.08	
Sb2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.66	rhombic dodecahedron Fe <sub>8</sub> Ti <sub>6</sub>
M3	2a	-3m.	0	0	0		octahedron Fe <sub>6</sub>

M3 = 0.78Ti + 0.22Fe

Experimental: powder, diffractometer, X-rays, wR = 0.071

Remarks: Short interatomic distances for partly occupied site(s). In [1] the Wyckoff position of the Fe site is misprinted as 4e instead of 4f.

References: [1] Skolozdra R.V., Melnyk G.A., Akselrud L.G. (1995), Int. Conf. Crystal Chem. Intermet. Compd., 6th, L'vov 1995, Coll. Abstr. p. 97.

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hP8

BaCu	hP8	(194) $P6_3/mmc - fcb$
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**BaCu** [1]

Structural features: Close-packed Ba layers in AABB stacking; Cu occupies all trigonal prismatic voids. CuBa<sub>6</sub> trigonal prisms share rectangular faces to form infinite slabs. Infinite hexagon-mesh Cu layers.

Fornasini M.L., Merlo F. (1980) [1]

BaCu

$a = 0.4499$ ,  $c = 1.625$  nm,  $c/a = 3.612$ ,  $V = 0.2849$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ba1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6217		16-vertex polyhedron Cu <sub>6</sub> Ba <sub>10</sub>
Cu2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cu <sub>3</sub> Ba <sub>6</sub>
Cu3	2b	-6m2	0	0	$\frac{1}{4}$		tricapped trigonal prism Cu <sub>3</sub> Ba <sub>6</sub>

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

Experimental: single crystal, precession photographs, X-rays, R = 0.090

Remarks: Preliminary data in [2].

References: [1] Fornasini M.L., Merlo F. (1980), Acta Crystallogr. B 36, 1288-1291. [2] Bruzzone G. (1971), J. Less-Common Met. 25, 361-366.

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hP8

Na <sub>3</sub> As	hP8	(194) $P6_3/mmc$ – fcb
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**Na<sub>3</sub>As** [1], Strukturbericht notation D0<sub>18</sub>; LaF<sub>3</sub> [2]; IrAl<sub>3</sub> [3]

Structural features: Close-packed As layers in h stacking; Na in tetrahedral and trigonal voids.

Brauer G., Zintl E. (1937) [1]

AsNa<sub>3</sub>

$a = 0.5088$ ,  $c = 0.8982$  nm,  $c/a = 1.765$ ,  $V = 0.2014$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Na1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.583		pentacapped trigonal prism As <sub>4</sub> Na <sub>7</sub>
As2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		pentacapped trigonal prism Na <sub>11</sub>
Na3	2b	-6m2	0	0	$\frac{1}{4}$		tricapped trigonal prism As <sub>3</sub> Na <sub>6</sub>

Experimental: powder, film, X-rays

Remarks: A refinement in the same space group on diffraction data collected at 3.6 GPa is reported in [6]. The structure was later redetermined in space group (185)  $P6_3cm$  with 3-fold cell volume ([4], [5]) (new axes 2a+b, -a+b, c). A similar structure proposal for IrAl<sub>3</sub> [3] is stated to be doubtful in [4]; the authors recommend all compounds to which this type has been assigned, be tested again. The structure of LaF<sub>3</sub> was later refined in space group (165)  $P-3c1$  [7].

References: [1] Brauer G., Zintl E. (1937), Z. Phys. Chem., Abt. B 37, 323-352. [2] Schlyter K. (1952), Ark. Kemi 5, 73-82. [3] Edshammar L.E. (1967), Acta Chem. Scand. 21, 1104-1105. [4] Hafner P., Range K.J. (1994), J. Alloys Compd. 216, 7-10. [5] Range K., Ehrl R., Hafner P. (1996), J. Alloys Compd. 240, 19-24. [6] Jürgen Beister H., Syassen K., Klein J. (1990), Z. Naturforsch. B 45, 1388-1392. [7] Mansmann M. (1964), Z. Anorg. Allg. Chem. 331, 98-101.

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hP8

Li <sub>2</sub> CuAs	hP8	(194) $P6_3/mmc$ – fcb
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**Li<sub>2</sub>CuAs** [1]; Na<sub>2</sub>CdSn [2]; Mg<sub>2</sub>PtSi [3]; ZrPt<sub>2</sub>Al [4]



Structural features: Close-packed As layers in h stacking; Li in tetrahedral, Cu in trigonal voids. CuAs<sub>3</sub> triangles share vertices to form infinite layers. Ordering variant of Na<sub>3</sub>As.

Benda K.V., Juza R. (1969) [1]

AsCuLi<sub>2</sub>

$a = 0.4185$ ,  $c = 0.7923$  nm,  $c/a = 1.893$ ,  $V = 0.1202$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Li1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.59		pentacapped trigonal prism Li <sub>4</sub> As <sub>4</sub> Cu <sub>3</sub>
As2	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		pentacapped trigonal prism Cu <sub>3</sub> Li <sub>8</sub>
Cu3	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		tricapped trigonal prism As <sub>3</sub> Li <sub>6</sub>

Experimental: powder, film, X-rays,  $R_B = 0.157$

Remarks: Homogeneity range Li<sub>3-x</sub>Cu<sub>x</sub>As,  $0 < x < 1$  at 913 K.

References: [1] Benda K.V., Juza R. (1969), Z. Anorg. Allg. Chem. 371, 172-192. [2] Matthes R., Schuster H.U. (1980), Z. Naturforsch. B 35, 778-780. [3] Range K.J., Rau F., Klement U. (1990), Acta Crystallogr. C 46, 1092-1093. [4] Ferro R., Marazza R., Rambaldi G., Saccone A. (1975), J. Less-Common Met. 40, 251-252.

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hP8

GaS-b	hP8	(194) $P6_3/mmc - fe$
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#### GaS hp [1]

Structural features: Close-packed S layers in BBCC stacking; Ga<sub>2</sub> dumbbells in trigonal prismatic voids (stacking sequence BaaB CaaC). S<sub>3</sub>Ga-GaS<sub>3</sub> units share vertices to form infinite slabs. Layer structure with sandwiches consisting of four sublayers (S-Ga-Ga-S).

D'Amour H. et al. (1982) [1]

GaS

$a = 0.3547$ ,  $c = 1.474$  nm,  $c/a = 4.156$ ,  $V = 0.1606$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.098		non-coplanar triangle Ga <sub>3</sub>
Ga2	4 <i>e</i>	3 <i>m</i> .	0	0	0.1677		tetrahedron S <sub>3</sub> Ga

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

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.063$ ,  $p = 3.0$  GPa

Remarks: High-pressure phase.

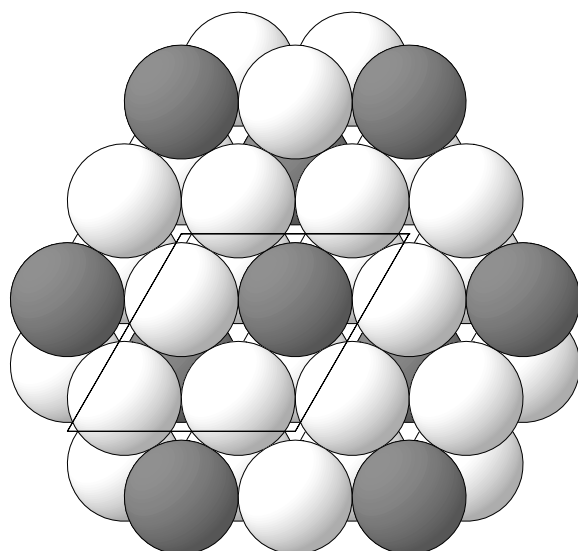
References: [1] D'Amour H., Holzapfel W.B., Polian A., Chevy A. (1982), Solid State Commun. 44, 853-855.

194  
hP8

Mg <sub>3</sub> Cd	hP8	(194) $P6_3/mmc - hd$
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**Mg<sub>3</sub>Cd** [2], Strukturbericht notation D0<sub>19</sub>; Ni<sub>3</sub>Sn  $\alpha$  [3]; MgCd<sub>3</sub> [2]; UPt<sub>3</sub> [4]

Structural features: Close-packed Mg<sub>3</sub>Cd layers in h stacking; the Cd atoms form a triangle mesh. Substitution derivative of Mg (prototype for a hexagonal close-packed atom arrangement). See Fig. III.13.

Fig. III.13. **Mg<sub>3</sub>Cd**

Arrangement of Mg (light) and Cd (dark) atoms in close-packed layers perpendicular to [001].

Edwards D.A. et al. (1952) [1]

**CdMg<sub>3</sub>**

$a = 0.6313$ ,  $c = 0.5074$  nm,  $c/a = 0.804$ ,  $V = 0.1751$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	6h	$mm2$	0.16667	0.33333	$\frac{1}{4}$		anticuboctahedron Mg <sub>8</sub> Cd <sub>4</sub>
Cd2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron Mg <sub>12</sub>

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

Experimental: powder, film, X-rays,  $T = 298$  K

Remarks: Idealized coordinates. Strukturbericht notation D0<sub>19</sub> was defined on  $\alpha$ -Ni<sub>3</sub>Sn.

References: [1] Edwards D.A., Wallace W.E., Craig R.S. (1952), J. Am. Chem. Soc. 74, 5256-5261. [2] Dehlinger U. (1931), Z. Anorg. Allg. Chem. 194, 223-238. [3] Rahlfs P. (1937), Metallwirtsch. Metallwiss. Metalltech. 16, 343-345. [4] Heal T.J., Williams G.I. (1955), Acta Crystallogr. 8, 494-498.

194  
hP10

**AuVS<sub>2</sub>**

hP10

(194)  $P6_3/mmc$  – edca

**AuVS<sub>2</sub>** [1]

Structural features: Directly superposed close-packed S layers; V in trigonal prismatic voids (partial disorder), Au in linear coordination between S layers. Single S-Au-S linear units.

Gauzzi A. et al. (2002) [1]

**AuS<sub>2</sub>V**

$a = 0.3224$ ,  $c = 1.5039$  nm,  $c/a = 4.665$ ,  $V = 0.1354$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4e	3m.	0	0	0.154		7-vertex polyhedron AuV <sub>6</sub>
V2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.048	tricapped trigonal prism V <sub>3</sub> S <sub>6</sub>
V3	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.952	tricapped trigonal prism V <sub>3</sub> S <sub>6</sub>
Au4	2a	$-3m.$	0	0	0		colinear S <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.040$ ,  $T = 293$  K

Remarks: High-pressure phase. Short interatomic distances for partly occupied site(s). In table II of [1] the Wyckoff position of former V(2) is misprinted as  $2c$  instead of  $2d$ .

References: [1] Gauzzi A., Gilioli E., Licci F., Marezio M., Calestani G., Franchini C., Massidda S. (2002), Phys. Rev. B: Condens. Matter 66, 085106: 1-7.

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hP10

$\text{La}_2\text{O}_3$	<i>hP10</i>	(194) $P6_3/mmc - f^2a$
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### **$\text{La}_2\text{O}_3$ form H [2]**

Structural features: Close-packed La layers in h stacking (split site); O in octahedral and tetrahedral voids. Variant of  $\text{YH}_{0.18}$  with site splitting.

Aidebert P., Traverse J.P. (1979) [1]

$\text{LaO}_{1.50}$

$a = 0.4057$ ,  $c = 0.6430$  nm,  $c/a = 1.585$ ,  $V = 0.0917$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
La1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.248	0.5	
O2	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.649	0.5	single atom O
O3	$2a$	$-3m.$	0	0	0	0.5	octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $R = 0.028$ ,  $T = 2303$  K

Remarks: Phase stable at approximately  $2273 < T < 2373$  K. Short interatomic distances for partly occupied site(s).

References: [1] Aidebert P., Traverse J.P. (1979), Mater. Res. Bull. 14, 303-323. [2] Müller Buschbaum H., Von Schnering H.G. (1965), Z. Anorg. Allg. Chem. 340, 232-245.

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hP10

$(\text{Eu}_{0.5}\text{Gd}_{0.5})\text{PtP}$	<i>hP10</i>	(194) $P6_3/mmc - f^2a$
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### **$\text{Eu}_{0.5}\text{Gd}_{0.5}\text{PtP}$ [1]; $\text{EuPdAs } \alpha$ [2]**

Structural features: 3D-framework of fused  $(\text{Eu,Gd})_6$  trigonal prisms centered alternatively by Pt and P (both displaced from the prism centers). Variant of  $\text{ZrBeSi}$  with site splitting.

Lux C. et al. (1991) [1]

$\text{Eu}_{0.50}\text{Gd}_{0.50}\text{PPt}$

$a = 0.4114$ ,  $c = 0.8156$  nm,  $c/a = 1.982$ ,  $V = 0.1195$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Pt1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.2391	0.5	
P2	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.7351	0.5	
M3	$2a$	$-3m.$	0	0	0		

$\text{M3} = 0.5\text{Eu} + 0.5\text{Gd}$

Experimental: powder, diffractometer, X-rays,  $R = 0.016$

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

References: [1] Lux C., Mewis A., Lossau N., Michels G., Schlabititz W. (1991), Z. Anorg. Allg. Chem. 593, 169-180. [2] Johrendt D., Mewis A. (1992), J. Alloys Compd. 183, 210-223.

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hP10

$\text{Pt}_2\text{Sn}_3$	<i>hP10</i>	(194) $P6_3/mmc - \bar{1}^2b$
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**Pt<sub>2</sub>Sn<sub>3</sub>** [1], Strukturbericht notation D5<sub>b</sub>

Structural features: Close-packed Sn layers in hc<sub>2</sub> stacking; Pt in octahedral voids leaving the interstices between c-stacked layers vacant. Units of two interpenetrating Pt(PtSn<sub>7</sub>) cubes share edges to form a 3D-framework.

Schubert K., Pfisterer H. (1949) [1]

 $\text{Pt}_2\text{Sn}_3$  $a = 0.4334$ ,  $c = 1.2966$  nm,  $c/a = 2.992$ ,  $V = 0.2109$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Pt1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.143		square prism (cube) Sn <sub>7</sub> Pt
Sn2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.570		fourcapped trigonal prism Pt <sub>4</sub> Sn <sub>6</sub>
Sn3	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		cuboctahedron Pt <sub>6</sub> Sn <sub>6</sub>

Experimental: single crystal, rotation photographs, X-rays

Remarks: In [1] the cell parameters are expressed in kX instead of Å as indicated (see [2]). In the summary of [1] the *z*-coordinate of the Sn site in Wyckoff position 4*f* is misprinted as 0.070 instead of -0.070 (given on page 40; checked on interatomic distances).

References: [1] Schubert K., Pfisterer H. (1949), Z. Metallkd. 40, 405-411. [2] (1951), Structure Reports 11, 176.

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hP10

$\text{NbAl}_{0.33}\text{Se}_2$	<i>hP10</i>	(194) $P6_3/mmc - \bar{1}^2b$
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**Al<sub>0.33</sub>NbSe<sub>2</sub>** [1]

Structural features: Close-packed Se layers in AABB stacking; Nb in trigonal prismatic, Al in tetrahedral voids. NbSe<sub>6</sub> trigonal prisms share edges to form infinite slabs.

Voorhoeve Van Den Berg J.M. (1972) [1]

 $\text{Al}_{0.33}\text{NbSe}_2$  $a = 0.3456$ ,  $c = 1.2822$  nm,  $c/a = 3.710$ ,  $V = 0.1326$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Se1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.125		7-vertex polyhedron Al <sub>4</sub> Nb <sub>3</sub>
Al2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.548	0.167	7-vertex polyhedron Se <sub>4</sub> Al <sub>3</sub>
Nb3	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>

Experimental: powder, film, X-rays

Remarks: In [1] the Hermann-Mauguin symbol for the space group is misprinted as  $P6_3mmc$  instead of  $P6_3/mmc$ .

References: [1] Voorhoeve Van Den Berg J.M. (1972), J. Less-Common Met. 26, 399-402.

194  
hP10

$\text{Sc}_2\text{SO}_2$	<i>hP10</i>	(194) $P6_3/mmc - \bar{1}^2b$
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**Sc<sub>2</sub>O<sub>2</sub>S** [1]

Structural features: Close-packed Sc layers in AABBB stacking; S in trigonal prismatic, O in tetrahedral voids.

Julien Pouzol M. et al. (1978) [1]

$\text{O}_2\text{SSc}_2$

$a = 0.35196$ ,  $c = 1.2519$  nm,  $c/a = 3.557$ ,  $V = 0.1343$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Sc1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.10702		7-vertex polyhedron $\text{O}_4\text{S}_3$
O2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5661		tetrahedron $\text{Sc}_4$
S3	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism $\text{Sc}_6$

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

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

References: [1] Julien Pouzol M., Jaulmes S., Guittard M., Laruelle P. (1978), J. Solid State Chem. 26, 185-188.

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hP10

$\text{W}_{2.3}\text{N}_2$	hP10	(194) $P6_3/mmc - f^2c$
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**WN<sub>0.87</sub>** [1]

Structural features: Close-packed W layers (vacancies ignored) in AAABBB stacking; N in trigonal prismatic voids.  $\text{NW}_6$  trigonal prisms share triangular faces and edges to form double slabs.

Khitrova V.I., Pinsker Z.G. (1958) [1]

$\text{N}_2\text{W}_{2.30}$

$a = 0.289$ ,  $c = 1.530$  nm,  $c/a = 5.294$ ,  $V = 0.1107$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
W1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.06	0.65	trigonal prism $\text{N}_3\text{W}_3$
N2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.66		trigonal prism $\text{W}_6$
W3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $\text{N}_6$

Experimental: thin film, electron diffraction,  $R = 0.195$

Remarks: A similar model with N in Wyckoff position 4e was tested and rejected. The same data are also reported in [2]. In [1] the  $z$ -coordinate of the N site is misprinted as 0.16 (idealized value 9.5/60) instead of -0.16 (-9.5/60) (from the drawing in fig. 4 and [2]).

References: [1] Khitrova V.I., Pinsker Z.G. (1958), Sov. Phys. Crystallogr. 3, 551-558. [2] Khitrova V.I., Pinsker Z.G. (1962), Sov. Phys. Crystallogr. 6, 712-719 (Kristallografiya 6, 882-891).

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hP10

$\text{Ru}_2\text{B}_3$	hP10	(194) $P6_3/mmc - f^2c$
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**Ru<sub>2</sub>B<sub>3</sub>** [2]

Structural features: Infinite slabs of edge-linked  $\text{BRu}_6$  trigonal prisms (no B-B contact) and puckered hexagon-mesh B layers alternate along [001].

Lundström T. (1969) [1]

$\text{B}_3\text{Ru}_2$

$a = 0.29051$ ,  $c = 1.28125$  nm,  $c/a = 4.410$ ,  $V = 0.0937$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0278		non-coplanar triangle B <sub>3</sub>
Ru2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.639855		7-vertex polyhedron B <sub>7</sub>
B3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Ru <sub>6</sub>

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

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

Remarks: No significant electron density was detected in Wyckoff position 2a or 2b. Refinement of the occupancy of site B1 showed no significant deviation from unity.

References: [1] Lundström T. (1969), Ark. Kemi 30, 115-127. [2] Lundström T. (1967), Colloq. Int. Propr. Thermodyn. Derivés Semi-Métall., Orsay (France) 1965, pp. 91-93.

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hP10

Cu <sub>0.65</sub> NbS <sub>2</sub>	hP10	(194) <i>P6<sub>3</sub>/mmc</i> – <i>f</i> <sup>2</sup> c
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**Cu<sub>0.6</sub>NbS<sub>2</sub>** [2]; Ag<sub>0.6</sub>NbS<sub>2</sub> (see remark)

Structural features: Close-packed S layers in AABBB stacking; Nb in trigonal prismatic, Cu in tetrahedral voids. NbS<sub>6</sub> trigonal prisms share edges to form infinite slabs. Filled-up derivative of MoS<sub>2</sub> 2H.

Kars M. et al. (1995) [1]

Cu<sub>0.50</sub>NbS<sub>2</sub>

*a* = 0.33455, *c* = 1.3016 nm, *c/a* = 3.891, *V* = 0.1262 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0344	0.25	7-vertex polyhedron Cu <sub>3</sub> S <sub>4</sub>
S2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.63044		7-vertex polyhedron Cu <sub>4</sub> Nb <sub>3</sub>
Nb3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron S <sub>6</sub> Cu <sub>2</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). Average structure for Ag<sub>0.6</sub>NbS<sub>2</sub>; the incommensurately modulated low-temperature structure is studied in [3].

References: [1] Kars M., Kheit M., Rebbah H., Rebbah A. (1995), Ann. Chim. (Paris) 20, 47-52. [2] Koerts K. (1963), Acta Crystallogr. 16, 432-433. [3] Van Der Lee A., Van Smaalen S., Wiegers G.A., De Boer J.L. (1991), Phys. Rev. B: Condens. Matter 43, 9420-9430.

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hP10

Be <sub>3</sub> N <sub>2</sub>	hP10	(194) <i>P6<sub>3</sub>/mmc</i> – <i>fcba</i>
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**Be<sub>3</sub>N<sub>2</sub> β** [1]

Structural features: Close-packed N layers in hc stacking; Be in tetrahedral and trigonal voids. Close-packed Be layers in hc<sub>2</sub> stacking; N in octahedral and trigonal bipyramidal voids.

Eckertlin P., Rabenau A. (1960) [1]

Be<sub>3</sub>N<sub>2</sub>

*a* = 0.28413, *c* = 0.9693 nm, *c/a* = 3.411, *V* = 0.0678 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Be1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.075		tetrahedron N <sub>4</sub>
N2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid Be <sub>5</sub>

Be3	2b	-6m2	0	0	$\frac{1}{4}$	coplanar triangle N <sub>3</sub>
N4	2a	-3m.	0	0	0	octahedron Be <sub>6</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.132

Remarks: Phase stable at T > ~1673 K. Splitting of site Be3 is proposed in [2] (same sample studied).

References: [1] Eckerlin P., Rabenau A. (1960), Z. Anorg. Allg. Chem. 304, 218-229. [2] Hall D., Gurr G.E., Jeffrey G.A. (1969), Z. Anorg. Allg. Chem. 369, 108-112.

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hP10

YAlO <sub>3</sub>	hP10	(194) P6 <sub>3</sub> /mmc – fcba
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**YAlO<sub>3</sub> hexagonal** [1]; InMnO<sub>3</sub> [2]

Structural features: Close-packed O layers in hc<sub>2</sub> stacking; Y in octahedral, Al in trigonal bipyramidal voids. AlO<sub>5</sub> trigonal bipyramids share vertices to form infinite slabs.

Bertaut F., Mareschal J. (1963) [1]

AlO<sub>3</sub>Y

$a = 0.368$ ,  $c = 1.052$  nm,  $c/a = 2.859$ ,  $V = 0.1234$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.077		single atom Al
Al2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>
O3	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle Al <sub>3</sub>
Y4	2a	-3m.	0	0	0		square prism (cube) O <sub>8</sub>

Experimental: powder, film, X-rays, R = 0.024

Remarks: Phase stable at T < 1223 K [1].

References: [1] Bertaut F., Mareschal J. (1963), C. R. Hebd. Seances Acad. Sci. 257, 867-870. [2] Giaquinta D.M., Zur Loye H.C. (1992), J. Am. Chem. Soc. 114, 10952-10953.

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hP10

Na <sub>0.5</sub> CoO <sub>2</sub>	hP10	(194) P6 <sub>3</sub> /mmc – fcba
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**Na<sub>0.5</sub>CoO<sub>2</sub>** [2]; K<sub>0.5</sub>CoO<sub>2</sub> [5]; K<sub>0.5</sub>Zr<sub>0.5</sub>In<sub>0.5</sub>S<sub>2</sub> [3]

Structural features: Close-packed O layers in AAB<sub>B</sub> stacking; Co in octahedral, Na in trigonal prismatic voids (disordered vacancies for the latter).

Nakatsugawa H., Nagasawa K. (2004) [1]

CoNa<sub>0.78</sub>O<sub>2</sub>

$a = 0.2831$ ,  $c = 1.09$  nm,  $c/a = 3.85$ ,  $V = 0.0757$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5898		non-coplanar triangle Co <sub>3</sub>
Na2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.5	
Na3	2b	-6m2	0	0	$\frac{1}{4}$	0.28	
Co4	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, neutrons, R = 0.035

Remarks: Phase referred to as  $\gamma$ -Na<sub>x</sub>CoO<sub>2</sub>. Structure type referred to as P2-type (alkaline cation in Prismatic coordination, 2 TO<sub>2</sub> slabs in the translation unit) layered bronze [4]. Short interatomic distances for partly occupied site(s). The description in space group (182)  $P6_322$  in [2] does not take into consideration all symmetry elements of the proposed structure; the same is true for the description of K<sub>0.5</sub>CoO<sub>2</sub> in [5]. The similar structure proposal reported for K<sub>0.5</sub>CoO<sub>2</sub> in [5] describes the average structure; different superstructure reflections were observed for different crystals.

References: [1] Nakatsugawa H., Nagasawa K. (2004), J. Solid State Chem. 177, 1137-1145. [2] Jansen M., Hoppe R. (1974), Z. Anorg. Allg. Chem. 408, 104-106. [3] Wu P., Ibers J.A. (1993), Acta Crystallogr. C 49, 126-129. [4] Fouassier C., Delmas C., Hagenmuller P. (1975), Mater. Res. Bull. 10, 443-449. [5] Jansen M., Hoppe R. (1974), Z. Anorg. Allg. Chem. 408, 97-103.

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hP10

Ho <sub>2</sub> NiAs <sub>2</sub>	hP10	(194) $P6_3/mmc$ – fcba
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**Ho<sub>2</sub>NiAs<sub>2</sub>** [1]; Zr<sub>2</sub>NiAs<sub>2</sub> [1]

Structural features: As layers in hc stacking; Ho in octahedral, Ni in trigonal voids in h-stacked layers. NiAs<sub>3</sub> trigonal units share vertices to form infinite layers.

El Ghadraoui E.H. et al. (1988) [1]

As<sub>2</sub>Ho<sub>2</sub>Ni

$a = 0.4091$ ,  $c = 1.3857$  nm,  $c/a = 3.387$ ,  $V = 0.2008$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ho1	4f	3m.	1/3	2/3	0.61751		9-vertex polyhedron As <sub>6</sub> Ni <sub>3</sub>
As2	2c	-6m2	1/3	2/3	1/4		tricapped trigonal prism Ni <sub>3</sub> Ho <sub>6</sub>
Ni3	2b	-6m2	0	0	1/4		coplanar triangle As <sub>3</sub>
As4	2a	-3m.	0	0	0		octahedron Ho <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.039

References: [1] El Ghadraoui E.H., Pivan J.Y., Guérin R., Sergent M. (1988), Mater. Res. Bull. 23, 891-898.

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hP10

TbNiSiH <sub>1.78</sub>	hP10	(194) $P6_3/mmc$ – fdca
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**TbNiSiH<sub>1.78</sub>** [1]

Structural features: Filled-up derivative of ZrBeSi with H in tetrahedral (Tb<sub>3</sub>Ni) voids.

Brinks H.W. et al. (2001) [1]

D<sub>1.78</sub>NiSiTb

$a = 0.40371$ ,  $c = 0.79756$  nm,  $c/a = 1.976$ ,  $V = 0.1126$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	4f	3m.	1/3	2/3	0.0466	0.889	single atom Ni
Si2	2d	-6m2	1/3	2/3	3/4		trigonal bipyramid Ni <sub>3</sub> D <sub>2</sub>
Ni3	2c	-6m2	1/3	2/3	1/4		colinear D <sub>2</sub>
Tb4	2a	-3m.	0	0	0		octahedron D <sub>6</sub>

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.038, T = 293 K



Remarks: Space group (62) *Pnma* (TiNiSi type) was tested and rejected. Refinements on data collected at 50 and 100 K are reported in [2].

References: [1] Brinks H.W., Yartys V.A., Hauback B.C. (2001), *J. Alloys Compd.* 322, 160-165. [2] Brinks H.W., Yartys V.A., Hauback B.C., Fjellvag H., Ouladdiaf B. (2002), *J. Alloys Compd.* 340, 62-66.

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*hP10*

$\text{Na}_{0.5}\text{NbS}_2$	<i>hP10</i>	(194) <i>P6<sub>3</sub>/mmc</i> – fec
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### **$\text{Na}_{0.5}\text{NbS}_2$ [1]**

Structural features: Directly superposed close-packed S layers; Nb and Na occupy trigonal prismatic voids in alternating interlayers (ordered arrangement for the former, partly disordered for the latter).  $\text{NbS}_6$  trigonal prisms share edges to form infinite slabs.

Gareh J.E. et al. (1995) [1]

$\text{Na}_{0.64}\text{NbS}_2$

$a = 0.3352$  nm,  $c = 1.4552$  nm,  $c/a = 4.341$ ,  $V = 0.1416$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Na1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.51	0.32	non-coplanar triangle Na <sub>3</sub>
S2	4 <i>e</i>	3 <i>m</i> .	0	0	0.1435		non-coplanar triangle Nb <sub>3</sub>
Nb3	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism S <sub>6</sub>

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

Remarks: Homogeneity range  $\text{Na}_x\text{NbS}_2$ ,  $0.25 < x < 1.0$ . Refinement of the occupancy of the S site showed no significant deviation from unity. Short interatomic distances for partly occupied site(s). A refinement on diffraction data collected at 150 K is reported in [2].

References: [1] Gareh J.E., Barker M.G., Begley M.I. (1995), *Mater. Res. Bull.* 30, 57-63. [2] Salyer P.A., Barker M.G., Blake A.J., Gregory D.H., Weston D.P., Wilson C. (2003), *J. Mater. Chem.* 13, 175-180.

194  
*hP10*

$\text{Gd}_2\text{Fe}_2\text{I}$	<i>hP10</i>	(194) <i>P6<sub>3</sub>/mmc</i> – fec
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### **$\text{Gd}_2\text{Fe}_2\text{I}$ [1]**

Structural features: Close-packed Gd and I layers in AAB'AAC' stacking (B',C'= I); Fe in trigonal prismatic voids between Gd layers.  $\text{FeGd}_6$  trigonal prisms share faces to form infinite slabs. See Fig. III.14.

Ruck M., Simon A. (1993) [1]

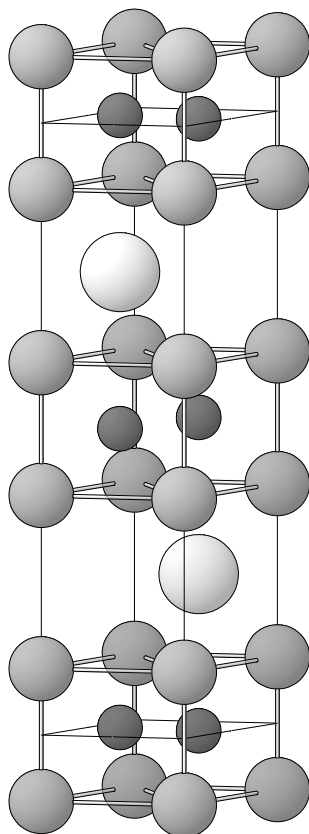
$\text{Fe}_2\text{Gd}_2\text{I}$

$a = 0.40143$  nm,  $c = 1.718$  nm,  $c/a = 4.280$ ,  $V = 0.2398$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.506		tricapped trigonal prism Fe <sub>3</sub> Gd <sub>6</sub>
Gd2	4 <i>e</i>	3 <i>m</i> .	0	0	0.1084		16-vertex polyhedron Fe <sub>6</sub> I <sub>3</sub> Gd <sub>7</sub>
I3	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Gd <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.016$

Fig. III.14. **Gd<sub>2</sub>Fe<sub>2</sub>I**

Arrangement of Gd<sub>6</sub> trigonal prisms (Gd atoms medium) centered by Fe atoms (small), and I atoms (large).

References: [1] Ruck M., Simon A. (1993), Z. Anorg. Allg. Chem. 619, 327-336.

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hP10

Ni <sub>2</sub> SbTe <sub>2</sub>	hP10	(194) <i>P6<sub>3</sub>/mmc – fec</i>
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### Ni<sub>2</sub>SbTe<sub>2</sub> [1]

Structural features: Close-packed Sb and Te layers in h stacking; Ni in octahedral (Sb<sub>3</sub>Te<sub>3</sub>) voids. Layer structure with sandwiches consisting of 5 sublayers (Te-Ni(o)-Sb-Ni(o)-Te).

Reynolds T.K. et al. (2004) [1]

Ni<sub>2</sub>SbTe<sub>2</sub>

$a = 0.3903$ ,  $c = 1.5634$  nm,  $c/a = 4.006$ ,  $V = 0.2063$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Te1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.58729		non-coplanar triangle Ni <sub>3</sub>
Ni2	4 <i>e</i>	3 <i>m</i> .	0	0	0.1658		7-vertex polyhedron Te <sub>3</sub> Sb <sub>3</sub> Ni
Sb3	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Ni <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.047$ ,  $T = 165$  K

References: [1] Reynolds T.K., Kelley R.F., DiSalvo F.J. (2004), J. Alloys Compd. 366, 136-144.

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hP10

BaNiO <sub>3</sub>	hP10	(194) <i>P6<sub>3</sub>/mmc – hda</i>
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**BaNiO<sub>3</sub>** [2], perovskite 2H; BaTiS<sub>3</sub> [4]; BaVS<sub>3</sub> rt [5]; CsNiCl<sub>3</sub> [3]; Mn<sub>3</sub>PtN<sub>0.25</sub> [6]; Mn<sub>3</sub>RhN<sub>0.20</sub> [6]; NaBa<sub>3</sub>N [7]

Structural features: Close-packed BaO<sub>3</sub> layers in h stacking; Ni in octahedral (O<sub>6</sub>) voids. NiO<sub>6</sub> octahedra share faces to form infinite columns (linear -Ni- chains). See Fig. III.15.

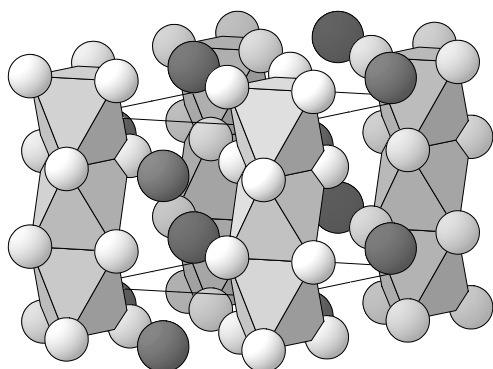


Fig. III.15. **BaNiO<sub>3</sub>**

Arrangement of NiO<sub>6</sub> octahedra (O atoms light) and Ba atoms (dark).

Takeda Y. et al. (1976) [1]

BaNiO<sub>3</sub>

$a = 0.5629$ ,  $c = 0.4811$  nm,  $c/a = 0.855$ ,  $V = 0.1320$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	$mm2$	0.1462	0.2924	$\frac{1}{4}$		non-colinear Ni <sub>2</sub>
Ba2	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>
Ni3	2a	$-3m.$	0	0	0		octahedron O <sub>6</sub>

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

Remarks: In [2] the  $z$ -coordinates of the Ba positions are interchanged (from the projection of the structure). The description in space group (186)  $P6_3mc$  in [2] does not take into consideration all symmetry elements of the proposed structure. The same is true for the description of BaTiS<sub>3</sub> in [3] (see [9]). We assume that the refinement of BaNiO<sub>3</sub> in the same space group in [8] is also superseded.

References: [1] Takeda Y., Kanamaru F., Shimada M., Koizumi M. (1976), Acta Crystallogr. B 32, 2464-2466. [2] Lander J.J. (1951), Acta Crystallogr. 4, 148-156. [3] Tishchenko G.N. (1955), Tr. Inst. Kristallogr., Akad. Nauk SSSR 11, 93-96. [4] Clearfield A. (1963), Acta Crystallogr. 16, 135-142. [5] Gardner R.A., Vlasse M., Wold A. (1969), Acta Crystallogr. B 25, 781-787. [6] Kren E., Kadar G., Barberon M., Fruchart R. (1971), Int. J. Magn. 1, 341-345. [7] Rauch P.E., Simon A. (1992), Angew. Chem. Int. Ed. 31, 1519-1521 (Angew. Chem. 104, 1505-1506). [8] Krischner H., Torkar K., Kolbesen B.O. (1971), J. Solid State Chem. 3, 349-357. [9] Huster J. (1980), Z. Naturforsch. B 35, 775.

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*hP10*

LiI[H<sub>2</sub>O]<sub>3</sub>

*hP10*

(194)  $P6_3/mmc - hda$

**LiI·3H<sub>2</sub>O** [1]

Structural features: Close-packed I(OH<sub>2</sub>)<sub>3</sub> layers in h stacking; Li in octahedral voids surrounded by six H<sub>2</sub>O. Li(OH<sub>2</sub>)<sub>6</sub> octahedra share faces to form infinite chains.

West C.D. (1934) [1]

H<sub>6</sub>ILiO<sub>3</sub>

$a = 0.745$ ,  $c = 0.545$  nm,  $c/a = 0.732$ ,  $V = 0.2620$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH <sub>2</sub> )1	6h	mm2	0.142	0.284	$\frac{1}{4}$		non-colinear Li <sub>2</sub>
I2	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron (OH <sub>2</sub> ) <sub>12</sub>
Li3	2a	-3m.	0	0	0		octahedron (OH <sub>2</sub> ) <sub>6</sub>

Transformation from published data (*P6<sub>3</sub>mc*): origin shift 0 0  $\frac{1}{4}$

Remarks: Cell parameters from [2]. The description in space group (186) *P6<sub>3</sub>mc* in [1] does not take into consideration all symmetry elements of the proposed structure. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] West C.D. (1934), Z. Kristallogr. 88, 198-204. [2] Hendricks S.B. (1928), Am. J. Sci. 15, 403-409.

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hP12

MoC <sub>0.67</sub>	hP12	(194) <i>P6<sub>3</sub>/mmc</i> – f <sup>2</sup> ba
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### MoC<sub>1-x</sub> η [1]

Structural features: Close-packed Mo layers in hc<sub>2</sub> stacking; C in octahedral voids.

Nowotny H. et al. (1954) [1]

CMo

$a = 0.301$ ,  $c = 1.461$  nm,  $c/a = 4.854$ ,  $V = 0.1146$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.16667		octahedron Mo <sub>6</sub>
Mo2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.58333		octahedron C <sub>6</sub>
Mo3	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism C <sub>6</sub>
C4	2a	-3m.	0	0	0		octahedron Mo <sub>6</sub>

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

Experimental: powder, film, X-rays

Remarks: Phase stable at  $T > 1920$  K. Idealized coordinates. Composition MoC, indicated in [1], was later corrected to MoC<sub>1-x</sub>,  $0.33 < x < 0.42$  (see [2] and [3]). In [1] the Wyckoff position of the first Mo site is misprinted as 2a instead of 2b.

References: [1] Nowotny H., Parthé E., Kieffer R., Benesovsky F. (1954), Monatsh. Chem. 85, 255-272. [2] Rudy E., Windisch S., Stosick A.J., Hoffman J.R. (1967), Trans. Metall. Soc. AIME 239, 1247-1267. [3] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163.

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hP12

TaSe <sub>2</sub>	hP12	(194) <i>P6<sub>3</sub>/mmc</i> – f <sup>2</sup> ba
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### TaSe<sub>2</sub> 4H<sub>b</sub> [2]

Structural features: Close-packed Se layers in BBCBCCBC stacking; Ta in trigonal prismatic and octahedral voids (BaB CaB CaC BaC). Layer structure with two kinds of sandwich consisting of three sublayers each (Se-Ta-Se for both).

Brown B.E., Beerntsen D.J. (1965) [1]

Se<sub>2</sub>Ta

$a = 0.346$ ,  $c = 2.518$  nm,  $c/a = 7.277$ ,  $V = 0.2611$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.184		non-coplanar triangle Ta <sub>3</sub>
Se2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.565		non-coplanar triangle Ta <sub>3</sub>
Ta3	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>
Ta4	2a	-3m.	0	0	0		octahedron Se <sub>6</sub>

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

Experimental: single crystal, precession photographs, X-rays, R = 0.143

Remarks: Phase stable at T > 600 K; average structure below this temperature The commensurate superstructure stable at 75 < T < 410 K ( $a = \sqrt{13} \cdot a_0$ ,  $c = c_0$ ) was refined in 5D superspace, together with the average structure, in [3].

References: [1] Brown B.E., Beerntsen D.J. (1965), Acta Crystallogr. 18, 31-36. [2] Kaduk F., Huisman R., Jellinek F. (1964), Recl. Trav. Chim. Pays-Bas 83, 768-775. [3] Lüdecke J., Van Smaalen S., Spijkerman A., De Boer J.L., Wiegers G.A. (1999), Phys. Rev. B: Condens. Matter 59, 6063-6071.

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hP12

YPtAs	hP12	(194) $P6_3/mmc - f^2ba$
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**YPtAs** [1]; CaGaGe [2]; Tb<sub>1-x</sub>NiP [3]

Structural features: 3D-framework of fused PtY<sub>6</sub> and AsY<sub>6</sub> trigonal prisms (units of two base-linked AsY<sub>6</sub> prisms share edges to form a 3D-framework, the same is true for the PtY<sub>6</sub> prisms). Approximately planar hexagon-mesh PtAs layers. Substitution derivative of AlB<sub>2</sub>. See Fig. III.16.

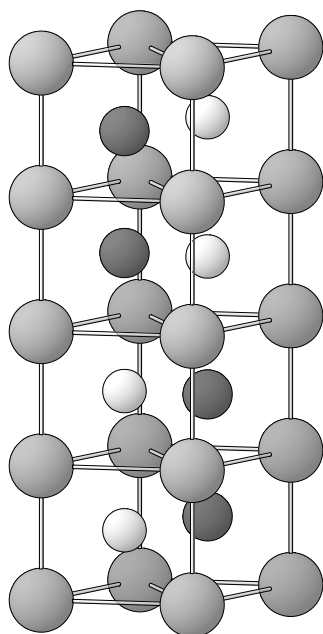


Fig. III.16. **YPtAs**

Arrangement of Y<sub>6</sub> trigonal prisms (Y atoms large) centered by Pt (dark) and As (light) atoms.

Wenski G., Mewis A. (1986) [1]

AsPtY

$a = 0.425$ ,  $c = 1.5165$  nm,  $c/a = 3.568$ ,  $V = 0.2372$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pt1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1365		non-coplanar triangle As <sub>3</sub>
As2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6204		tricapped trigonal prism Pt <sub>3</sub> Y <sub>6</sub>
Y3	2b	-6m2	0	0	$\frac{1}{4}$		pseudo Frank-Kasper Pt <sub>6</sub> As <sub>6</sub> Y <sub>8</sub>
Y4	2a	-3m.	0	0	0		pseudo Frank-Kasper As <sub>6</sub> Pt <sub>6</sub> Y <sub>8</sub>

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

References: [1] Wenski G., Mewis A. (1986), Z. Kristallogr. 176, 125-134. [2] Czybulka A., Pinger B., Schuster H.U. (1989), Z. Anorg. Allg. Chem. 579, 151-157. [3] Chikhrii S.I., Orishchin S.V., Kuz'ma Y.B. (1987), Russ. J. Inorg. Chem. 32, 1386-1388 (Zh. Neorg. Khim. 32, 2375-2379).

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hP12

Ti <sub>3</sub> SiC <sub>2</sub>	hP12	(194) $P6_3/mmc - f^2ba$
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### Ti<sub>3</sub>SiC<sub>2</sub> [2]

Structural features: Close-packed Ti and Si layers in h<sub>3</sub>c stacking; C in octahedral (Ti<sub>6</sub>) voids. CTi<sub>6</sub> octahedra share edges to form infinite double slabs. See Fig. III.17.

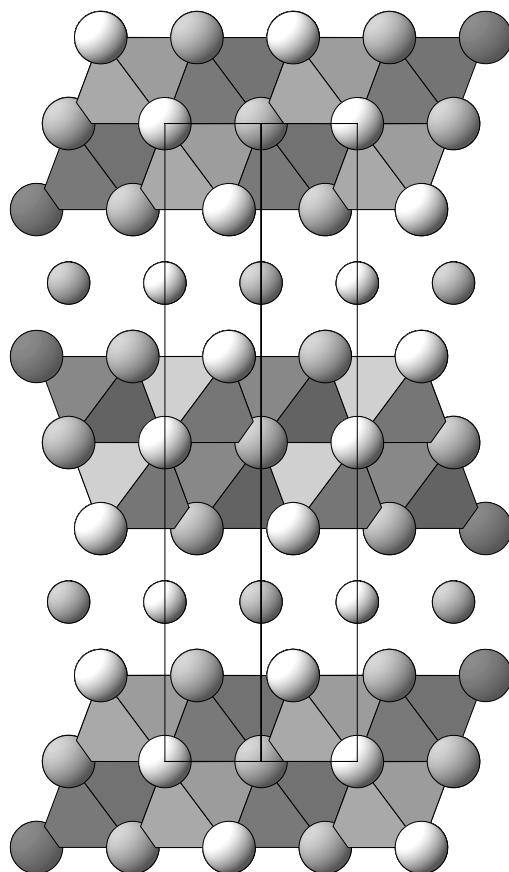


Fig. III.17. Ti<sub>3</sub>SiC<sub>2</sub>

Arrangement of CTi<sub>6</sub> octahedra (Ti atoms large) and Si atoms (small) viewed along [110].

Rawns C.J. et al. (2000) [1]

C<sub>2</sub>SiTi<sub>3</sub>

$a = 0.30654$ ,  $c = 1.7635$  nm,  $c/a = 5.753$ ,  $V = 0.1435$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1348		non-coplanar triangle C <sub>3</sub>
C2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.57244		octahedron Ti <sub>6</sub>
Si3	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron Ti <sub>6</sub> Si <sub>6</sub>
Ti4	2a	-3m.	0	0	0		octahedron C <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.073$

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

References: [1] Rawn C.J., Payzant E.A., Hubbard C.R., Barsoum M.W., El Raghy T. (2000), Mater. Sci. Forum 321/324, 889-892. [2] Jeitschko W., Nowotny H. (1967), Monatsh. Chem. 98, 329-337.

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hP12

Ni <sub>1.2</sub> (Te <sub>0.82</sub> Se <sub>0.18</sub> )	hP12	(194) $P6_3/mmc - f^2ca$
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**Ni<sub>0.55</sub>Te<sub>0.37</sub>Se<sub>0.08</sub>** [1]

Structural features: Close-packed (Te,Se) layers in hc stacking; Ni in tetrahedral and octahedral voids (partial disorder).

Haugsten K., Rost E. (1972) [1]

Ni<sub>1.20</sub>Se<sub>0.18</sub>Te<sub>0.82</sub>

$a = 0.3836$ ,  $c = 1.224$  nm,  $c/a = 3.191$ ,  $V = 0.1560$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.053	0.40	pseudo Frank-Kasper Te <sub>4</sub> Ni <sub>7</sub>
Ni2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.646	0.80	11-vertex polyhedron Ni <sub>5</sub> Te <sub>6</sub>
M3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron Ni <sub>8</sub>
M4	2a	-3m.	0	0	0		cuboctahedron Ni <sub>12</sub>

M3 = 0.822Te + 0.178Se; M4 = 0.822Te + 0.178Se

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.075$

Remarks: In table 1 of [1] the Wyckoff position of former (Se,Te)1 is misprinted as 2b instead of 2a; the stacking of close-packed layers is erroneously stated to be ABCABC instead of ABAC.

References: [1] Haugsten K., Rost E. (1972), Acta Chem. Scand. 26, 410-411.

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hP12

WB <sub>2</sub>	hP12	(194) $P6_3/mmc - f^2cb$
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**WB<sub>2</sub> ht** [1]

Structural features: Infinite slabs of face-linked BW<sub>6</sub> trigonal prisms (planar hexagon-mesh B layers) and puckered hexagon-mesh B layers alternate along [001].

Lundström T. (1969) [1]

B<sub>2</sub>W

$a = 0.29831$ ,  $c = 1.38790$  nm,  $c/a = 4.653$ ,  $V = 0.1070$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0243		non-coplanar triangle B <sub>3</sub>
W2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.63759		10-vertex polyhedron B <sub>10</sub>
B3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism B <sub>3</sub> W <sub>6</sub>

B4      2b   -6m2      0      0       $\frac{1}{4}$       tricapped trigonal prism B<sub>3</sub>W<sub>6</sub>

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

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

Remarks: Phase stable at T > 1693 K. Limiting composition of the so-called ε phase, where Wyckoff position 2a may be partly occupied by additional B.

References: [1] Lundström T. (1969), Ark. Kemi 30, 115-127.

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hP12

YSF      hP12      (194) P6<sub>3</sub>/mmc – fdcba

### YFS β [2]

Structural features: Close-packed Y layers in hc stacking; F in trigonal, S in tetrahedral voids.

Schleid T. (1999) [1]

FSY

a = 0.40513, c = 1.667 nm, c/a = 4.115, V = 0.2369 nm<sup>3</sup>, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.08523		tetrahedron Y <sub>4</sub>
F2	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar hexagon F <sub>3</sub> Y <sub>3</sub>
Y3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron F <sub>6</sub> S <sub>2</sub>
F4	2b	-6m2	0	0	$\frac{1}{4}$		coplanar hexagon F <sub>3</sub> Y <sub>3</sub>
Y5	2a	-3m.	0	0	0		octahedron S <sub>6</sub>

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

Remarks: Structure type referred to as B-type rare-earth fluoride sulfide.

References: [1] Schleid T. (1999), Z. Anorg. Allg. Chem. 625, 1700-1706. [2] Rysanek N., Loye O. (1973), Acta Crystallogr. B 29, 1567-1569.

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hP12

ThI<sub>2</sub>      hP12      (194) P6<sub>3</sub>/mmc – feca

### ThI<sub>2</sub> β [1]

Structural features: Close-packed I layers in AABCAACB stacking; Th in octahedral and trigonal prismatic voids (stacking sequence AbA BaC AcA CaB). Layer structure with two kinds of sandwich consisting of three sublayers each (I-Th-I for both). Infinite slabs of edge-linked ThI<sub>6</sub> octahedra and infinite slabs of edge-linked ThI<sub>6</sub> trigonal prisms.

Guggenberger L.J., Jacobson R.A. (1968) [1]

I<sub>2</sub>Th

a = 0.397, c = 3.175 nm, c/a = 7.997, V = 0.4334 nm<sup>3</sup>, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.07128		non-coplanar triangle Th <sub>3</sub>
I2	4e	3m.	0	0	0.17959		non-coplanar triangle Th <sub>3</sub>
Th3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron I <sub>6</sub> Th <sub>6</sub>
Th4	2a	-3m.	0	0	0		cuboctahedron I <sub>6</sub> Th <sub>6</sub>

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



Remarks: Phase stable at  $T > 923$  K.

References: [1] Guggenberger L.J., Jacobson R.A. (1968), Inorg. Chem. 7, 2257-2260.

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hP12

$\text{Be}_3\text{N}_2$	hP12	(194) $P6_3/mmc$ – feca
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### $\text{Be}_3\text{N}_2$ $\beta$ [1]

Structural features: Close-packed N layers in  $hc$  stacking, Be in tetrahedral voids. Close-packed Be layers in  $hc_2$  stacking; N in octahedral and tetrahedral (statistical occupation of two face-sharing tetrahedra) voids.

Hall D. et al. (1969) [1]

$\text{Be}_3\text{N}_2$

$a = 0.28413$ ,  $c = 0.9693$  nm,  $c/a = 3.411$ ,  $V = 0.0678$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Be1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.071	0.5	fourcapped trigonal prism $\text{N}_4\text{Be}_6$
Be2	4e	3m.	0	0	0.205		
N3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron $\text{Be}_8$
N4	2a	-3m.	0	0	0		square prism (cube) $\text{Be}_8$

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

Remarks: Phase stable at  $T > \sim 1673$  K. Short interatomic distances for partly occupied site(s). Space group (186)  $P6_3mc$  was tested and rejected ( $R = 0.093$ ). Supersedes a structure proposal with Be atoms in Wyckoff position  $2b$  instead of  $4e$  [2] (same sample studied).

References: [1] Hall D., Gurr G.E., Jeffrey G.A. (1969), Z. Anorg. Allg. Chem. 369, 108-112. [2] Eckerlin P., Rabenau A. (1960), Z. Anorg. Allg. Chem. 304, 218-229.

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hP12

$\text{Al}_3\text{BC}$	hP12	(194) $P6_3/mmc$ – feca
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### $\text{Al}_3\text{BC}$ [1]

Structural features: Close-packed Al layers in  $hc_2$  stacking; B in octahedral, C in trigonal bipyramidal voids. Variant of  $\text{YAlO}_3$  antitype with site splitting in the close-packed layers.

Meyer F.D., Hillebrecht H. (1997) [1]

$\text{Al}_3\text{BC}$

$a = 0.3484$ ,  $c = 1.15202$  nm,  $c/a = 3.307$ ,  $V = 0.1211$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.07621	0.5	tetrahedron $\text{CB}_3$
Al2	4e	3m.	0	0	0.22948		
C3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron $\text{Al}_6$
B4	2a	-3m.	0	0	0		

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.039$ ,  $T = 293$  K

Remarks: Average structure; additional reflections could be indexed with a 4-fold supercell (new axes  $2a, 2b, c$ ). Short interatomic distances for partly occupied site(s). In table 3 of [1] the occupancy of former Al(2) is misprinted as  $\frac{1}{6}$  instead of  $\frac{1}{2}$  (agreement with the chemical formula).

References: [1] Meyer F.D., Hillebrecht H. (1997), J. Alloys Compd. 252, 98-102.

194  
hP12

CuS	hP12	(194) $P6_3/mmc$ – fedc
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**CuS rt** [2], covellite, Strukturbericht notation B18

Structural features: Close-packed S layers in AABAAC stacking; Cu in tetrahedral and trigonal voids. One S<sub>2</sub> dumbbell for one single S atom. See Fig. III.18.

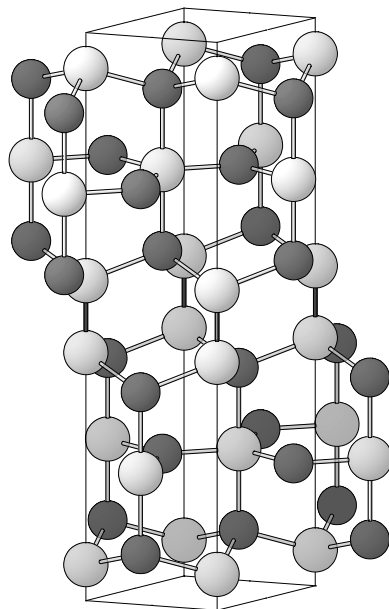


Fig. III.18. **CuS rt**

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

Gotsis H.J. et al. (1992) [1]

CuS

$a = 0.378813$ ,  $c = 1.633307$  nm,  $c/a = 4.312$ ,  $V = 0.2030$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.10737		tetrahedron S <sub>4</sub>
S2	4e	3m.	0	0	0.06329		tetrahedron SCu <sub>3</sub>
Cu3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle S <sub>3</sub>
S4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid Cu <sub>5</sub>

Experimental: powder, diffractometer, neutrons, time-of-flight,  $R_p = 0.040$

Remarks: Supersedes a structure proposal in [3].

References: [1] Gotsis H.J., Barnes A.C., Strange P. (1992), J. Phys.: Condens. Matter 4, 10461-10468.  
[2] Roberts H.S., Ksanda C.J. (1929), Am. J. Sci. 17, 489-503. [3] (1931), Strukturberichte 1, 771.

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hP12

SiO <sub>2</sub>	hP12	(194) $P6_3/mmc$ – gfc
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**SiO<sub>2</sub> tridymite ht** [2], tridymite high, Strukturbericht notation C10

Structural features:  $\text{SiO}_4$  tetrahedra share vertices to form a 3D-framework with channels delimited by 6-rings parallel to  $[001]$ . See Fig. III.19.

Kihara K. et al. (1986) [1]

$\text{O}_2\text{Si}$

$a = 0.5047$ ,  $c = 0.8262$  nm,  $c/a = 1.637$ ,  $V = 0.1823$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6g	$.2/m.$	$\frac{1}{2}$	0	0		colinear $\text{Si}_2$
Si2	4f	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.0621		tetrahedron $\text{O}_4$
O3	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear $\text{Si}_2$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.069$ ,  $T = 693$  K

Remarks: Phase stable at  $T > \sim 680$  K. Space group (20)  $C22_1$  was tested and rejected ( $R = 0.104$ ,  $wR = 0.077$ ; displacive phase transition on cooling).

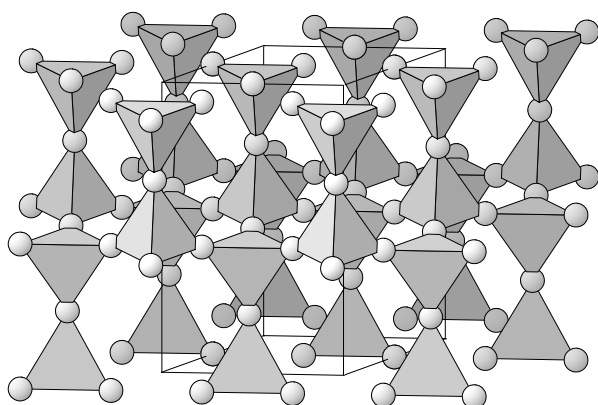


Fig. III.19.  **$\text{SiO}_2$  tridymite ht**

Arrangement of  $\text{SiO}_4$  tetrahedra.

References: [1] Kihara K., Matsumoto T., Imamura M. (1986), Z. Kristallogr. 177, 27-38. [2] (1931), Strukturberichte 1, 171,203.

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*hP12*

$\text{Na}_2[\text{CO}_3]$	<i>hP12</i>	(194) $P6_3/mmc - hdca$
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**$\text{Na}_2\text{CO}_3 \alpha$**  [2];  $\text{K}_2\text{CO}_3 \alpha$  (see remark)

Structural features: Na atoms and  $\text{CO}_3$  trigonal units (perpendicular to  $[001]$ ) in a  $\text{Ni}_2\text{In}$ -type (ht- $\text{Co}_2\text{Ge}$ ) arrangement. See Fig. III.20.

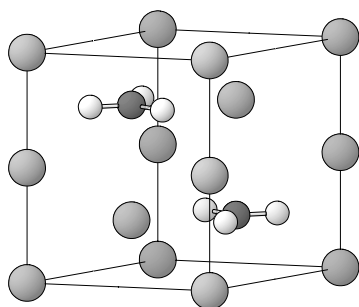


Fig. III.20.  **$\text{Na}_2\text{CO}_3 \alpha$**

Arrangement of  $\text{CO}_3$  triangles (C atoms dark, O atoms light) and Na atoms (large).

Swainson I.P. et al. (1995) [1]

CNa<sub>2</sub>O<sub>3</sub>

$a = 0.52087$ ,  $c = 0.6503$  nm,  $c/a = 1.248$ ,  $V = 0.1528$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	$mm2$	0.2018	0.4036	$1/4$		single atom C
Na2	2d	$-6m2$	$1/3$	$2/3$	$3/4$		coplanar hexagon O <sub>6</sub>
C3	2c	$-6m2$	$1/3$	$2/3$	$1/4$		coplanar triangle O <sub>3</sub>
Na4	2a	$-3m.$	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, neutrons, T = 800 K

Remarks: Phase stable at T > 754 K. A drawing referring to the first determination [2] and isotypic K<sub>2</sub>CO<sub>3</sub> is reported in [3].

References: [1] Swainson I.P., Dove M.T., Harris M.J. (1995), J. Phys.: Condens. Matter 7, 4395-4417. [2] Eysel W. (1971), Thesis, Rh. Westf. Hochschule, Germany. [3] Becht H.Y., Struikmans R. (1976), Acta Crystallogr. B 32, 3344-3346.

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hP12

NaBaPdH <sub>3</sub>	hP12	(194) $P6_3/mmc$ – hdca
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**NaBaPdH<sub>3</sub>** [1]

Structural features: Filled-up derivative of ZrBeSi with H in trigonal (Na<sub>2</sub>Pd) voids. PdH<sub>3</sub> trigonal units.

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

BaD<sub>3</sub>NaPd

$a = 0.60513$ ,  $c = 0.60813$  nm,  $c/a = 1.005$ ,  $V = 0.1929$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	6h	$mm2$	0.169	0.338	$1/4$		single atom Pd
Ba2	2d	$-6m2$	$1/3$	$2/3$	$3/4$		8-vertex polyhedron D <sub>6</sub> Pd <sub>2</sub>
Pd3	2c	$-6m2$	$1/3$	$2/3$	$1/4$		coplanar triangle D <sub>3</sub>
Na4	2a	$-3m.$	0	0	0		octahedron D <sub>6</sub>

Experimental: powder, diffractometer, neutrons, R = 0.055, T = 295 K

References: [1] Olofsson M., Kritikos M., Noréus D. (1998), Inorg. Chem. 37, 2900-2902.

194  
hP12

CsTaTe <sub>3</sub>	hP12	(194) $P6_3/mmc$ – hed
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**CsTaTe<sub>3</sub> rt** [1], perovskite 2H

Structural features: Close-packed CsTe<sub>3</sub> layers in h stacking; Ta in octahedral (Te<sub>6</sub>) voids (displaced from the octahedron centers). Variant of BaNiO<sub>3</sub> with splitting of the octahedral site.

Pell M.A. et al. (1997) [1]

CsTaTe<sub>3</sub>

$a = 0.7992$ ,  $c = 0.6496$  nm,  $c/a = 0.813$ ,  $V = 0.3593$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Te1	6h	$mm2$	0.1642	0.3284	$1/4$		

Ta2	4e	3m.	0	0	0.0506	0.5	
Cs3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron Te <sub>12</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.131, T = 115 K

Remarks: Phase stable at T < ~493 K. Short interatomic distances for partly occupied site(s).

References: [1] Pell M.A., Vajenine G.V.M., Ibers J.A. (1997), J. Am. Chem. Soc. 119, 5186-5192.

194  
hP12

MgZn <sub>2</sub>	hP12	(194) P6 <sub>3</sub> /mmc – hfa
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**MgZn<sub>2</sub>** [2], Laves phase 2H, Friauf phase hexagonal, Strukturbericht notation C14; WFe<sub>2</sub> [3]  
Structural features: Mg(Mg<sub>4</sub>Zn<sub>12</sub>) Friauf polyhedra (Zn<sub>12</sub> truncated tetrahedron + Mg<sub>4</sub> tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. Zn<sub>4</sub> tetrahedra share faces and vertices to form infinite columns parallel to [001]. Kagomé-mesh Zn<sub>3</sub> and puckered triangle-mesh Mg<sub>2</sub>Zn layers alternate along [001]. Laves-type slabs in h stacking. Tetrahedrally close-packed structure (Frank-Kasper phase). See Fig. III.21.

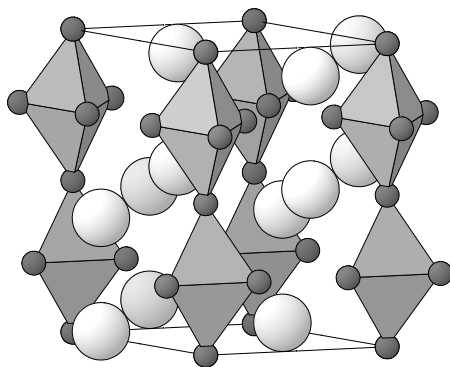


Fig. III.21. **MgZn<sub>2</sub>**

Arrangement of Zn<sub>4</sub> tetrahedra (Zn atoms small) and Mg atoms (large).

Wandahl G., Christensen A.N. (1989) [1]

MgZn<sub>2</sub>

$a = 0.52234$ ,  $c = 0.85562$  nm,  $c/a = 1.638$ ,  $V = 0.2022$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	6h	mm2	0.1697	0.3394	$\frac{1}{4}$		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5629		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Zn3	2a	-3m.	0	0	0		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>

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

Experimental: single crystal, diffractometer, neutrons, R = 0.030

Remarks: Strukturbericht notation C41 was defined on WFe<sub>2</sub>.

References: [1] Wandahl G., Christensen A.N. (1989), Acta Chem. Scand. 43, 296-297. [2] (1931), Strukturberichte 1, 180,228. [3] Arnfelt H., Westgren A. (1935), Jernkontorets Ann. 1935, 185-196.

194  
hP12

Mg <sub>2</sub> Cu <sub>3</sub> Si	hP12	(194) P6 <sub>3</sub> /mmc – hfa
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**Mg<sub>2</sub>Cu<sub>3</sub>Si** rt [1], Laves phase 2H

Structural features:  $\text{Mg}(\text{Mg}_4\text{Cu}_9\text{Si}_3)$  Friauf polyhedra ( $\text{Cu}_9\text{Si}_3$  truncated tetrahedron +  $\text{Mg}_4$  tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. Empty  $\text{Cu}_3\text{Si}$  tetrahedra share vertices and  $\text{Cu}_3$  faces to form infinite columns parallel to  $[001]$ . Ordering variant of  $\text{MgZn}_2$ .

Witte H. (1938) [1]

$\text{Cu}_3\text{Mg}_2\text{Si}$

$a = 0.5004$ ,  $c = 0.7873$  nm,  $c/a = 1.573$ ,  $V = 0.1707$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	6h	mm2	0.1667	0.3334	$\frac{1}{4}$		icosahedron $\text{Si}_2\text{Cu}_4\text{Mg}_6$
Mg2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5625		16-vertex Frank-Kasper $\text{Cu}_9\text{Si}_3\text{Mg}_4$
Si3	2a	-3m.	0	0	0		icosahedron $\text{Cu}_6\text{Mg}_6$

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

Experimental: powder, film, X-rays

Remarks: Phase stable at  $T < 1143$ -1163 K depending on the composition. Ordered  $\text{MgZn}_2$  type stated in [1]; we took idealized values for the refinable coordinates from [2] ( $\text{MgZn}_2$  type).

References: [1] Witte H. (1938), Z. Angew. Mineral. 1, 255-268. [2] (1931), Strukturberichte 1, 180.

194  
hP12

$\text{Ba}_{0.67}\text{Pt}_3\text{B}_2$	hP12	(194) $P6_3/mmc$ – hfa
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**$\text{Ba}_{0.67}\text{Pt}_3\text{B}_2$**  [1]

Structural features: Infinite columns of base-linked  $\text{BPt}_6$  trigonal prisms share edges to form a 3D-framework; no B-B contact. Distorted derivative of  $\text{CeCo}_3\text{B}_2$ .

Shelton R.N. (1978) [1]

$\text{B}_2\text{Ba}_{0.67}\text{Pt}_3$

$a = 0.6161$ ,  $c = 0.5268$  nm,  $c/a = 0.855$ ,  $V = 0.1732$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Pt1	6h	mm2	0.512	0.024	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{B}_4\text{Pt}_6\text{Ba}_4$
B2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.033		7-vertex polyhedron $\text{Pt}_6\text{B}$
Ba3	2a	-3m.	0	0	0	0.67	pseudo Frank-Kasper $\text{Ba}_2\text{Pt}_{12}\text{B}_6$

Experimental: powder, diffractometer, X-rays,  $R = 0.077$

Remarks: Short interatomic distances:  $d(\text{Ba3-Ba3}) = 0.263$  nm. Possibly isotypic with  $\text{Ba}_2\text{Ni}_9\text{B}_6$  with ordered vacancies and 9-fold cell volume [2].

References: [1] Shelton R.N. (1978), J. Less-Common Met. 62, 191-196. [2] Jung W., Quentmeier D. (1980), Z. Kristallogr. 151, 172-174.

194  
hP12

$\text{SbCl}_5$	hP12	(194) $P6_3/mmc$ – hfc
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**$\text{SbCl}_5$  It1** [2];  $\text{PF}_5$  [3]

Structural features: Single  $\text{SbCl}_5$  trigonal bipyramids in a Mg-type (h.c.p.) arrangement. See Fig. III.22.

Haupt S., Seppelt K. (2002) [1]

$\text{Cl}_5\text{Sb}$

$a = 0.7414$ ,  $c = 0.794$  nm,  $c/a = 1.071$ ,  $V = 0.3780$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	6h	mm2	0.1565	0.3131	$\frac{1}{4}$		single atom Sb
Cl2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5439		single atom Sb
Sb3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid Cl <sub>5</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.024, T = 243 K

Remarks: Phase stable at T > 219 K (melting point 277.5 K). In table 5 of [1] the Hermann-Mauguin symbol for the space group is misprinted as *P6<sub>3</sub>/mc* instead of *P6<sub>3</sub>/mmc* (given elsewhere).

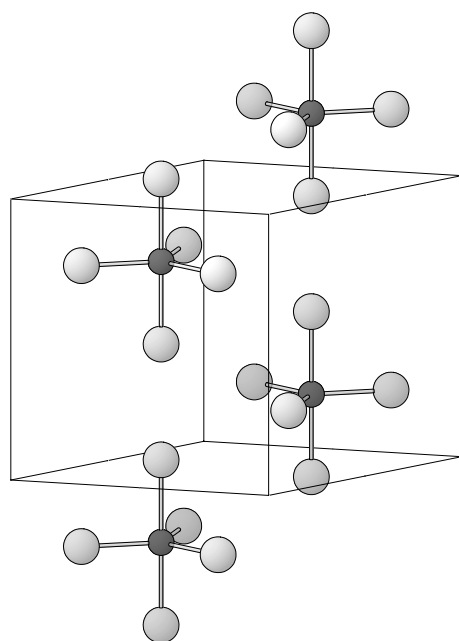


Fig. III.22. **SbCl<sub>5</sub> It1**

Arrangement of SbCl<sub>5</sub> trigonal bipyramids (Sb atoms dark, Cl atoms light).

References: [1] Haupt S., Seppelt K. (2002), Z. Anorg. Allg. Chem. 628, 729-734. [2] Ohlberg S.M. (1959), J. Am. Chem. Soc. 81, 811-813. [3] Mootz D., Wiebcke M. (1987), Z. Anorg. Allg. Chem. 545, 39-42.

194  
hP14

$W_2B_{4.3}$	<i>hP14</i>	(194) <i>P6<sub>3</sub>/mmc</i> – f <sup>2</sup> cba
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**WB<sub>2.5</sub>** [1], Strukturbericht notation D8<sub>h</sub>

Structural features: Infinite slabs of face-linked BW<sub>6</sub> trigonal prisms (planar hexagon-mesh B layers) alternate with puckered triangle-mesh B layers along [001] (partial vacancies ignored).

Kiessling R. (1947) [1]

B<sub>4.30</sub>W<sub>2</sub>

*a* = 0.2984, *c* = 1.387 nm, *c/a* = 4.648, *V* = 0.1070 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.028	0.86	bicapped square prism B <sub>6</sub> W <sub>4</sub>
W2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.639		pseudo Frank-Kasper B <sub>13</sub> W <sub>7</sub>
B3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.86	tricapped trigonal prism B <sub>3</sub> W <sub>6</sub>
B4	2b	-6m2	0	0	$\frac{1}{4}$	0.86	tricapped trigonal prism B <sub>3</sub> W <sub>6</sub>

B5       $2a$     $-3m.$       0      0      0      0.86    octahedron B<sub>6</sub>

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

Experimental: powder, film, X-rays

Remarks: The B vacancies could not be located in [1], but can be assumed to be mainly in Wyckoff position  $2a$ , in agreement with [2]. According to [3] the homogeneity range extends from W<sub>2</sub>B<sub>4</sub> (Wyckoff position  $2a$  vacant) to W<sub>2</sub>B<sub>4.54</sub>.

References: [1] Kiessling R. (1947), Acta Chem. Scand. 1, 893-916. [2] Lundström T. (1969), Ark. Kemi 30, 115-127. [3] Romans P.A., Krug M.P. (1966), Acta Crystallogr. 20, 313-315.

194  
hP14

Ba<sub>2</sub>Mn<sub>2</sub>Sb<sub>2</sub>O

hP14

(194)  $P6_3/mmc - f^2cba$

**Ba<sub>2</sub>Mn<sub>2</sub>Sb<sub>2</sub>O** [1]; Ba<sub>2</sub>Mn<sub>2</sub>Bi<sub>2</sub>O [1]

Structural features: 3D-framework of fused Ba<sub>6</sub> trigonal prisms centered by Mn or Sb (displaced from the prism centers); O in Ba layers between prisms centered by Mn. Mn(Sb<sub>3</sub>O) tetrahedra share vertices to form double layers (corrugated hexagon-mesh MnSb layers interconnected via -O- bridges).

Brechtel E. et al. (1981) [1]

Ba<sub>2</sub>Mn<sub>2</sub>OSb<sub>2</sub>

$a = 0.471$ ,  $c = 2.004$  nm,  $c/a = 4.255$ ,  $V = 0.3850$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mn1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.1495		single atom O
Sb2	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.6127		non-coplanar triangle Mn <sub>3</sub>
O3	$2c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid Mn <sub>2</sub> Ba <sub>3</sub>
Ba4	$2b$	$-6m2$	0	0	$\frac{1}{4}$		coplanar triangle O <sub>3</sub>
Ba5	$2a$	$-3m.$	0	0	0		octahedron Sb <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.055$

Remarks: In the abstract of [1] the  $a$ -parameter is misprinted as 471(1) pm instead of 471.1(1) nm (given in table I).

References: [1] Brechtel E., Cordier G., Schäfer H. (1981), Z. Naturforsch. B 36, 27-30.

194  
hP14

ScAl<sub>3</sub>C<sub>3</sub>

hP14

(194)  $P6_3/mmc - f^2dca$

**ScAl<sub>3</sub>C<sub>3</sub>** [1]; SmZn<sub>3</sub>P<sub>3</sub> [4]

Structural features: Close-packed Sc and Al layers in hc<sub>3</sub> stacking; C in octahedral (Sc<sub>3</sub>Al<sub>3</sub>) and trigonal bipyramidal (Al<sub>3</sub>) voids.

Tsokol A.O. et al. (1986) [1]

Al<sub>3</sub>C<sub>3</sub>Sc

$a = 0.3355$ ,  $c = 1.6776$  nm,  $c/a = 5.000$ ,  $V = 0.1635$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.1293		tetrahedron C <sub>4</sub>
C2	$4f$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.5876		7-vertex polyhedron Al <sub>4</sub> Sc <sub>3</sub>
Al3	$2d$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle C <sub>3</sub>



C4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	trigonal bipyramid Al <sub>5</sub>
Sc5	2a	-3m.	0	0	0	octahedron C <sub>6</sub>

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

Remarks: The structure was later redetermined in space group (186)  $P6_3mc$  [3] (preliminary report in [2]). The description of the structure of SmZn<sub>3</sub>P<sub>3</sub> in space group  $P6_322$  in [4] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Tsokol A.O., Bodak O.I., Marusin E.P., Baivel'man M.G. (1986), Sov. Phys. Crystallogr. 31, 467-468 (Kristallografiya 31, 791-792). [2] Gesing T.M., Jeitschko W. (1994), Proc. Journ. Actinides, 24th, Obergurgl (Austria) 1994, 84-85. [3] Gesing T.M., Jeitschko W. (1998), J. Solid State Chem. 140, 396-401. [4] Tejedor P., Hollander F.J., Fayos J., Stacy A.M. (1995), J. Cryst. Growth 155, 223-228.

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hP14

FeH	hP14	(194) $P6_3/mmc - \bar{f}^2dca$
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### FeH<sub>1.0</sub> [1]

Structural features: Close-packed Fe layers in hc stacking (stacking faults ignored); H in octahedral voids.

Antonov V.E. et al. (1998) [1]

DFe

$a = 0.2668$ ,  $c = 0.875$  nm,  $c/a = 3.280$ ,  $V = 0.0539$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.118	0.155	single atom Fe
D2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.618	0.845	single atom Fe
Fe3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.155	colinear D <sub>2</sub>
Fe4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.845	colinear D <sub>2</sub>
Fe5	2a	-3m.	0	0	0		hexagonal prism D <sub>12</sub>

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.016, T = 90 K

Remarks: Phase referred to as ε'-FeH<sub>x</sub>. Short interatomic distances for partly occupied site(s).

References: [1] Antonov V.E., Cornell K., Fedotov V.K., Kolesnikov A.I., Ponyatovsky E.G., Shiryayev V.I., Wipf H. (1998), J. Alloys Compd. 264, 214-222.

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hP14

K <sub>0.16</sub> Y <sub>2</sub> Cl <sub>2</sub> O <sub>1.64</sub>	hP14	(194) $P6_3/mmc - \bar{f}^2ec$
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### K<sub>0.08</sub>YO<sub>0.82</sub>Cl<sub>2</sub>H [1]

Structural features: Slabs consisting of four close-packed layers Cl-Y-Y-Cl and O in tetrahedral (Y<sub>4</sub>) voids; K in trigonal prismatic voids between the slabs.

Ford J.E., Corbett J.D. (1985) [1]

Cl<sub>2</sub>K<sub>0.16</sub>O<sub>1.64</sub>Y<sub>2</sub>

$a = 0.37873$ ,  $c = 2.186$  nm,  $c/a = 5.772$ ,  $V = 0.2715$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.04	0.82	tetrahedron Y <sub>4</sub>
Y2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.56447		7-vertex polyhedron O <sub>4</sub> Cl <sub>3</sub>
Cl3	4e	3m.	0	0	0.1469		non-coplanar triangle Y <sub>3</sub>

K4      2c   -6m2       $\frac{1}{3}$        $\frac{2}{3}$        $\frac{1}{4}$       0.16    trigonal prism Cl<sub>6</sub>

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

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

References: [1] Ford J.E., Corbett J.D. (1985), Inorg. Chem. 24, 4120-4128.

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hP14

Mg<sub>3</sub>BN<sub>3</sub>      hP14      (194) P6<sub>3</sub>/mmc – fecba

### Mg<sub>3</sub>BN<sub>3</sub> [1]

Structural features: Slabs containing N=B=N linear units (parallel to [001]) alternate with slabs of vertex-linked NMg<sub>5</sub> trigonal bipyramids (partial vacancies ignored).

Hiraguchi H. et al. (1991) [1]

BMg<sub>2.76</sub>N<sub>3</sub>

$a = 0.35445$ ,  $c = 1.60354$  nm,  $c/a = 4.524$ ,  $V = 0.1745$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1228	0.933	tetrahedron N <sub>4</sub>
N2	4e	3m.	0	0	0.0851		single atom B
N3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid Mg <sub>5</sub>
Mg4	2b	-6m2	0	0	$\frac{1}{4}$	0.894	coplanar triangle N <sub>3</sub>
B5	2a	-3m.	0	0	0		colinear N <sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.038

References: [1] Hiraguchi H., Hashizume H., Fukunaga O., Takenaka A., Sakata M. (1991), J. Appl. Crystallogr. 24, 286-292.

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hP14

Cu<sub>2</sub>S      hP14      (194) P6<sub>3</sub>/mmc – gfcba

### Cu<sub>2</sub>S chalcocite ht [1], chalcocite high

Structural features: Close-packed S layers in h stacking; Cu in tetrahedral, trigonal and linear voids (disorder).

Buerger M.J., Wuensch B.J. (1963) [1]

Cu<sub>2</sub>S

$a = 0.389$ ,  $c = 0.688$  nm,  $c/a = 1.769$ ,  $V = 0.0902$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	6g	.2/m.	$\frac{1}{2}$	0	0	0.188	
Cu2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.578	0.408	
S3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Cu4	2b	-6m2	0	0	$\frac{1}{4}$	0.62	

Experimental: single crystal, precession photographs, X-rays, R = 0.180, T = 398 K

Remarks: Phase stable at 377 < T < 708 K. Natural specimen from Bristol, Connecticut. Short interatomic distances for partly occupied site(s).

References: [1] Buerger M.J., Wuensch B.J. (1963), Science (Washington D.C.) 141, 276-277.

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hP14

$\text{Fe}_{1.6}\text{Ge}$	<i>hP14</i>	(194) $P6_3/mmc - h^2a$
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 **$\text{Fe}_{2-x}\text{Ge} \beta$  [1]**

Structural features: 3D-framework of fused  $\text{Fe}_6$  prisms centered alternatively by additional Fe (partial vacancies) and Ge (both displaced from the prism centers). Variant of ht- $\text{Co}_2\text{Ge}$  with splitting of the sites centering the trigonal prisms.

Malaman B. et al. (1980) [1]

 $\text{Fe}_{1.60}\text{Ge}$  $a = 0.3998$ ,  $c = 0.5010$  nm,  $c/a = 1.253$ ,  $V = 0.0694$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Fe1	6h	$mm2$	0.3377	0.6754	$1/4$	0.2	
Ge2	6h	$mm2$	0.6318	0.2636	$1/4$	0.333	
Fe3	2a	$-3m.$	0	0	0		

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.083$ 

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

References: [1] Malaman B., Steinmetz J., Roques B. (1980), J. Less-Common Met. 75, 155-176.

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hP14

$(\text{Mg}_{0.75}\text{Fe}_{0.25})[\text{CO}_3]_{0.125}[\text{OH}]_2[\text{H}_2\text{O}]_{0.56}$	<i>hP14</i>	(194) $P6_3/mmc - hfba$
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 **$\text{Mg}_6\text{Fe}_2(\text{OH})_{16}\text{CO}_3 \cdot 4.5\text{H}_2\text{O}$  [2], sjögrenite**

Structural features: Infinite slabs of edge-linked  $(\text{Mg},\text{Fe})(\text{OH})_6$  octahedra and layers containing a partly disordered arrangement of  $\text{CO}_3$  trigonal units (perpendicular to  $[001]$ ) and  $\text{H}_2\text{O}$  alternate along  $[001]$ .

Allmann R. (1969) [1]

 $\text{C}_{0.13}\text{Fe}_{0.25}\text{H}_{3.13}\text{Mg}_{0.75}\text{O}_{2.94}$  $a = 0.3113$ ,  $c = 1.561$  nm,  $c/a = 5.014$ ,  $V = 0.1310$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	6h	$mm2$	0.235	0.47	$1/4$	0.313	
O2	4f	$3m.$	$1/3$	$2/3$	0.0652		non-coplanar triangle $\text{Mg}_3$
C3	2b	$-6m2$	0	0	$1/4$	0.125	coplanar triangle $(\text{OH}_2)_3$
M4	2a	$-3m.$	0	0	0		octahedron $\text{O}_6$
H5	4f	$3m.$	$1/3$	$2/3$	0.1147		

 $\text{M1} = 0.6\text{OH}_2 + 0.4\text{O}$ ;  $\text{M4} = 0.75\text{Mg} + 0.25\text{Fe}$ Experimental: single crystal, photographs, X-rays,  $R = 0.070$ 

Remarks: Diffraction data and cell parameters from [3] (natural specimen from Långban, Sweden). Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In the abstracts of [1] the number of formula units per cell  $Z$  is misprinted as  $2/2$  (German) and  $8/8$  (English) instead of  $2/8$  (given on page 554).

References: [1] Allmann R. (1969), Neues Jahrb. Mineral., Monatsh. 1969, 552-557. [2] Ingram L., Taylor H.F.W. (1967), Mineral. Mag. J. Mineral. Soc. 36, 465-479. [3] Allmann R., Lohse H.H. (1966), Neues Jahrb. Mineral., Monatsh. 1966, 161-181.

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hP14

$\text{Na}_{0.61}\text{CoO}_2$	<i>hP14</i>	(194) $P6_3/mmc$ – hfba
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**Na<sub>0.61</sub>CoO<sub>2</sub> [1]**

Structural features: Close-packed O layers in AABB stacking; Co in octahedral, Na in trigonal prismatic voids (disorder, in part displaced from the prism centers). CoO<sub>6</sub> octahedra share edges to form infinite slabs.

Jorgensen J.D. et al. (2003) [1]

CoNa<sub>0.57</sub>O<sub>2</sub> $a = 0.28329$ ,  $c = 1.08969$  nm,  $c/a = 3.847$ ,  $V = 0.0757$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Na1	6 <i>h</i>	<i>mm2</i>	0.713	0.426	$\frac{1}{4}$	0.132	non-coplanar triangle Co <sub>3</sub>
O2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.09024		
Na3	2 <i>b</i>	-6 <i>m2</i>	0	0	$\frac{1}{4}$	0.17	octahedron O <sub>6</sub>
Co4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

Experimental: powder, diffractometer, neutrons, time-of-flight, T = 295 K

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

References: [1] Jorgensen J.D., Avdeev M., Hinks D.G., Burley J.C., Short S. (2003), Phys. Rev. B: Condens. Matter 68, 214517: 1-10.

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hP14

$\text{Na}_{0.36}\text{CoO}_2[\text{H}_2\text{O}]_{0.65}$	<i>hP14</i>	(194) $P6_3/mmc$ – hfca
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**Na<sub>0.36</sub>CoO<sub>2</sub>·0.65H<sub>2</sub>O [1]**

Structural features: Infinite slabs of edge-linked CoO<sub>6</sub> octahedra (h stacking) and layers containing a partly disordered arrangement of Na and H<sub>2</sub>O (Na between two O) alternate along [001].

Takada K. et al. (2004) [1]

CoH<sub>1.28</sub>Na<sub>0.36</sub>O<sub>2.64</sub> $a = 0.28344$ ,  $c = 1.3842$  nm,  $c/a = 4.884$ ,  $V = 0.0963$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH <sub>2</sub> )1	6 <i>h</i>	<i>mm2</i>	0.175	0.35	$\frac{1}{4}$	0.214	non-coplanar triangle Co <sub>3</sub>
O2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0666		
Na3	2 <i>c</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.358	octahedron O <sub>6</sub>
Co4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.013

Remarks: Referred to as MLH (monolayer hydrate). 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] Takada K., Sakurai H., Takayama Muromachi E., Izumi F., Dilanian R.A., Sasaki T. (2004), J. Solid State Chem. 177, 372-376.

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hP14

[NO <sub>2</sub> ][NO <sub>3</sub> ]	<i>hP14</i>	(194) $P6_3/mmc$ – hfdb
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**N<sub>2</sub>O<sub>5</sub>** [2]

Structural features: O-N-O linear units (parallel to [001]) and NO<sub>3</sub> trigonal units (perpendicular to [001]); N forms a graphite-like substructure.

Simon A. et al. (1992) [1]

**N<sub>2</sub>O<sub>5</sub>**

$a = 0.54019$ ,  $c = 0.65268$  nm,  $c/a = 1.208$ ,  $V = 0.1649$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	mm2	0.13445	0.26890	$\frac{1}{4}$		single atom N
O2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.57877		single atom N
N3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear O <sub>2</sub>
N4	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle O <sub>3</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.028$ ,  $T = 105$  K

Remarks: Average structure; line splitting indicates orthorhombic symmetry at  $105 < T < 273$  K. In the material deposited for [1] the cell volume is misprinted as  $264.94 \cdot 10^6$  pm<sup>3</sup> instead of  $164.94 \cdot 10^6$  pm<sup>3</sup>.

References: [1] Simon A., Horakh J., Obermeyer A., Borrmann H. (1992), Angew. Chem. 104, 325-327.

[2] Grison E., Eriks K., De Vries J.L. (1950), Acta Crystallogr. 3, 290-294.

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hP14

BaC <sub>6</sub>	hP14	(194) $P6_3/mmc - ic$
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**BaC<sub>6</sub>** [1], GIC (graphite intercalation compound)

Structural features: Directly superposed graphite (hexagon-mesh) C layers; Ba between hexagons in every interlayer (stage 1).

Guérard D., Herold A. (1974) [1]

**BaC<sub>6</sub>**

$a = 0.4302$ ,  $c = 1.051$  nm,  $c/a = 2.443$ ,  $V = 0.1685$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
C1	12i	.2.	0.33333	0	0		coplanar triangle C <sub>3</sub>
Ba2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		hexagonal prism C <sub>12</sub>

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

Experimental: powder, diffractometer, X-rays

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

References: [1] Guérard D., Herold A. (1974), C. R. Seances Acad. Sci., Ser. C 279, 455-456.

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hP16

YbFe <sub>2</sub> Si <sub>4.5</sub>	hP16	(194) $P6_3/mmc - f^2eca$
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**Yb<sub>2</sub>Fe<sub>4</sub>Si<sub>9</sub>** [1]; Y<sub>2</sub>Fe<sub>4</sub>Si<sub>9</sub> [1]

Structural features: 7-layer thick W-type (b.c.c. arrangement) slabs of ideal composition Fe<sub>2</sub>Si<sub>5</sub> alternate with triangle-mesh Yb layers along [001].

Gladyshevskii E.I. et al. (1978) [1]

**Fe<sub>2</sub>Si<sub>4.50</sub>Yb**

$a = 0.3916$ ,  $c = 1.539$  nm,  $c/a = 3.930$ ,  $V = 0.2044$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0444		13-vertex polyhedron Fe <sub>4</sub> Si <sub>9</sub>
Fe2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6083		13-vertex polyhedron Si <sub>10</sub> Yb <sub>3</sub>
Si3	4e	3m.	0	0	0.1351		bicapped square prism Si <sub>4</sub> Fe <sub>3</sub> Yb <sub>3</sub>
Yb4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		rhombic dodecahedron Si <sub>8</sub> Fe <sub>6</sub>
Si5	2a	-3m.	0	0	0	0.5	rhombic dodecahedron Si <sub>8</sub> Fe <sub>6</sub>

Experimental: single crystal, X-rays, R = 0.145

Remarks: In [1] the Wyckoff position of former Si(2) is misprinted as 4c instead of 4e.

References: [1] Gladyshevskii E.I., Bodak O.I., Yarovets V.I., Gorelenko Y.K., Skolozdra R.V. (1978), Ukr. Fiz. Zh. (Russ. Ed.) 23, 77-82.

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hP16

Cu <sub>2</sub> U <sub>3</sub> Sb <sub>3</sub>	hP16	(194) $P6_3/mmc - f^2eca$
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### U<sub>3</sub>Cu<sub>2</sub>Sb<sub>3</sub> [1]

Structural features: Close-packed Sb layers in AAABBB stacking; U in trigonal prismatic and octahedral, Cu in trigonal voids (displaced out of the plane).

De Mooij D.B., Buschow K.H.J. (1986) [1]

Cu<sub>2</sub>Sb<sub>3</sub>U<sub>3</sub>

$a = 0.4393$ ,  $c = 2.3011$  nm,  $c/a = 5.238$ ,  $V = 0.3846$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
U1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0786		octahedron Sb <sub>6</sub>
Sb2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6592		tricapped trigonal prism Cu <sub>3</sub> U <sub>6</sub>
Cu3	4e	3m.	0	0	0.1853		7-vertex polyhedron Sb <sub>3</sub> U <sub>3</sub> Cu
U4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		hexagonal prism Cu <sub>6</sub> Sb <sub>6</sub>
Sb5	2a	-3m.	0	0	0		octahedron U <sub>6</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.100

References: [1] De Mooij D.B., Buschow K.H.J. (1986), J. Less-Common Met. 125, 239-245.

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hP16

CsYb <sub>3</sub> Se <sub>4</sub>	hP16	(194) $P6_3/mmc - f^2eca$
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### CsYb<sub>3</sub>Se<sub>4</sub> [1]; Ti<sub>4</sub>AlN<sub>3</sub> [4]

Structural features: Close-packed Cs and Se layers in hc<sub>4</sub> stacking (Cs in h-stacked layers); Yb in octahedral voids between Se layers.

Folchnandt M., Schleid T. (1998) [1]

CsSe<sub>4</sub>Yb<sub>3</sub>

$a = 0.40578$ ,  $c = 3.1303$  nm,  $c/a = 7.714$ ,  $V = 0.4464$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0554		octahedron Yb <sub>6</sub>
Yb2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.61079		octahedron Se <sub>6</sub>
Se3	4e	3m.	0	0	0.1575		non-coplanar triangle Yb <sub>3</sub>
Cs4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Se <sub>6</sub> Cs <sub>6</sub>

Yb5      2a   -3m.      0      0      0      octahedron Se<sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays

Remarks: The structure proposal for so-called Ti<sub>4</sub>Al<sub>2</sub>N<sub>2</sub> in space group (186) *P*6<sub>3</sub>*mc* in [2] is superseded (see [4]; composition corrected to Ti<sub>4</sub>AlN<sub>3</sub>). The description of this superseded structure proposal in space group (159) *P*31*c* in [2] does not take into consideration all symmetry elements of the proposed structure (see [3]).

References: [1] Folchnandt M., Schleid T. (1998), Z. Kristallogr. Suppl. 15, 57. [2] Schuster J.C., Bauer J. (1984), J. Solid State Chem. 53, 260-265. [3] Cenxual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439. [4] Rawn C.J., Barsoum M.W., El Raghy T., Procipio A., Hoffmann C.M., Hubbard C.R. (2000), Mater. Res. Bull. 35, 1785-1796.

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hP16

K <sub>5</sub> CuAs <sub>2</sub>	hP16	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – f <sup>2</sup> edc
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### K<sub>5</sub>CuAs<sub>2</sub> [1]

Structural features: Close-packed K layers in h<sub>3</sub>c<sub>2</sub> stacking; Cu and As in trigonal voids. As-Cu-As linear units parallel to [001].

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

As<sub>2</sub>CuK<sub>5</sub>

$a = 0.5737$ ,  $c = 1.8771$  nm,  $c/a = 3.272$ ,  $V = 0.5350$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
As1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1271		single atom Cu
K2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5498		pseudo Frank-Kasper As <sub>4</sub> K <sub>7</sub>
K3	4e	3m.	0	0	0.1457		13-vertex polyhedron As <sub>3</sub> K <sub>7</sub> Cu <sub>3</sub>
K4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle Cu <sub>3</sub>
Cu5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear As <sub>2</sub>

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

Remarks: In the abstract and table 1 of [1] the  $a$ -parameter is misprinted as 0.5377 nm instead of 0.5737 nm (checked on interatomic distances).

References: [1] Eisenmann B., Klein J., Somer M. (1992), J. Alloys Compd. 178, 431-439.

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hP16

Ca <sub>2</sub> CuZn <sub>2</sub> P <sub>3</sub>	hP16	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – f <sup>2</sup> edc
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### Ca<sub>2</sub>CuZn<sub>2</sub>P<sub>3</sub> [1]

Structural features: Infinite slabs of edge-linked ZnP<sub>4</sub> tetrahedra and infinite slabs of fused CuCa<sub>6</sub> and PCa<sub>6</sub> trigonal prisms alternate along [001].

Frik L., Mewis A. (1999) [1]

Ca<sub>2</sub>CuP<sub>3</sub>Zn<sub>2</sub>

$a = 0.4048$ ,  $c = 2.1466$  nm,  $c/a = 5.303$ ,  $V = 0.3046$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
P1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.076		7-vertex polyhedron Zn <sub>4</sub> Ca <sub>3</sub>
Zn2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5421		tetrahedron P <sub>4</sub>

Ca3	4e	3m.	0	0	0.1582	19-vertex polyhedron $P_6Cu_3Zn_3Ca_7$
P4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	tricapped trigonal prism $Cu_3Ca_6$
Cu5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	tricapped trigonal prism $P_3Ca_6$

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

References: [1] Frik L., Mewis A. (1999), Z. Anorg. Allg. Chem. 625, 126-130.

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hP16

$UAl_3C_3$	hP16	(194) $P6_3/mmc - f^3ca$
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#### $UAl_3C_3$ [1]

Structural features: Close-packed U and Al layers in  $hc_3$  stacking; C in octahedral ( $U_3Al_3$ ) and trigonal bipyramidal ( $Al_5$ ) voids. Variant of  $ScAl_3C_3$  with splitting of the Al site forming the h-stacked layers.

Gesing T.M. et al. (1992) [1]

$Al_3C_3U$

$a = 0.3389$ ,  $c = 1.7394$  nm,  $c/a = 5.132$ ,  $V = 0.1730$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1346		tetrahedron $C_4$
C2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.594		non-coplanar triangle $Al_3$
Al3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7406	0.5	
C4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
U5	2a	-3m.	0	0	0		octahedron $C_6$

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

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

References: [1] Gesing T.M., Pöttgen R., Jeitschko W., Wortmann U. (1992), J. Alloys Compd. 186, 321-331.

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hP16

$Hg_2BrN$	hP16	(194) $P6_3/mmc - gfdca$
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#### ( $Hg_2N$ )Br [2], Millon's salt

Structural features: N-Hg-N linear units share vertices to form a tetrahedral framework.

Nijssen L., Lipscomb W. (1954) [1]

$BrHg_2N$

$a = 0.665$ ,  $c = 1.126$  nm,  $c/a = 1.693$ ,  $V = 0.4312$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	6g	.2/m.	$\frac{1}{2}$	0	0		colinear $N_2$
N2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0625		tetrahedron $Hg_4$
Br3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		8-vertex polyhedron $Hg_6N_2$
Hg4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear $N_2$
Br5	2a	-3m.	0	0	0		coplanar hexagon $Hg_6$

Experimental: powder, diffractometer, X-rays

References: [1] Nijssen L., Lipscomb W. (1954), Acta Crystallogr. 7, 103-106. [2] Rüdorff W., Brodersen K. (1953), Z. Anorg. Allg. Chem. 274, 323-340.



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hP16

Ni <sub>1.50</sub> Sn	hP16	(194) $P6_3/mmc - h^2ca$
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**Ni<sub>1.50</sub>Sn** [1]

Structural features: 3D-framework of fused Ni<sub>6</sub> prisms centered alternatively by additional Ni (partial vacancies) and Sn (displaced from the prism centers). Variant of ht-Co<sub>2</sub>Ge with complex splitting of the Sn site.

Leineweber A. et al. (2004) [1]

Ni<sub>1.52</sub>Sn $a = 0.4103$ ,  $c = 0.5176$  nm,  $c/a = 1.262$ ,  $V = 0.0755$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Sn1	6h	mm2	0.6289	0.2578	$\frac{1}{4}$	0.167	
Sn2	6h	mm2	0.6842	0.3684	$\frac{1}{4}$	0.167	
Ni3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.523	
Ni4	2a	-3m.	0	0	0		

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.021$ 

Remarks: Static displacements from the ideal positions. Short interatomic distances for partly occupied site(s). Several other models were also tested (atom coordinates published).

References: [1] Leineweber A., Oeckler O., Zachwieja U. (2004), J. Solid State Chem. 177, 936-945.

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hP16

Ba <sub>3</sub> Al <sub>5</sub>	hP16	(194) $P6_3/mmc - hf^2a$
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**Ba<sub>3</sub>Al<sub>5</sub>** [1]

Structural features: Kagomé-mesh Al<sub>3</sub>, triangle-mesh Ba and puckered hexagon-mesh BaAl layers alternate along [001]. Pairs of face-linked Al<sub>4</sub> tetrahedra are interconnected via additional Al-Al contacts to form infinite layers.

Fornasini M.L. (1988) [1]

Al<sub>5</sub>Ba<sub>3</sub> $a = 0.6066$ ,  $c = 1.4611$  nm,  $c/a = 2.409$ ,  $V = 0.4656$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	6h	mm2	0.1547	0.3094	$\frac{1}{4}$		icosahedron Al <sub>6</sub> Ba <sub>6</sub>
Al2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1137		pseudo Frank-Kasper Al <sub>4</sub> Ba <sub>7</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6251		14-vertex Frank-Kasper Al <sub>10</sub> Ba <sub>4</sub>
Ba4	2a	-3m.	0	0	0		18-vertex polyhedron Al <sub>12</sub> Ba <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.027$ 

References: [1] Fornasini M.L. (1988), Acta Crystallogr. C 44, 1355-1357.

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hP16

Sr <sub>3</sub> [BO <sub>3</sub> ]P	hP16	(194) $P6_3/mmc - hfdba$
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**Sr<sub>3</sub>PBO<sub>3</sub>** [1]; Ba<sub>3</sub>PBO<sub>3</sub> [2]

Structural features:  $\text{PSr}_8$  cubes share edges and vertices to form a 3D-framework;  $\text{BO}_3$  trigonal units in voids (Edshamar polyhedra).

Somer M. et al. (1995) [1]

$\text{BO}_3\text{PSr}_3$

$a = 0.5259$ ,  $c = 1.2706$  nm,  $c/a = 2.416$ ,  $V = 0.3043$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6h	mm2	0.5156	0.0312	$\frac{1}{4}$		single atom B
Sr2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.10001		non-coplanar triangle O <sub>3</sub>
B3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle O <sub>3</sub>
Sr4	2b	-6m2	0	0	$\frac{1}{4}$		coplanar hexagon O <sub>6</sub>
P5	2a	-3m.	0	0	0		square prism (cube) Sr <sub>8</sub>

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

References: [1] Somer M., Carrillo Cabrera W., Peters K., Von Schnering H.G. (1995), Z. Kristallogr. 210, 526. [2] Somer M., Carrillo Cabrera W., Peters K., Von Schnering H.G. (1995), Z. Kristallogr. 210, 449.

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hP16

KPu[CO <sub>3</sub> ]O <sub>2</sub>	hP16	(194) $P6_3/mmc$ – hfdca
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**KPuO<sub>2</sub>(CO<sub>3</sub>)** [1]

Structural features: Compressed PuO<sub>8</sub> hexagonal bipyramids share equatorial edges with CO<sub>3</sub> trigonal units to form infinite slabs.

Ellinger F.H., Zachariasen W.H. (1954) [1]

$\text{CKO}_3\text{Pu}$

$a = 0.509$ ,  $c = 0.983$  nm,  $c/a = 1.931$ ,  $V = 0.2206$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6h	mm2	0.188	0.376	$\frac{1}{4}$		single atom C
O2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.553		single atom Pu
Pu3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear O <sub>2</sub>
C4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle O <sub>3</sub>
K5	2a	-3m.	0	0	0		icosahedron O <sub>12</sub>

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

Experimental: powder, film, X-rays

References: [1] Ellinger F.H., Zachariasen W.H. (1954), J. Phys. Chem. 58, 405-408.

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hP16

MoN	hP16	(194) $P6_3/mmc$ – hgba
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**MoN** [1]

Structural features: Directly superposed slightly distorted close-packed Mo layers in h stacking; N in linear coordination.

Zhao X., Range K.J. (2000) [1]

MoN

$a = 0.572$ ,  $c = 0.56$  nm,  $c/a = 0.979$ ,  $V = 0.1587$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mo1	6h	mm2	0.52	0.04	$\frac{1}{4}$		non-colinear N <sub>2</sub>
N2	6g	.2/m.	$\frac{1}{2}$	0	0		colinear Mo <sub>2</sub>
Mo3	2b	-6m2	0	0	$\frac{1}{4}$		colinear N <sub>2</sub>
N4	2a	-3m.	0	0	0		colinear Mo <sub>2</sub>

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

Experimental: powder, diffractometer, X-rays,  $R_p = 0.238$

Remarks: Short interatomic distances:  $d(\text{Mo3-N4}) = 0.140$  nm,  $d(\text{Mo1-N2}) = 0.141$  nm. Space group (164)  $P\bar{3}m1$ , used in [2], was tested and rejected. On page 74 of [1] the Wyckoff position of former Mo(1) is misprinted as 2c instead of 2b.

References: [1] Zhao X., Range K.J. (2000), J. Alloys Compd. 296, 72-74. [2] Troitskaya N.V., Pinsker Z.G. (1961), Sov. Phys. Crystallogr. 6, 34-39 (Kristallografiya 6, 43-48).

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hP16

TiNi <sub>3</sub>	hP16	(194) $P6_3/mmc - hgda$
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**TiNi<sub>3</sub>** [1], Strukturbericht notation D0<sub>24</sub>; UPd<sub>3</sub> [2]

Structural features: Close-packed TiNi<sub>3</sub> layers in hc stacking; the Ti atoms form a triangle mesh. Substitution derivative of  $\alpha$ -Nd. See Fig. III.23.

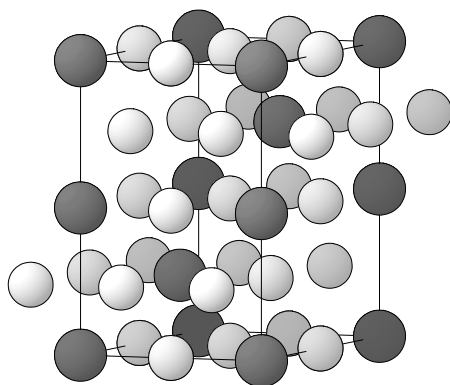


Fig. III.23. **TiNi<sub>3</sub>**

Arrangement of Ti (dark) and Ni (light) atoms.

Laves F., Wallbaum H.J. (1939) [1]

Ni<sub>3</sub>Ti

$a = 0.5109$ ,  $c = 0.8299$  nm,  $c/a = 1.624$ ,  $V = 0.1876$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	6h	mm2	0.16667	0.33333	$\frac{1}{4}$		anticuboctahedron Ni <sub>8</sub> Ti <sub>4</sub>
Ni2	6g	.2/m.	$\frac{1}{2}$	0	0		cuboctahedron Ti <sub>4</sub> Ni <sub>8</sub>
Ti3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron Ni <sub>12</sub>
Ti4	2a	-3m.	0	0	0		cuboctahedron Ni <sub>12</sub>

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

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

Remarks: Idealized coordinates. On page 79 of [1] the Wyckoff position of former Ti(I) is misprinted as 6a instead of 2a.

References: [1] Laves F., Wallbaum H.J. (1939), Z. Kristallogr. 101, 78-93. [2] Heal T.J., Williams G.I. (1955), Acta Crystallogr. 8, 494-498.

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hP16

Mo <sub>0.8</sub> B <sub>3</sub>	hP16	(194) <i>P6<sub>3</sub>/mmc</i> – icb
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### Mo<sub>1-x</sub>B<sub>3</sub> [2]

Structural features: Directly superposed planar hexagon-mesh B layers; Mo between hexagons (partial disorder).

Klesnar H. et al. (1996) [1]

B<sub>3</sub>Mo<sub>0.91</sub>

$a = 0.52646$ ,  $c = 0.6121$  nm,  $c/a = 1.163$ ,  $V = 0.1469$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	12i	.2.	0.33	0	0		coplanar triangle B <sub>3</sub>
Mo2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		hexagonal prism B <sub>12</sub>
Mo3	2b	-6m2	0	0	$\frac{1}{4}$	0.82	hexagonal prism B <sub>12</sub>

Experimental: powder, diffractometer, neutrons, time-of-flight,  $wR_p = 0.075$

Remarks: Multiphase refinement considering also structural parameters for rhombohedral MoB<sub>2+x</sub> (88.2%) and hexagonal MoB<sub>2-x</sub> (3.2%).

References: [1] Klesnar H., Aselage T.L., Morosin B., Kwei G.H., Lawson A.C. (1996), J. Alloys Compd. 241, 180-186. [2] Lundström T., Rosenberg I. (1973), J. Solid State Chem. 6, 299-305.

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hP16

Cu <sub>2</sub> S	hP16	(194) <i>P6<sub>3</sub>/mmc</i> – kcb
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### Cu<sub>2</sub>S chalcocite ht [1], chalcocite high

Structural features: Close-packed S layers in h stacking; Cu in trigonal voids (disorder).

Cava R.J. et al. (1981) [1]

Cu<sub>2</sub>S

$a = 0.3959$ ,  $c = 0.6784$  nm,  $c/a = 1.714$ ,  $V = 0.0921$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	12k	.m.	0.2573	0.5146	0.5661	0.216	
S2	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Cu3	2b	-6m2	0	0	$\frac{1}{4}$	0.707	tricapped trigonal prism Cu <sub>6</sub> S <sub>3</sub>

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

Experimental: single crystal, diffractometer, neutrons,  $R = 0.071$ ,  $T = 393$  K

Remarks: Phase stable at  $377 < T < 703$  K. Natural specimen from Bristol, Connecticut. Short interatomic distances for partly occupied site(s). Supersedes structure proposals with different partly occupied Cu sites ([2]; [3]).

References: [1] Cava R.J., Reidinger F., Wuensch B.J. (1981), Solid State Ionics 5, 501-504. [2] Buerger M.J., Wuensch B.J. (1963), Science (Washington D.C.) 141, 276-277. [3] Sadanaga R., Ohmasa M., Morimoto N. (1965), Mineral. J. 4, 275-290.

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hP18

YbNi <sub>1.7</sub> Sn	hP18	(194) $P6_3/mmc - f^2ecba$
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**YbNi<sub>2-x</sub>Sn [1]**

Structural features: Intergrowth of W-type (MnCu<sub>2</sub>Al) and AlB<sub>2</sub>-type (ZrBeSi) slabs (single Ni atoms in part replaced by Ni<sub>2</sub> dumbbells) along [001]. Ni(Yb<sub>4</sub>Sn<sub>4</sub>) cubes and NiYb<sub>6</sub>Sn<sub>3</sub> tricapped trigonal prisms (Ni<sub>2</sub> dumbbells ignored) share atoms to form a dense 3D-framework.

Rizzoli C. et al. (2002) [1]

Co<sub>0.40</sub>Ni<sub>1.30</sub>SnYb $a = 0.4424$ ,  $c = 1.5232$  nm,  $c/a = 3.443$ ,  $V = 0.2582$  nm<sup>3</sup>,  $Z = 4$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05283		rhombic dodecahedron Sn <sub>4</sub> Yb <sub>4</sub> Ni <sub>6</sub>
Yb2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6332		non-coplanar triangle Ni <sub>3</sub>
Co3	4e	3m.	0	0	0.17184	0.4	
Sn4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Ni <sub>3</sub>
Ni5	2b	-6m2	0	0	$\frac{1}{4}$	0.6	
Sn6	2a	-3m.	0	0	0		square prism (cube) Ni <sub>8</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: Refinement of the occupancy of the Yb site showed no significant deviation from unity. Short interatomic distances for partly occupied site(s).

References: [1] Rizzoli C., Salamakha P.S., Sologub O.L., Bocelli G. (2002), J. Alloys Compd. 340, 146-150.

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hP18

Rh <sub>5</sub> B <sub>4</sub>	hP18	(194) $P6_3/mmc - f^3ec$
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**Rh<sub>5</sub>B<sub>4</sub> [1]**

Structural features: Close-packed Rh layers in h<sub>3</sub>c<sub>2</sub> stacking; B in octahedral voids, leaving the interstices between c-stacked layers vacant. Finite B<sub>4</sub> linear chains.

Noläng B.I. et al. (1981) [1]

B<sub>4</sub>Rh<sub>5</sub> $a = 0.33058$ ,  $c = 2.0394$  nm,  $c/a = 6.169$ ,  $V = 0.1930$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Rh1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.04670		non-coplanar triangle B <sub>3</sub>
B2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5872		7-vertex polyhedron Rh <sub>6</sub> B
B3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6957		square prism (cube) Rh <sub>6</sub> B <sub>2</sub>
Rh4	4e	3m.	0	0	0.14737		trigonal prism B <sub>6</sub>
Rh5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism B <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.098

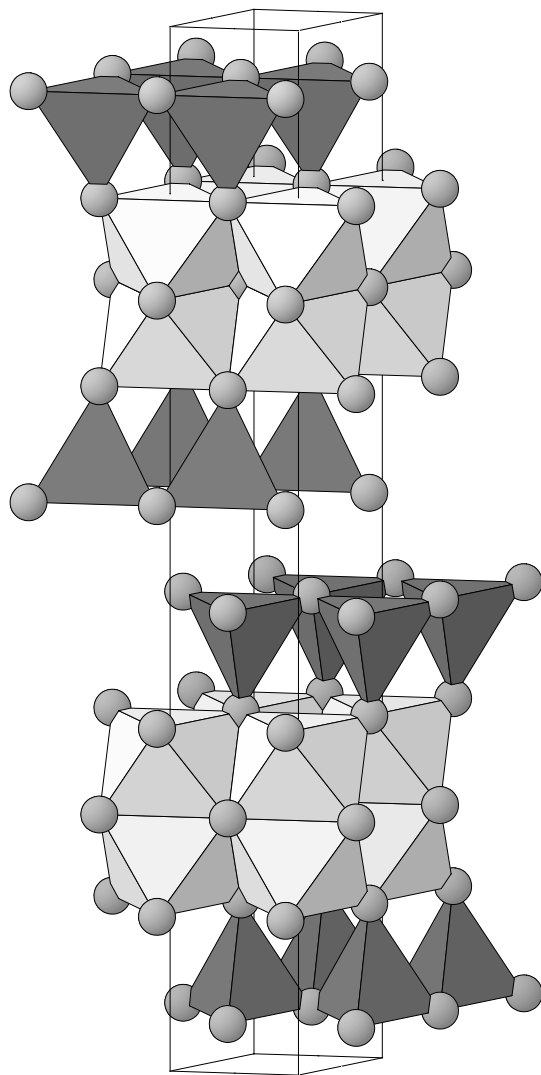
References: [1] Noläng B.I., Tergenius L.E., Westman I. (1981), J. Less-Common Met. 82, 303-308.

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hP18

Fe <sub>2</sub> Ga <sub>2</sub> S <sub>5</sub>	hP18	(194) $P6_3/mmc - f^3ec$
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**Fe<sub>2</sub>Ga<sub>2</sub>S<sub>5</sub> 2H** [1]

Structural features: Close-packed S layers in h stacking; Fe in octahedral, Ga in tetrahedral voids. Layer structure with sandwiches consisting of nine sublayers (S-Ga(t)-S-Fe(o)-S-Fe(o)-S-Ga(t)-S). See Fig. III.24.

Fig. III.24. **Fe<sub>2</sub>Ga<sub>2</sub>S<sub>5</sub> 2H**

Arrangement of FeS<sub>6</sub> octahedra (light) and GaS<sub>4</sub> tetrahedra (dark).

Cascarano G. et al. (1987) [1]

Fe<sub>2</sub>Ga<sub>2</sub>S<sub>5</sub>

$a = 0.3637$ ,  $c = 2.963$  nm,  $c/a = 8.147$ ,  $V = 0.3394$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0532		non-coplanar triangle Ga <sub>3</sub>
Ga2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5845		tetrahedron S <sub>4</sub>
S3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.66		tetrahedron GaFe <sub>3</sub>
Fe4	4e	3m.	0	0	0.2012		7-vertex polyhedron S <sub>6</sub> Fe
S5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Fe <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.047$ ,  $T = 293$  K

References: [1] Cascarano G., Dogguy Smiri L., Dung N.H. (1987), Acta Crystallogr. C 43, 2050-2053.

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hP18

Hg <sub>2</sub> IN	hP18	(194) <i>P6<sub>3</sub>/mmc</i> – gfdcba
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**(Hg<sub>2</sub>N)I** [1], Millon's salt

Structural features: N-Hg-N linear units share vertices to form a tetrahedral framework. Partly disordered variant of Hg<sub>2</sub>BrN.

Rüdrorff W., Brodersen K. (1953) [1]

Hg<sub>2</sub>IN

$a = 0.673$ ,  $c = 1.145$  nm,  $c/a = 1.701$ ,  $V = 0.4491$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Hg1	6g	.2/m.	$\frac{1}{2}$	0	0		colinear N <sub>2</sub>
N2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.066		tetrahedron Hg <sub>4</sub>
I3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		8-vertex polyhedron Hg <sub>6</sub> N <sub>2</sub>
Hg4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear N <sub>2</sub>
I5	2b	-6m2	0	0	$\frac{1}{4}$	0.5	colinear I <sub>2</sub>
I6	2a	-3m.	0	0	0	0.5	colinear I <sub>2</sub>

Experimental: powder, film, X-rays

References: [1] Rüdrorff W., Brodersen K. (1953), Z. Anorg. Allg. Chem. 274, 323-340.

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hP18

Y[BO <sub>3</sub> ]	hP18	(194) <i>P6<sub>3</sub>/mmc</i> – h <sup>2</sup> fa
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**YBO<sub>3</sub>** [1]

Structural features: Y atoms and BO<sub>3</sub> trigonal units (perpendicular to (001), partial disorder) in a NiAs-type arrangement.

Newnham R.E. et al. (1963) [1]

BO<sub>3</sub>Y

$a = 0.3778$ ,  $c = 0.8814$  nm,  $c/a = 2.333$ ,  $V = 0.1090$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	mm2	0.024	0.048	$\frac{1}{4}$	0.333	
B2	6h	mm2	0.23	0.46	$\frac{1}{4}$	0.333	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.117		
Y4	2a	-3m.	0	0	0		

Experimental: powder, diffractometer, X-rays,  $R_B = 0.180$

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

References: [1] Newnham R.E., Redman M.J., Santoro R.P. (1963), J. Am. Ceram. Soc. 46, 253-256.

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hP18

Na <sub>0.67</sub> CoO <sub>2</sub>	hP18	(194) <i>P6<sub>3</sub>/mmc</i> – h <sup>2</sup> fa
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**Na<sub>x</sub>CoO<sub>2</sub> γ** [1]

Structural features: Close-packed O layers in BBCC stacking; Co in octahedral, Na in trigonal prismatic voids (displaced from the prism centers, disorder). CoO<sub>6</sub> octahedra share edges to form infinite slabs.

Ono Y. et al. (2003) [1]

CoNa<sub>0.67</sub>O<sub>2</sub>

$a = 0.28329$ ,  $c = 1.09089$  nm,  $c/a = 3.851$ ,  $V = 0.0758$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Na1	6h	mm2	0.043	0.086	$\frac{1}{4}$	0.064	
Na2	6h	mm2	0.7293	0.4586	$\frac{1}{4}$	0.159	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0902		non-coplanar triangle Co <sub>3</sub>
Co4	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $R_B = 0.026$ ,  $T = 300$  K

Remarks: Homogeneity range Na<sub>x</sub>CoO<sub>2</sub>,  $0.67 < x < 0.75$  (at least). Short interatomic distances for partly occupied site(s).

References: [1] Ono Y., Kato N., Ishii Y., Miyazaki Y., Kajitani T. (2003), Funtai Oyobi Funmatsu Yakin 50, 469-474.

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hP18

La(Cu<sub>0.75</sub>Mo<sub>0.25</sub>)O<sub>3</sub> hP18 (194)  $P6_3/mmc - h^2fa$

**La<sub>4</sub>Cu<sub>3</sub>MoO<sub>12</sub> quenched** [2]

Structural features: Close-packed O layers in hc<sub>2</sub> stacking; La in octahedral, (Cu,Mo) in trigonal bipyramidal voids. Variant of YAlO<sub>3</sub> with site splitting.

Griend D.A.V. et al. (1999) [1]

Cu<sub>0.75</sub>LaMo<sub>0.25</sub>O<sub>3</sub>

$a = 0.39559$ ,  $c = 1.1012$  nm,  $c/a = 2.784$ ,  $V = 0.1492$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	mm2	0.054	0.108	$\frac{1}{4}$	0.333	
M2	6h	mm2	0.2941	0.5882	$\frac{1}{4}$	0.333	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0836		
La4	2a	-3m.	0	0	0		

$M2 = 0.75Cu + 0.25Mo$

Experimental: powder, diffractometer, neutrons, time-of-flight,  $R_B = 0.116$

Remarks: Investigation combining electron, X-ray and neutron powder diffraction data. Short interatomic distances for partly occupied site(s). Average structure; the superstructure was refined in space group (59)  $Pmmn$ .

References: [1] Griend D.A.V., Boudin S., Caignaert V., Poeppelmeier K.R., Wang Y., Dravid V.P., Azuma M., Takano M., Hu Z., Jorgensen J.D. (1999), J. Am. Chem. Soc. 121, 4787-4792. [2] Griend D.A.V., Boudin S., Poeppelmeier K.R., Azuma M., Toganoh H., Takano M. (1998), J. Am. Chem. Soc. 120, 11518-11519.

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hP18

Y(Al<sub>0.5</sub>Si<sub>0.5</sub>)(N<sub>0.17</sub>O<sub>0.83</sub>)<sub>3</sub> hP18 (194)  $P6_3/mmc - h^2fa$

**Y<sub>2</sub>AlSiO<sub>5</sub>N** [1]



Structural features: Y atoms and (Al,Si)(O,N)<sub>4</sub> tetrahedra (randomly vertex-linked) in a NiAs-type arrangement.

Gonon M.F. et al. (2000) [1]

Al<sub>0.50</sub>N<sub>0.50</sub>O<sub>2.50</sub>Si<sub>0.50</sub>Y

$a = 0.38359$ ,  $c = 0.97539$  nm,  $c/a = 2.543$ ,  $V = 0.1243$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	6h	mm2	0.108	0.216	$\frac{1}{4}$	0.333	non-colinear O <sub>2</sub>
M2	6h	mm2	0.594	0.188	$\frac{1}{4}$	0.333	
M3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6		
Y4	2a	-3m.	0	0	0		

M1 = 0.833O + 0.167N; M2 = 0.5Al + 0.5Si; M3 = 0.833O + 0.167N

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

Experimental: powder, diffractometer, X-rays,  $R_p = 0.060$

Remarks: Phase referred to as B-(AlNOSiY). Short interatomic distances for partly occupied site(s). Supersedes a pseudo  $\alpha$ -wollastonite structure model in space group (63) *Cmcm* [2].

References: [1] Gonon M.F., Descamps J.C., Cambier F., Thompson D.P. (2000), *Ceram. Int.* 26, 105-111. [2] Thompson D.P. (1989), *Mater. Sci. Forum* 47, 21-42.

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*hP18*

Ba <sub>4</sub> Al <sub>5</sub>	<i>hP18</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $hf^2e$
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**Ba<sub>4</sub>Al<sub>5</sub>** [1]

Structural features: Kagomé-mesh Al<sub>3</sub>, triangle-mesh Ba and hexagon-mesh BaAl layers are stacked along [001]. Pairs of face-linked Al<sub>4</sub> tetrahedra are interconnected via additional Al-Al contacts to form infinite layers.

Fornasini M.L. (1975) [1]

Al<sub>5</sub>Ba<sub>4</sub>

$a = 0.6092$ ,  $c = 1.7782$  nm,  $c/a = 2.919$ ,  $V = 0.5715$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	6h	mm2	0.5091	0.0182	$\frac{1}{4}$		icosahedron Al <sub>6</sub> Ba <sub>6</sub>
Al2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1347		pseudo Frank-Kasper Al <sub>4</sub> Ba <sub>7</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5700		pseudo Frank-Kasper Al <sub>7</sub> Ba <sub>6</sub>
Ba4	4e	3m.	0	0	0.1429		pseudo Frank-Kasper Al <sub>9</sub> Ba <sub>4</sub>

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

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

Remarks: Identical to the phase called BaAl in [2].

References: [1] Fornasini M.L. (1975), *Acta Crystallogr. B* 31, 2551-2552. [2] Bruzzone G., Merlo F. (1975), *J. Less-Common Met.* 39, 1-6.

194  
*hP18*

Cs <sub>2</sub> Ni <sub>3</sub> S <sub>4</sub>	<i>hP18</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $hf^2e$
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**Cs<sub>2</sub>Ni<sub>3</sub>S<sub>4</sub>** [1]

Structural features:  $\text{NiS}_4$  squares share edges to form infinite slabs (double hexagon-mesh S layers); Cs above  $\text{S}_6$  hexagons.

Bronger W. et al. (1988) [1]

$\text{Cs}_2\text{Ni}_3\text{S}_4$

$a = 0.5841$ ,  $c = 1.5109$  nm,  $c/a = 2.587$ ,  $V = 0.4464$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	6h	mm2	0.1667	0.3334	$\frac{1}{4}$		8-vertex polyhedron $\text{S}_4\text{Ni}_4$
S2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1546		non-coplanar triangle $\text{Ni}_3$
Cs3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5868		13-vertex polyhedron $\text{S}_7\text{Ni}_6$
S4	4e	3m.	0	0	0.1544		non-coplanar triangle $\text{Ni}_3$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.055$

References: [1] Bronger W., Rennau R., Schmitz D. (1988), *Z. Kristallogr.* 183, 201-205.

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hP18

$\text{Na}_3\text{Hg}$	<i>hP18</i>	(194) $P6_3/mmc - \text{kec}$
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**$\text{Na}_3\text{Hg } \alpha$**  [2]

Structural features: Na forms a strongly distorted Mg-type (h.c.p.) sublattice; Hg in "trigonal" voids. Variant of  $\text{Na}_3\text{As}$  with site splitting.

Deiseroth H.J., Rochnia M. (1994) [1]

$\text{HgNa}_3$

$a = 0.5405$ ,  $c = 0.9766$  nm,  $c/a = 1.807$ ,  $V = 0.2471$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	12k	.m.	0.268	0.536	0.581	0.333	
Na2	4e	3m.	0	0	0.168	0.5	
Hg3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		

Experimental: single crystal, diffractometer, X-rays,  $R = 0.035$ ,  $T = 223$  K

Remarks: Phase stable at  $T < 309$  K. Short interatomic distances for partly occupied site(s). A similar model with Na in Wyckoff positions  $2b$  and  $4f$  was tested and rejected ( $R = 0.046$ , but unrealistic displacement parameters). The authors state that the structure approaches the non-split model with increasing temperature, but remains better described in the split model up to the transition temperature. The structure was later redetermined in space group (185)  $P6_3cm$  [3]. In table 3 of [1] the Wyckoff position of the Hg site is misprinted as  $2d$  instead of  $2c$ .

References: [1] Deiseroth H.J., Rochnia M. (1994), *Z. Anorg. Allg. Chem.* 620, 1736-1740. [2] Deiseroth H.J., Toelstede D. (1992), *Z. Anorg. Allg. Chem.* 615, 43-48. [3] Range K., Ehrl R., Hafner P. (1996), *J. Alloys Compd.* 240, 19-24.

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hP20

$\text{Ti}_{0.81}\text{S}$	<i>hP20</i>	(194) $P6_3/mmc - f^3\text{eba}$
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**$\text{Ti}_4\text{S}_5$**  [2]

Structural features: Close-packed S layers in  $\text{h}_2\text{chc}$  stacking; Ti in octahedral voids (partial order).

Beckmann O. et al. (1970) [1]

STi<sub>0.81</sub>

$a = 0.3439$ ,  $c = 2.893$  nm,  $c/a = 8.412$ ,  $V = 0.2963$  nm<sup>3</sup>,  $Z = 10$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0519		trigonal prism Ti <sub>6</sub>
Ti2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1966	0.875	octahedron S <sub>6</sub>
S3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6497		octahedron Ti <sub>6</sub>
Ti4	4e	3m.	0	0	0.1057	0.65	octahedron S <sub>6</sub>
S5	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Ti <sub>6</sub>
Ti6	2a	-3m.	0	0	0		octahedron S <sub>6</sub>

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.094$

Remarks: Cell parameters from [3]. In the abstract of [1] the  $z$ -coordinates of former Ti(II) and S(III) are given as 0.1055 and 0.649 but in the text as 0.1057 and 0.6497, respectively.

References: [1] Beckmann O., Boller H., Nowotny H. (1970), Monatsh. Chem. 101, 945-955. [2] Wiegers G.A., Jellinek F. (1970), J. Solid State Chem. 1, 519-525. [3] Flink E., Wiegers G.A., Jellinek F. (1966), Recl. Trav. Chim. Pays-Bas 85, 869-872.

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hP20

H <sub>1.26</sub> Mg <sub>1.06</sub> Fe <sub>0.30</sub> Si <sub>0.43</sub> O <sub>3</sub>	hP20	(194) $P6_3/mmc - f^3$ eba
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**H<sub>2.52</sub>Mg<sub>2.13</sub>Fe<sub>0.59</sub>Si<sub>0.87</sub>O<sub>6</sub>** [1], E' phase

Structural features: Close-packed O layers in hc<sub>2</sub> stacking; Mg and Fe in octahedral, Si in tetrahedral voids (high degree of disorder).

Yang H. et al. (2002) [1]

Fe<sub>0.28</sub>Mg<sub>1.09</sub>O<sub>3</sub>Si<sub>0.36</sub>

$a = 0.2953$ ,  $c = 1.417$  nm,  $c/a = 4.799$ ,  $V = 0.1070$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Si1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.044	0.058	rhombic dodecahedron O <sub>4</sub> Fe <sub>3</sub> MgSi <sub>6</sub>
Mg2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1738	0.544	pentacapped trigonal prism Si <sub>4</sub> O <sub>6</sub> Mg
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5849		13-vertex polyhedron Si <sub>7</sub> Fe <sub>3</sub> Mg <sub>3</sub>
Si4	4e	3m.	0	0	0.1252	0.124	pentacapped trigonal prism O <sub>4</sub> FeMg <sub>3</sub> Si <sub>3</sub>
O5	2b	-6m2	0	0	$\frac{1}{4}$		8-vertex polyhedron Si <sub>2</sub> Mg <sub>6</sub>
Fe6	2a	-3m.	0	0	0	0.284	rhombic dodecahedron Si <sub>8</sub> O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.026$

Remarks: 41.34 wt.% MgO, 25.16 wt.% SiO<sub>2</sub>, and 22.54 wt.% Fe<sub>2</sub>O<sub>3</sub> found by electron microprobe analysis, difference assumed to be H<sub>2</sub>O. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Refinement considering partial substitution of Mg for Fe and vice versa showed no significant deviation from zero.

References: [1] Yang H., Prewitt C.T., Liu Z. (2002), J. Mineral. Petrol. Sci. 97, 137-143.

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hP20

Zr <sub>2</sub> Al <sub>3</sub> C <sub>4</sub>	hP20	(194) $P6_3/mmc - f^3$ eca
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**Zr<sub>2</sub>Al<sub>3</sub>C<sub>5-x</sub>** [1]

Structural features: Close-packed Zr and Al layers in hc<sub>4</sub> stacking (Al-Al-Zr-Zr-Al); C in octahedral voids.

Schuster J.C., Nowotny H. (1980) [1]



$a = 0.33445$ ,  $c = 2.223$  nm,  $c/a = 6.647$ ,  $V = 0.2153$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1161		octahedron Al <sub>3</sub> Zr <sub>3</sub>
Zr2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5588		octahedron C <sub>6</sub>
C3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.705		7-vertex polyhedron CAI <sub>6</sub>
Al4	4 <i>e</i>	3 <i>m</i> .	0	0	0.16		octahedron C <sub>6</sub>
Al5	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism C <sub>6</sub>
C6	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron Zr <sub>6</sub>

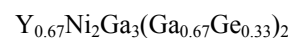
Transformation from published data (*P31c*): origin shift 0 0  $\frac{1}{4}$

Experimental: powder, film, X-rays

Remarks: The description in space group (159) *P31c* in [1] does not take into consideration all symmetry elements (see [3]). Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [2], 50% occupation of site C3 is assumed in [3]. In [1] the *y*-coordinate of former C(1) is misprinted as  $\frac{1}{2}$  instead of  $\frac{1}{3}$  (see [4]). In [4] the *z*-coordinate of former Al(3) is misprinted as 0 instead of  $\frac{1}{2}$  (see [3]).

References: [1] Schuster J.C., Nowotny H. (1980), Z. Metallkd. 71, 341-346. [2] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163. [3] Marsh R.E. (1988), Acta Crystallogr. C 44, 774-775. [4] (1982), Structure Reports 46A, 4.

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hP20



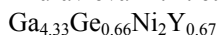
hP20

(194) *P6<sub>3</sub>/mmc* – hf<sup>2</sup>ec

**Y<sub>0.67</sub>Ni<sub>2</sub>Ga<sub>4.33</sub>Ge<sub>0.67</sub>** [1]

Structural features: Slabs consisting of two triangle-mesh Ga layers between two puckered hexagon-mesh Ni(Ga,Ge) layers alternate with layers containing a disordered arrangement of Y atoms and Ga<sub>3</sub> triangles.

Zhuravleva M.A. et al. (2002) [1]



$a = 0.4179$ ,  $c = 1.5993$  nm,  $c/a = 3.827$ ,  $V = 0.2419$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	6 <i>h</i>	<i>mm</i> 2	0.5408	0.0817	$\frac{1}{4}$	0.33	
Ga2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0459		fourcapped trigonal prism Ni <sub>4</sub> Ga <sub>6</sub>
Ni3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.60897		
M4	4 <i>e</i>	3 <i>m</i> .	0	0	0.13351		non-coplanar triangle Ni <sub>3</sub>
Y5	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.67	

M4 = 0.67Ga + 0.33Ge

Experimental: single crystal, diffractometer, neutrons, time-of-flight, R = 0.055, T = 295 K

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

References: [1] Zhuravleva M.A., Chen X.Z., Wang X., Schultz A.J., Ireland J., Kannewurf C.K., Kanatzidis M.G. (2002), Chem. Mater. 14, 3066-3081.

$\text{Sc}_{0.6}\text{Fe}_2\text{Si}_{4.9}$	<i>hP20</i>	(194) $P6_3/mmc - h1^2ec$
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**$\text{Sc}_{1.2}\text{Fe}_4\text{Si}_{9.8}$**  [1];  $\text{Ce}_2\text{Pt}_6\text{Ga}_{15}$  [3]

Structural features: Slabs consisting of two triangle-mesh Si layers between two puckered hexagon-mesh FeSi layers alternate with layers containing a disordered arrangement of Sc atoms and  $\text{Si}_3$  triangles.

Kotur B.Y., Bruvo M. (1991) [1]

$\text{Fe}_2\text{Sc}_{0.60}\text{Si}_{4.93}$

$a = 0.3897$ ,  $c = 1.516$  nm,  $c/a = 3.890$ ,  $V = 0.1994$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	6 <i>h</i>	<i>mm</i> 2	0.542	0.084	$\frac{1}{4}$	0.31	10-vertex polyhedron $\text{Fe}_4\text{Si}_6$
Si2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0459		
Fe3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6089		
Si4	4 <i>e</i>	3 <i>m</i> .	0	0	0.1369		
Sc5	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.6	

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

Remarks: Identical to the phase called  $\text{ScFe}_3\text{Si}_6$  in [2]. Short interatomic distances for partly occupied site(s). In the abstract of [1] the number of formula units per cell  $Z$  is misprinted as 15 instead of 1.

References: [1] Kotur B.Y., Bruvo M. (1991), Sov. Phys. Crystallogr. 36, 787-789 (Kristallografiya 36, 1391-1394). [2] Gladyshevs'kii E.I., Kotur B.Y., Bodak O.I., Skvorchuk V.P. (1977), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1977, 751-754. [3] Kwei G.H., Lawson A.C., Larson A.C., Morosin B., Larson E.M., Canfield P.C. (1996), Acta Crystallogr. B 52, 580-585.

$\text{BaMnO}_3$	<i>hP20</i>	(194) $P6_3/mmc - hgfd$
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**$\text{BaMnO}_3$  4H** [1], perovskite 4H

Structural features: Close-packed  $\text{BaO}_3$  layers in hc stacking; Mn in octahedral ( $\text{O}_6$ ) voids. Pairs of face-linked  $\text{MnO}_6$  octahedra ( $\text{Mn}_2$  dumbbells) share vertices to form a 3D-framework. See Fig. III.25.

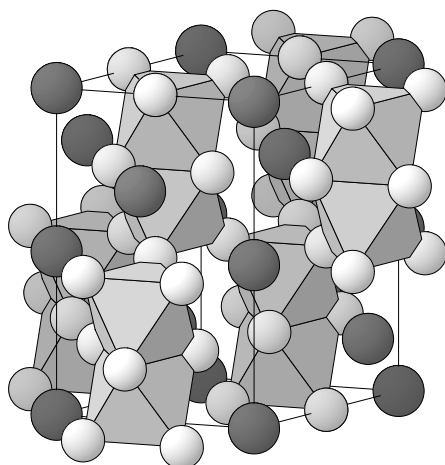


Fig. III.25.  **$\text{BaMnO}_3$  4H**

Arrangement of  $\text{MnO}_6$  octahedra (O atoms light) and Ba atoms (dark).

Hardy A. (1962) [1]

 $\text{BaMnO}_3$  $a = 0.5669$ ,  $c = 0.9375$  nm,  $c/a = 1.654$ ,  $V = 0.2609$  nm<sup>3</sup>,  $Z = 4$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6h	$mm2$	0.16667	0.33333	$\frac{1}{4}$		non-colinear $\text{Mn}_2$
O2	6g	$.2/m.$	$\frac{1}{2}$	0	0		colinear $\text{Mn}_2$
Mn3	4f	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.11		octahedron $\text{O}_6$
Ba4	2d	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron $\text{O}_{12}$
Ba5	2a	$-3m.$	0	0	0		cuboctahedron $\text{O}_{12}$

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

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Phase stable at  $T > 1823$  K. The same data are also reported in [2]. According to [3] the true composition is  $\text{BaMnO}_{3-x}$ ,  $x > 0.25$ .

References: [1] Hardy A. (1962), Acta Crystallogr. 15, 179-181. [2] Hardy A. (1962), Ann. Chim. (Paris) 7, 281-301. [3] Negas T., Roth R.S. (1971), J. Solid State Chem. 3, 323-339.

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hP20

WB <sub>4</sub>	hP20	(194) $P6_3/mmc - \text{ifcb}$
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**WB<sub>4</sub>** [1]Structural features: Hexagon-mesh  $\text{B}_6$  layers alternate with  $\text{W}_2(\text{B}_2)$  layers (a hexagon-mesh W, the hexagons of which are centered by a  $\text{B}_2$  dumbbell perpendicular to the layer) along [001]. B forms a 3D-framework with  $\text{B}_3$  and  $\text{B}_6$  rings.

Romans P.A., Krug M.P. (1966) [1]

 $\text{B}_4\text{W}$  $a = 0.5200$ ,  $c = 0.6340$  nm,  $c/a = 1.219$ ,  $V = 0.1485$  nm<sup>3</sup>,  $Z = 4$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	12i	$.2.$	0.333	0	0		tricapped trigonal prism $\text{B}_5\text{W}_4$
B2	4f	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.615		8-vertex polyhedron $\text{B}_7\text{W}$
W3	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		bicapped hexagonal prism $\text{B}_{14}$
W4	2b	$-6m2$	0	0	$\frac{1}{4}$		hexagonal prism $\text{B}_{12}$

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates. The authors state that W atoms may be replaced by  $\text{B}_2$  pairs within the composition range. Supersedes a report on  $\text{WB}_4$  with a tetragonal cell in [2]. The structure was later refined in space group (147)  $P-3$  [3] ( $\text{W}_{2-x}\text{B}_9$ ).

References: [1] Romans P.A., Krug M.P. (1966), Acta Crystallogr. 20, 313-315. [2] Chrétien A., Helgorsky J. (1961), C. R. Hebd. Seances Acad. Sci. 252, 742-744. [3] Nowotny H., Haschke H., Benesovsky F. (1967), Monatsh. Chem. 98, 547-554.

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hP20

$[\text{H}_2\text{O}]$	hP20	(194) $P6_3/mmc - \text{kf}^2$
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**H<sub>2</sub>O form I hexagonal** [2], ice Ih

Structural features: Non-linear H<sub>2</sub>O molecules (OH<sub>4</sub> tetrahedron with half occupation of the H positions) are interconnected via H bonds to form a tetrahedral framework. O forms a hexagonal diamond-type sublattice. See Fig. III.26.

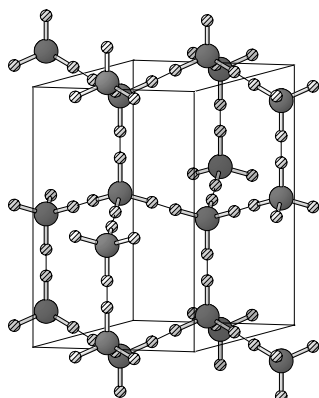


Fig. III.26. H<sub>2</sub>O form I hexagonal

Arrangement of H<sub>2</sub>O molecules (partly occupied H sites light, O atoms dark).

Peterson S.W., Levy H.A. (1957) [1]

D<sub>2</sub>O

$a = 0.4513$ ,  $c = 0.7355$  nm,  $c/a = 1.630$ ,  $V = 0.1297$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	12 <i>k</i>	. <i>m</i> .	0.5449	0.0898	0.5182	0.5	non-colinear DO
O2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0629		tetrahedron D <sub>4</sub>
D3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1989	0.5	colinear DO

Experimental: single crystal, diffractometer, neutrons,  $R = 0.063$ ,  $T = 223$  K

Remarks: Phase stable at  $T > 143$  K. Cell parameters interpolated from literature values. Supersedes a model in space group (186)  $P6_3mc$  in [3]. The authors state that untwinned ice crystals appeared to be piezoelectric. A refinement on neutron powder diffraction data for KOD-doped D<sub>2</sub>O is reported in [4].

References: [1] Peterson S.W., Levy H.A. (1957), Acta Crystallogr. 10, 70-76. [2] Pauling L. (1935), J. Am. Chem. Soc. 57, 2680-2684. [3] Rundle R.E. (1953), J. Chem. Phys. 21, 1311. [4] Leadbetter A.J., Ward R.C., Clark J.W., Tucker P.A., Matsuo T., Suga H. (1985), J. Chem. Phys. 82, 424-428.

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hP20

NbSe <sub>2</sub> H <sub>4</sub>	hP20	(194) $P6_3/mmc - kfca$
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H<sub>4.03</sub>Nb<sub>1.03</sub>Se<sub>2</sub> [1]

Structural features: Close-packed Se layers in BBCC stacking; Nb in trigonal prismatic voids, H in octahedral (Se<sub>6</sub> and distorted NbSe<sub>5</sub>) voids. Filled-up derivative of MoS<sub>2</sub> 2H.

Kulikov L.M. et al. (1991) [1]

H<sub>4</sub>NbSe<sub>2</sub>

$a = 0.34345$ ,  $c = 1.29941$  nm,  $c/a = 3.783$ ,  $V = 0.1327$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
H1	12 <i>k</i>	. <i>m</i> .	0.224	0.448	0.102	0.5	non-colinear H <sub>2</sub>
Se2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.617		non-coplanar hexagon H <sub>6</sub>
Nb3	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism H <sub>6</sub>

H4      2a   -3m.      0      0      0      octahedron H<sub>6</sub>

Experimental: powder, diffractometer, X-rays, R = 0.061

Remarks: Intercalated Nb ignored. We assigned approximate values to the occupancies of the H sites assuming full occupation of Wyckoff position 2a.

References: [1] Kulikov L.M., Aksel'rud L.G., Semenov Kobzar' A.A., Antonova M.M. (1991), Inorg. Mater. 27, 997-1000 (Neorg. Mater. 27, 1186-1189).

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hP20

Tl<sub>2</sub>Pt<sub>3</sub>      hP20      (194) *P*6<sub>3</sub>/*mmc* – kfc

### Pt<sub>3</sub>Tl<sub>2</sub> [1]

Structural features: Two triangle-mesh TlPt<sub>3</sub> layers (Pt forms a Kagomé mesh) alternate with hexagon-mesh Tl<sub>2</sub> layers along [001].

Bhan S. et al. (1968) [1]

Pt<sub>3</sub>Tl<sub>2</sub>

*a* = 0.5645, *c* = 1.3851 nm, *c/a* = 2.454, *V* = 0.3822 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Pt1	12 <i>k</i>	. <i>m</i> .	0.1667	0.3334	0.0875		pseudo Frank-Kasper Tl <sub>5</sub> Pt <sub>6</sub>
Tl2	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5913		non-coplanar hexagon Pt <sub>6</sub>
Tl3	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		15-vertex Frank-Kasper Pt <sub>6</sub> Tl <sub>9</sub>
Tl4	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		15-vertex Frank-Kasper Pt <sub>6</sub> Tl <sub>9</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.190

Remarks: The same data are also reported in [2]. The description in space group (163) *P*-31*c* in [1] and [2] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Bhan S., Gödecke T., Panday P.K., Schubert K. (1968), J. Less-Common Met. 16, 415-425. [2] Schubert K., Bhan S., Biswas T.K., Frank K., Panday P.K. (1968), Naturwissenschaften 55, 542-543.

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hP22

Li<sub>2</sub>(Ga<sub>0.67</sub>Sn<sub>0.33</sub>)<sub>3</sub>      hP22      (194) *P*6<sub>3</sub>/*mmc* – f<sup>3</sup>e<sup>2</sup>c

### Li<sub>2</sub>Ga<sub>2</sub>Sn [1]

Structural features: (Ga,Sn) forms a tetrahedral framework (hc<sub>2</sub> stacking in the notation used for ZnS polytypes).

Blase W. et al. (1993) [1]

Ga<sub>2</sub>Li<sub>2</sub>Sn

*a* = 0.4411, *c* = 2.1645 nm, *c/a* = 4.907, *V* = 0.3647 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.104	0.5	rhombic dodecahedron Li <sub>4</sub> Ga <sub>10</sub>
M2	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5223		rhombic dodecahedron Li <sub>10</sub> Ga <sub>4</sub>
M3	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6476		13-vertex polyhedron Ga <sub>4</sub> Li <sub>9</sub>
Li4	4 <i>e</i>	3 <i>m</i> .	0	0	0.065		rhombic dodecahedron Ga <sub>10</sub> Li <sub>4</sub>
M5	4 <i>e</i>	3 <i>m</i> .	0	0	0.1851		pentacapped trigonal prism Li <sub>7</sub> Ga <sub>4</sub>



Li6      2c   -6m2       $\frac{1}{3}$        $\frac{2}{3}$        $\frac{1}{4}$       rhombic dodecahedron Ga<sub>12</sub>Li<sub>2</sub>

M2 = 0.667Ga + 0.333Sn; M3 = 0.667Ga + 0.333Sn; M5 = 0.667Ga + 0.333Sn

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

Remarks: Li could not be located with certainty. In table 2 of [1] the z-coordinates of former Ga2/Sn2 and Ga3/Sn3 are interchanged (checked on the drawing in fig. 3 and interatomic distances).

References: [1] Blase W., Cordier G., Knip R. (1993), Z. Anorg. Allg. Chem. 619, 1161-1166.

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hP22

Ti <sub>6</sub> Sn <sub>5</sub>	hP22	(194) P6 <sub>3</sub> /mmc – h <sup>2</sup> gca
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### Ti<sub>6</sub>Sn<sub>5</sub> α [1]

Structural features: Ti<sub>3</sub>Sn framework of fused trigonal prisms centered alternatively by additional Ti (ordered vacancies) and Sn. Derivative of ht-Co<sub>2</sub>Ge, [(Ti<sub>3</sub>Sn)(Ti<sub>3</sub>□)]Sn<sub>4</sub>.

Schubert K. et al. (1963) [1]

Sn<sub>5</sub>Ti<sub>6</sub>

a = 0.9248, c = 0.569 nm, c/a = 0.615, V = 0.4214 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	6h	mm2	0.165	0.33	$\frac{1}{4}$		pentacapped trigonal prism Sn <sub>7</sub> Ti <sub>4</sub>
Sn2	6h	mm2	0.795	0.59	$\frac{1}{4}$		14-vertex Frank-Kasper Ti <sub>8</sub> Sn <sub>6</sub>
Ti3	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Sn <sub>6</sub> Ti <sub>6</sub>
Sn4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		15-vertex Frank-Kasper Ti <sub>9</sub> Sn <sub>6</sub>
Sn5	2a	-3m.	0	0	0		rhombic dodecahedron Sn <sub>8</sub> Ti <sub>6</sub>

Remarks: Phase stable at T > 1063 K. The description in space group (163) P-31c in [1] does not take into consideration all symmetry elements of the proposed structure (see [2]).

References: [1] Schubert K., Frank K., Gohle R., Maldonado A., Meissner H.G., Raman A., Rossteutscher W. (1963), Naturwissenschaften 50, 41. [2] Van Vucht J.H.N., Bruning H.A.C.M., Donkersloot H.C., Gomes De Mesquita A.H. (1964), Philips Res. Rep. 19, 407-421.

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hP22

Fe <sub>6.5</sub> Ge <sub>4</sub>	hP22	(194) P6 <sub>3</sub> /mmc – h <sup>2</sup> gca
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### Fe<sub>2-x</sub>Ge η [2]; Co<sub>2-x</sub>(Ga,Ge) η [1]

Structural features: 3D-framework of fused Fe<sub>6</sub> trigonal prisms centered alternatively by additional Fe (partly ordered vacancies) and Ge. Ordering variant of α-Ti<sub>6</sub>Sn<sub>5</sub>. Vacancy derivative of ht-Co<sub>2</sub>Ge, [Fe<sub>4</sub>(Fe<sub>3-x</sub>□)]Ge<sub>4</sub>.

Malaman B. et al. (1980) [1]

Fe<sub>6.50</sub>Ge<sub>4</sub>

a = 0.7976, c = 0.4993 nm, c/a = 0.626, V = 0.2751 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	6h	mm2	0.1615	0.3230	$\frac{1}{4}$	0.833	pentacapped trigonal prism Ge <sub>5</sub> Fe <sub>6</sub>
Ge2	6h	mm2	0.8078	0.6156	$\frac{1}{4}$		square antiprism Fe <sub>8</sub>
Fe3	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Ge <sub>6</sub> Fe <sub>6</sub>
Ge4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		15-vertex Frank-Kasper Fe <sub>9</sub> Ge <sub>6</sub>

Fe5      2a   -3m.      0      0      0      14-vertex Frank-Kasper Fe<sub>8</sub>Ge<sub>6</sub>

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

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

Remarks: Phase stable at T > 823 K; homogeneity range Fe<sub>100-x</sub>Ge<sub>x</sub>, 40 < x < 41 at 823 K, 40 < x < 43.48 at 1108 K. For a higher Ge content substitution takes place and vacancies occur on sites Fe3 and Fe5. Supersedes a report on so-called Fe<sub>3</sub>Ge<sub>2</sub> (r) with a Tl<sub>9</sub>Pd<sub>13</sub>-type structure in [3]. In [2] mixed Fe/Ge occupation is reported for the Fe site in Wyckoff position 6h and partial vacancies for the site in Wyckoff position 6g.

References: [1] Malaman B., Steinmetz J., Roques B. (1980), J. Less-Common Met. 75, 155-176. [2] Kanematsu K. (1965), J. Phys. Soc. Jpn. 20, 36-43. [3] Panday P.K., Schubert K. (1969), J. Less-Common Met. 18, 175-202.

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hP22

Rb<sub>6</sub>SnAs<sub>3</sub>O<sub>0.5</sub>      hP22      (194) P6<sub>3</sub>/mmc – h<sup>3</sup>ca

**Rb<sub>6</sub>SnAs<sub>3</sub>O<sub>0.5</sub>** [1]; Cs<sub>6</sub>SnAs<sub>3</sub>O<sub>0.5</sub> [1]

Structural features: Infinite columns of base-linked SnRb<sub>6</sub> and AsRb<sub>6</sub> trigonal prisms share faces to form AlB<sub>2</sub>-type columns of trigonal section; O in octahedral voids between the columns. Single SnAs<sub>3</sub> trigonal units.

Asbrand M., Eisenmann B. (1994) [1]

As<sub>3</sub>O<sub>0.50</sub>Rb<sub>6</sub>Sn

a = 1.1895, c = 0.6065 nm, c/a = 0.510, V = 0.7432 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	6h	mm2	0.2104	0.4208	$\frac{1}{4}$		single atom Sn
Rb2	6h	mm2	0.5422	0.0844	$\frac{1}{4}$		15-vertex Frank-Kasper Rb <sub>6</sub> As <sub>6</sub> Sn <sub>3</sub>
Rb3	6h	mm2	0.8779	0.7558	$\frac{1}{4}$		non-collinear O <sub>2</sub>
Sn4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle As <sub>3</sub>
O5	2a	-3m.	0	0	0	0.5	8-vertex polyhedron Rb <sub>6</sub> O <sub>2</sub>

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

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

Remarks: Preliminary report in [2].

References: [1] Asbrand M., Eisenmann B. (1994), Z. Anorg. Allg. Chem. 620, 1837-1843. [2] Asbrand M., Eisenmann B. (1994), Z. Kristallogr. Suppl. 8, 261.

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hP22

Cu<sub>2</sub>S      hP22      (194) P6<sub>3</sub>/mmc – hgfdba

**Cu<sub>2</sub>S chalcocite ht** [1], chalcocite high

Structural features: Close-packed S layers in h stacking; Cu in tetrahedral, trigonal and linear voids (disorder).

Will G. et al. (2002) [1]

Cu<sub>2</sub>S

a = 0.4033, c = 0.6739 nm, c/a = 1.671, V = 0.0949 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	6h	mm2	0.183	0.366	1/4	0.125	
Cu2	6g	.2/m.	1/2	0	0	0.162	
Cu3	4f	3m.	1/3	2/3	0.085	0.285	
S4	2d	-6m2	1/3	2/3	3/4		anticuboctahedron Cu <sub>12</sub>
Cu5	2b	-6m2	0	0	1/4	0.52	
Cu6	2a	-3m.	0	0	0	0.05	

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

Experimental: powder, film, X-rays, R = 0.026, T = 573 K

Remarks: Phase stable at 377 < T < 754 K. Short interatomic distances for partly occupied site(s). In table 8 of [1] the z-coordinate of former Cu(4) is misprinted as 1/4 instead of 3/4 (interatomic distances closer to expected ones).

References: [1] Will G., Hinze E., Abdelrahman A.R.M. (2002), Eur. J. Mineral. 14, 591-598.

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hP22

SrMnO <sub>3</sub>	hP22	(194) P6 <sub>3</sub> /mmc – hgfd
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**SrMnO<sub>3</sub> α** [1], perovskite 4H

Structural features: Close-packed SrO<sub>3</sub> layers in hc stacking; Mn in octahedral (O<sub>6</sub>) voids. Pairs of face-linked MnO<sub>6</sub> octahedra (Mn<sub>2</sub> dumbbells) share vertices to form a 3D-framework. Variant of BaMnO<sub>3</sub> 4H with splitting of one of the Sr sites.

Kuroda K. et al. (1981) [1]

MnO<sub>3</sub>Sr

a = 0.5454, c = 0.9092 nm, c/a = 1.667, V = 0.2342 nm<sup>3</sup>, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6h	mm2	0.1821	0.3642	1/4		non-colinear Mn <sub>2</sub>
O2	6g	.2/m.	1/2	0	0		colinear Mn <sub>2</sub>
Mn3	4f	3m.	1/3	2/3	0.1127		octahedron O <sub>6</sub>
Sr4	4e	3m.	0	0	0.012	0.5	
Sr5	2d	-6m2	1/3	2/3	3/4		anticuboctahedron O <sub>12</sub>

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

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

Remarks: Phase stable at T < 1308 K in air. Short interatomic distances for partly occupied site(s).

References: [1] Kuroda K., Ishizawa N., Mizutani N., Kato M. (1981), J. Solid State Chem. 38, 297-299.

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hP22

Rh <sub>6</sub> Sn <sub>4</sub> B	hP22	(194) P6 <sub>3</sub> /mmc – kfcba
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**Rh<sub>6</sub>Sn<sub>4</sub>B** [1]

Structural features: Two triangle-mesh SnRh<sub>3</sub> layers (Rh forms a Kagomé mesh) alternate with hexagon-mesh Sn<sub>2</sub> layers; B in octahedral voids. Single BRh<sub>6</sub> octahedra.

Klünter W., Jung W. (1996) [1]

BRh<sub>6</sub>Sn<sub>4</sub>

a = 0.56001, c = 1.3675 nm, c/a = 2.442, V = 0.3714 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Rh1	12k	.m.	0.16834	0.3367	0.09366		single atom B
Sn2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.57753		9-vertex polyhedron Rh <sub>9</sub>
Sn3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Rh <sub>6</sub>
Sn4	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Rh <sub>6</sub>
B5	2a	-3m.	0	0	0		octahedron Rh <sub>6</sub>

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

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

References: [1] Klünter W., Jung W. (1996), Z. Anorg. Allg. Chem. 622, 2099-2106.

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hP22

Mg <sub>3</sub> ReH <sub>7</sub>	hP22	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kfcba
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### Mg<sub>3</sub>ReH<sub>7</sub> [1]

Structural features: ReH<sub>6</sub> octahedra inside Mg<sub>8</sub> cubes, which share edges to form infinite layers, themselves interconnected via common vertices to form a 3D-framework; additional H in trigonal bipyramidal voids (linear coordination).

Huang B. et al. (1993) [1]

D<sub>7</sub>Mg<sub>3</sub>Re

$a = 0.48539$ ,  $c = 1.05699$  nm,  $c/a = 2.178$ ,  $V = 0.2157$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12k	.m.	0.1656	0.3312	0.5962		single atom Re
Mg2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0702		10-vertex polyhedron D <sub>10</sub>
D3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Mg <sub>2</sub>
Mg4	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism D <sub>6</sub>
Re5	2a	-3m.	0	0	0		octahedron D <sub>6</sub>

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.029, T = 295 K

References: [1] Huang B., Yvon K., Fischer P. (1993), J. Alloys Compd. 197, 97-99.

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hP22

LiMg <sub>2</sub> RuH <sub>7</sub>	hP22	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kfcba
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### LiMg<sub>2</sub>RuH<sub>7</sub> [1]

Structural features: RuH<sub>6</sub> octahedra inside Mg<sub>6</sub>Li<sub>2</sub> cubes, which share edges to form infinite layers, themselves interconnected via common vertices to form a 3D-framework; additional H atoms in trigonal bipyramidal (Mg<sub>2</sub>Li<sub>3</sub>) voids (linear coordination Mg-H-Mg). Ordering variant of Mg<sub>3</sub>ReH<sub>7</sub>.

Huang B. et al. (1994) [1]

D<sub>7</sub>LiMg<sub>2</sub>Ru

$a = 0.46998$ ,  $c = 1.06674$  nm,  $c/a = 2.270$ ,  $V = 0.2041$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12k	.m.	0.167	0.334	0.5945		single atom Ru
Mg2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0764		10-vertex polyhedron D <sub>10</sub>
D3	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Mg <sub>2</sub>
Li4	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism D <sub>6</sub>

Ru5      2a   -3m.      0      0      0      octahedron D<sub>6</sub>

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.076, T = 295 K

References: [1] Huang B., Yvon K., Fischer P. (1994), J. Alloys Compd. 210, 243-246.

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hP22

K <sub>2</sub> [SO <sub>4</sub> ]	hP22	(194) P6 <sub>3</sub> /mmc – kfdca
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### K<sub>2</sub>SO<sub>4</sub> α [1]

Structural features: K atoms and SO<sub>4</sub> tetrahedra (orientational disorder with one vertex up or down) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Miyake M. et al. (1980) [1]

K<sub>2</sub>O<sub>4</sub>S

*a* = 0.5947, *c* = 0.8375 nm, *c/a* = 1.408, *V* = 0.2565 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.212	0.424	0.188	0.5	single atom O
O2	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.09	0.5	4-vertex polyhedron SO <sub>3</sub>
K3	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		bicapped hexagonal prism O <sub>14</sub>
S4	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		8-vertex polyhedron O <sub>8</sub>
K5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.086, T = 1073 K

Remarks: Phase stable at T > 853 K. Short interatomic distances for partly occupied site(s). Supersedes a structure proposal in space group (164) *P*-3*m*1 reported in [3]. This space group, (186) *P*6<sub>3</sub>*mc* and (190) *P*-62*c* were tested and rejected. According to the authors of [2], this particular model for disorder is preferred above ~1000 K. A different model for disorder is proposed in [4].

References: [1] Miyake M., Morikawa H., Iwai S.I. (1980), Acta Crystallogr. B 36, 532-536. [2] Arnold H., Kurtz W., Richter Zinnius A., Bethke J., Heger G. (1981), Acta Crystallogr. B 37, 1643-1651. [3] Bredig M.A. (1942), J. Phys. Chem. 46, 747-764. [4] Van Den Berg A.J., Tuinstra F. (1978), Acta Crystallogr. B 34, 3177-3181.

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hP22

BaReH <sub>9</sub>	hP22	(194) P6 <sub>3</sub> /mmc – khca
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### BaReH<sub>9</sub> [1]

Structural features: Ba atoms and ReH<sub>6</sub>H<sub>3</sub> tricapped trigonal prisms in a NiAs-type arrangement. See Fig. III.27.

Stetson N.T. et al. (1994) [1]

BaH<sub>9</sub>Re

*a* = 0.5287, *c* = 0.9323 nm, *c/a* = 1.763, *V* = 0.2257 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	12 <i>k</i>	. <i>m</i> .	0.55	0.1	0.61		single atom Re
H2	6 <i>h</i>	<i>mm</i> 2	0.15	0.3	<sup>1</sup> / <sub>4</sub>		single atom Re
Re3	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism H <sub>9</sub>
Ba4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		18-vertex polyhedron H <sub>18</sub>

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.022$ ,  $T = 293\text{ K}$

Remarks: Idealized coordinates for the H sites from IR and NMR spectra.

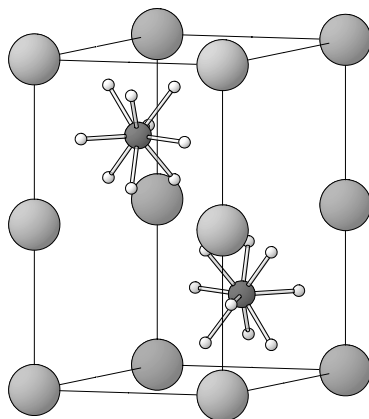


Fig. III.27. **BaReH<sub>9</sub>**

Arrangement of  $\text{ReH}_9$  tricapped trigonal prisms (Re atoms dark, H atoms light) and Ba atoms (medium).

References: [1] Stetson N.T., Yvon K., Fischer P. (1994), *Inorg. Chem.* 33, 4598-4599.

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hP22

$\text{CaNiAl}_9$	<i>hP22</i>	(194) $P6_3/mmc - khcb$
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#### **CaNiAl<sub>9</sub>** [1]

Structural features:  $\text{CaNiAl}_3$  layers (an Al Kagomé mesh, all hexagons of which are centered by Ca and half of the triangles by Ni) and  $\text{Al}_6$  layers (hexagons, squares and triangles) alternate along [001]. Ca atoms and  $\text{NiAl}_6\text{Al}_3$  tricapped trigonal prisms in an ordered graphite-type arrangement.

Manyako N.B. et al. (1987) [1]

$\text{Al}_9\text{CaNi}$

$a = 0.76002$ ,  $c = 0.79457\text{ nm}$ ,  $c/a = 1.045$ ,  $V = 0.3975\text{ nm}^3$ ,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12k	.m.	0.2084	0.4168	0.0153		monocapped square prism $\text{NiAl}_8$
Al2	6h	$mm2$	0.5226	0.0452	$\frac{1}{4}$		monocapped square prism $\text{NiAl}_8$
Ni3	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism $\text{Al}_9$
Ca4	2b	$-6m2$	0	0	$\frac{1}{4}$		23-vertex polyhedron $\text{Al}_{18}\text{Ca}_2\text{Ni}_3$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.059$

References: [1] Manyako N.B., Zarechnyuk O.S., Yanson T.I. (1987), *Sov. Phys. Crystallogr.* 32, 816-817 (*Kristallografiya* 32, 1389-1391).

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hP22

$\text{CsCrI}_3$	<i>hP22</i>	(194) $P6_3/mmc - khda$
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#### **CsCrI<sub>3</sub> α** [2], perovskite 2H

Structural features: Close-packed  $\text{CsI}_3$  layers in h stacking; Cr in octahedral ( $\text{I}_6$ ) voids.  $\text{CrI}_6$  octahedra share faces to form infinite chains. Variant of  $\text{BaNiO}_3$  with partial splitting of the I site leading to elongated octahedra.

Crama W.J., Zandbergen H.W. (1981) [1]

CrCsI<sub>3</sub>

$a = 0.8107$ ,  $c = 0.6917$  nm,  $c/a = 0.853$ ,  $V = 0.3937$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
I1	12 <i>k</i>	. <i>m</i> .	0.1677	0.3354	0.216	0.25	
I2	6 <i>h</i>	<i>mm</i> 2	0.1555	0.311	<sup>1</sup> / <sub>4</sub>	0.5	
Cs3	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		
Cr4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

Experimental: single crystal, diffractometer, X-rays,  $R = 0.027$ ,  $T = 295$  K

Remarks: Phase stable at  $T > 150$  K. Short interatomic distances for partly occupied site(s). An alternative model with both I sites in Wyckoff position 12*k* was also refined ( $R = 0.027$ ).

References: [1] Crama W.J., Zandbergen H.W. (1981), Acta Crystallogr. B 37, 1027-1031. [2] Zandbergen H.W., Ijdo D.J.W. (1980), J. Solid State Chem. 34, 65-70.

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hP24

NbGe <sub>0.25</sub> S <sub>2</sub>	hP24	(194) $P6_3/mmc - f^3e^2ca$
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Ge<sub>0.25</sub>NbS<sub>2</sub> 6H [1]

Structural features: Close-packed S layers in AABBCCAACCBB stacking; Nb in trigonal prismatic, Ge in octahedral voids (disorder for the latter).

Pocha R., Johrendt D. (2002) [1]

Ge<sub>0.26</sub>NbS<sub>2</sub>

$a = 0.3339$ ,  $c = 3.7326$  nm,  $c/a = 11.179$ ,  $V = 0.3604$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ge1	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1645	0.233	octahedron S <sub>6</sub>
S2	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5484		trigonal prism Nb <sub>3</sub> Ge <sub>3</sub>
S3	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6324		octahedron Ge <sub>3</sub> Nb <sub>3</sub>
Nb4	4 <i>e</i>	3 <i>m</i> .	0	0	0.0909		trigonal prism S <sub>6</sub>
S5	4 <i>e</i>	3 <i>m</i> .	0	0	0.208		trigonal prism Nb <sub>3</sub> Ge <sub>3</sub>
Nb6	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		trigonal prism S <sub>6</sub>
Ge7	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.325	octahedron S <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.035$ ,  $T = 298$  K

References: [1] Pocha R., Johrendt D. (2002), Z. Naturforsch. B 57, 1367-1374.

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hP24

ZrAlC <sub>1.67</sub>	hP24	(194) $P6_3/mmc - f^4eba$
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ZrAlC<sub>2-x</sub> [1]

Structural features: Close-packed Zr and Al layers in hc<sub>5</sub> stacking; C in octahedral voids (disordered vacancies).

Mikhalenko S.I. et al. (1979) [1]

AlC<sub>1.67</sub>Zr

$a = 0.3347$ ,  $c = 2.765$  nm,  $c/a = 8.261$ ,  $V = 0.2682$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.095		octahedron C <sub>6</sub>
C2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.214	0.833	7-vertex polyhedron CAI <sub>6</sub>
C3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.548	0.833	octahedron Zr <sub>6</sub>
Al4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.677		octahedron C <sub>6</sub>
C5	4e	3m.	0	0	0.141	0.833	octahedron Al <sub>3</sub> Zr <sub>3</sub>
Al6	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism C <sub>6</sub>
Zr7	2a	-3m.	0	0	0		octahedron C <sub>6</sub>

Experimental: single crystal, oscillation photographs, X-rays, R = 0.101

Remarks: Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [2], 50% occupation of site C3 and full occupation of sites C2 and C5 are expected. An ordered structure in space group (186)  $P6_3mc$  is proposed in [4] (preliminary data in [5] and [6]). In [3] x in the chemical formula is misprinted as 0.23 instead of 0.33.

References: [1] Mikhalenko S.I., Kuz'ma Y.B., Popov V.E., Gurin V.N., Nechitailov A.P. (1979), Inorg. Mater. 15, 1532-1535 (Izv. Akad. Nauk SSSR, Neorg. Mater. 15, 1948-1951). [2] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163. [3] (1981), Structure Reports 45A, 6. [4] Gesing T.M., Jeitschko W. (1998), J. Solid State Chem. 140, 396-401. [5] Gesing T.M., Jeitschko W. (1994), Z. Kristallogr. Suppl. 8, 432. [6] Gesing T.M., Jeitschko W. (1994), Proc. Journ. Actinides, 24th, Obergurgl (Austria) 1994, 84-85.

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hP24

Yb <sub>2</sub> Fe <sub>3</sub> O <sub>7</sub>	hP24	(194) $P6_3/mmc - f^4ecb$
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#### Yb<sub>2</sub>Fe<sub>3</sub>O<sub>7</sub> [2]

Structural features: Close-packed O layers in h<sub>2</sub>c<sub>2</sub>hc<sub>2</sub> stacking; Yb in octahedral, Fe in trigonal bipyramidal voids. Double and single slabs of vertex-linked FeO<sub>5</sub> trigonal bipyramids (also common edges for double layers) share vertices with infinite slabs of edge-linked YbO<sub>6</sub> octahedra (compressed trigonal antiprisms) to form a 3D-framework.

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

Fe<sub>3</sub>O<sub>7</sub>Yb<sub>2</sub>

a = 0.347, c = 2.845 nm, c/a = 8.199, V = 0.2967 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.035		tetrahedron Fe <sub>4</sub>
Yb2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1482		octahedron O <sub>6</sub>
(Fe <sup>2+</sup> ) <sub>3</sub>	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5426		trigonal bipyramid O <sub>5</sub>
O4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.615		tetrahedron FeYb <sub>3</sub>
O5	4e	3m.	0	0	0.180		tetrahedron FeYb <sub>3</sub>
O6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Fe <sub>3</sub>
(Fe <sup>3+</sup> ) <sub>7</sub>	2b	-6m2	0	0	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>

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

References: [1] Malaman B., Evrard O., Tannières N., Courtois A., Protas J. (1976), Acta Crystallogr. B 32, 749-752. [2] Kato K., Kawada I., Kimizuka N., Shindo I., Katsura T. (1976), Z. Kristallogr. 143, 278-284.



$\text{Nd}_2[\text{CO}_3]\text{O}_2$	<i>hP24</i>	(194) $P6_3/mmc - h^2f^2e$
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**$\text{Nd}_2\text{O}_2(\text{CO}_3)$**  [1];  $\text{La}_2\text{O}_2(\text{CO}_3)$  form II [2]

Structural features:  $\text{NdO}_8$  cubes share edges to form double slabs, which are interconnected via common vertices (split site) to form a 3D-framework; C in trigonal voids.  $\text{CO}_3$  trigonal units parallel to [001] (partial orientational disorder).

Christensen A.N. (1970) [1]

$\text{C}_3\text{Nd}_2\text{O}_5$

$a = 0.3974$ ,  $c = 1.5703$  nm,  $c/a = 3.951$ ,  $V = 0.2148$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	6 <i>h</i>	<i>mm2</i>	0.13	0.26	$\frac{1}{4}$		single atom O
O2	6 <i>h</i>	<i>mm2</i>	0.28	0.56	$\frac{1}{4}$	0.333	
Nd3	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0944		
O4	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.557		tetrahedron Nd <sub>4</sub>
O5	4 <i>e</i>	3 <i>m.</i>	0	0	0.178		non-coplanar triangle C <sub>3</sub>

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

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

References: [1] Christensen A.N. (1970), Acta Chem. Scand. 24, 2440-2446. [2] Attfield J.P., Ferey G. (1989), J. Solid State Chem. 82, 132-138.

$\text{MgNi}_2$	<i>hP24</i>	(194) $P6_3/mmc - hgf^2e$
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**$\text{MgNi}_2$**  [2], Laves phase 4H, Strukturbericht notation C36

Structural features:  $\text{Mg}(\text{Mg}_4\text{Ni}_{12})$  Friauf polyhedra ( $\text{Ni}_{12}$  truncated tetrahedron +  $\text{Mg}_4$  tetrahedron) share the hexagonal faces of the truncated tetrahedra to form a 3D-framework.  $\text{Ni}_4$  tetrahedra share faces and vertices to form a 3D-framework. Kagomé-mesh  $\text{Ni}_3$  layers and puckered triangle-mesh  $\text{Mg}_2\text{Ni}$  layers alternate along [001]. Laves-type slabs in hc stacking. Tetrahedrally close-packed structure (Frank-Kasper phase). See Fig. III.28.

Komura Y., Tokunaga K. (1980) [1]

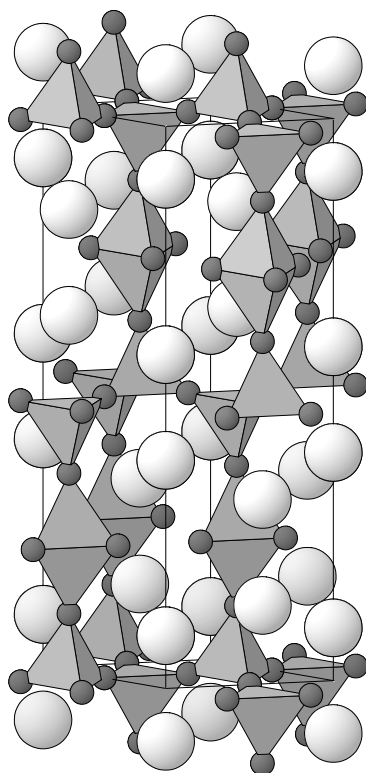
$\text{MgNi}_2$

$a = 0.4824$ ,  $c = 1.5826$  nm,  $c/a = 3.281$ ,  $V = 0.3190$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	6 <i>h</i>	<i>mm2</i>	0.16429	0.32858	$\frac{1}{4}$		icosahedron $\text{Ni}_6\text{Mg}_6$
Ni2	6 <i>g</i>	$\frac{1}{2}/m.$	$\frac{1}{2}$	0	0		icosahedron $\text{Ni}_6\text{Mg}_6$
Ni3	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.12514		icosahedron $\text{Ni}_6\text{Mg}_6$
Mg4	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.65583		16-vertex Frank-Kasper $\text{Ni}_{12}\text{Mg}_4$
Mg5	4 <i>e</i>	3 <i>m.</i>	0	0	0.09400		16-vertex Frank-Kasper $\text{Ni}_{12}\text{Mg}_4$

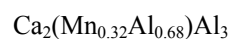
Experimental: single crystal, diffractometer, X-rays,  $R = 0.053$

References: [1] Komura Y., Tokunaga K. (1980), Acta Crystallogr. B 36, 1548-1554. [2] Laves F., Löhberg K. (1934), Nachr. Ges. Wiss. Göttingen, Math.-Phys. Kl., Fachgruppe 1, 1, 59-66.

Fig. III.28. **MgNi<sub>2</sub>**

Arrangement of Ni<sub>4</sub> tetrahedra (Ni atoms small) and Mg atoms (large).

194  
hP24

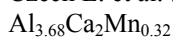


hP24

(194)  $P6_3/mmc - \text{hg}\bar{f}^2e$ **CaMn<sub>x</sub>Al<sub>2-x</sub>** [1]

Structural features: Kagomé-mesh Al<sub>3</sub> and puckered triangle-mesh Ca<sub>2</sub>(Al,Mn) layers alternate along [001]. Laves-type slabs in hc stacking. Ordering variant of MgNi<sub>2</sub>.

Czech E. et al. (1983) [1]



$a = 0.5723$ ,  $c = 1.8264$  nm,  $c/a = 3.191$ ,  $V = 0.5181$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	6h	mm2	0.1675	0.335	$\frac{1}{4}$		icosahedron Al <sub>6</sub> Ca <sub>6</sub>
Al2	6g	2/m.	$\frac{1}{2}$	0	0		icosahedron Al <sub>6</sub> Ca <sub>6</sub>
M3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1264		icosahedron Al <sub>6</sub> Ca <sub>6</sub>
Ca4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.656		16-vertex Frank-Kasper Al <sub>12</sub> Ca <sub>4</sub>
Ca5	4e	3m.	0	0	0.0935		16-vertex Frank-Kasper Al <sub>12</sub> Ca <sub>4</sub>

$$\text{M3} = 0.68\text{Al} + 0.32\text{Mn}$$

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

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

Remarks: Homogeneity range CaMn<sub>x</sub>Al<sub>2-x</sub>, 0.16 < *x* < 0.32.

References: [1] Czech E., Cordier G., Schäfer H. (1983), J. Less-Common Met. 90, 109-119.

194  
hP24

$\text{Ca}_2[\text{SiO}_4]$	<i>hP24</i>	(194) $P6_3/mmc - \text{kf}^2\text{ca}$
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**Ca<sub>2</sub>SiO<sub>4</sub> α [2], cement α-C<sub>2</sub>S**

Structural features: Ca atoms (in part split site) and SiO<sub>4</sub> tetrahedra (rotational disorder) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Mumme W.G. et al. (1995) [1]

Ca<sub>2</sub>O<sub>4</sub>Si

$a = 0.542$ ,  $c = 0.7027$  nm,  $c/a = 1.296$ ,  $V = 0.1788$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.17	0.34	0.16	0.5	single atom O
O2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.03	0.5	trigonal bipyramid SiCaO <sub>3</sub>
Ca3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.71	0.5	
Si4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		8-vertex polyhedron O <sub>8</sub>
Ca5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, X-rays

Remarks: Phase stable at  $T > 1698$  K. Short interatomic distances for partly occupied site(s). Space groups (164)  $P-3m1$  and (186)  $P6_3mc$  were tested and rejected.

References: [1] Mumme W.G., Hill R.J., Bushnell Wye G., Segnit E.R. (1995), Neues Jahrb. Mineral., Abh. 169, 35-68. [2] Udagawa S., Urabe K., Yano T. (1977), Semento Gijutsu Nenpo 31, 26-29.

194  
hP24

$\text{KLi}[\text{SO}_4]$	<i>hP24</i>	(194) $P6_3/mmc - \text{kf}^2\text{da}$
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**KLiSO<sub>4</sub> form VI [1]**

Structural features: K and Li atoms and SO<sub>4</sub> tetrahedra (partial rotational disorder) in a ZrBeSi-type arrangement; Li displaced from Zr<sub>6</sub> prism centers (split site).

Solans X. et al. (1999) [1]

KLiO<sub>4</sub>S

$a = 0.52997$ ,  $c = 0.88021$  nm,  $c/a = 1.661$ ,  $V = 0.2141$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.515	0.03	0.195	0.5	
Li2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.115	0.5	tetrahedron O <sub>4</sub>
O3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.582	0.5	
S4	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		
K5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

Experimental: powder, diffractometer, X-rays,  $wR_p = 0.061$ ,  $T = 973$  K

Remarks: Phase stable at  $T > 941$  K. Short interatomic distances for partly occupied site(s).

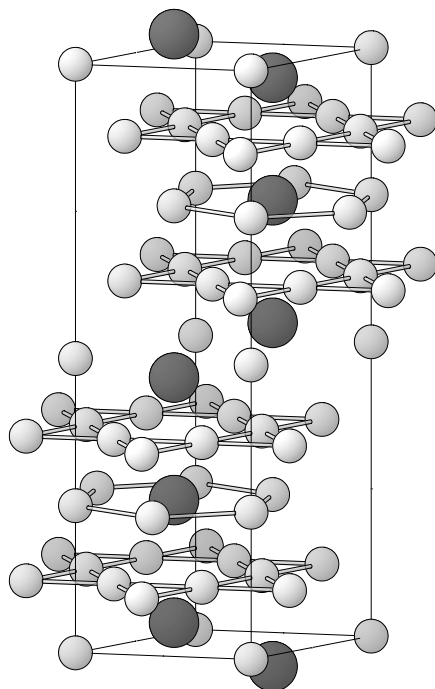
References: [1] Solans X., Calvet M.T., Martinez Sarrion M.L., Mestres L., Bakkali A., Bocanegra E., Mata J., Herraiz M. (1999), J. Solid State Chem. 148, 316-324.

194  
hP24

$\text{CeNi}_3$	<i>hP24</i>	(194) $P6_3/mmc - \text{kfdcba}$
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**CeNi<sub>3</sub>** [1]

Structural features: Intergrowth of Laves- and CaCu<sub>5</sub>-type slabs (common Kagomé-mesh layers) in the ratio 1:1, consecutive Laves-type slabs in h stacking. See Fig. III.29.

Fig. III.29. **CeNi<sub>3</sub>**

Arrangement of Ce (dark) and Ni (light) atoms.

Cromer D.T., Olsen C.E. (1959) [1]

CeNi<sub>3</sub>

$a = 0.498$ ,  $c = 1.654$  nm,  $c/a = 3.321$ ,  $V = 0.3552$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	12k	.m.	0.1666	0.3332	0.12715		icosahedron Ni <sub>7</sub> Ce <sub>5</sub>
Ce2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.54178		16-vertex Frank-Kasper Ni <sub>12</sub> Ce <sub>4</sub>
Ce3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper Ni <sub>18</sub> Ce <sub>2</sub>
Ni4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		icosahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ni5	2b	-6m2	0	0	$\frac{1}{4}$		icosahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ni6	2a	-3m.	0	0	0		icosahedron Ni <sub>6</sub> Ce <sub>6</sub>

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

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

References: [1] Cromer D.T., Olsen C.E. (1959), Acta Crystallogr. 12, 689-694.

194  
hP24

Ce <sub>3</sub> Co <sub>8</sub> Si	hP24	(194) $P6_3/mmc$ – kfdcba
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**Ce<sub>3</sub>Co<sub>8</sub>Si** [1]

Structural features: Intergrowth of ternary Laves- and binary CaCu<sub>5</sub>-type slabs (common Kagomé-mesh layers) in the ratio 1:1, consecutive Laves-type slabs in h stacking. Ordering variant of CeNi<sub>3</sub>.

Bodak O.I. (1971) [1]

 $\text{Ce}_3\text{Co}_8\text{Si}$  $a = 0.496$ ,  $c = 1.645$  nm,  $c/a = 3.317$ ,  $V = 0.3505$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Co1	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.127		icosahedron $\text{Co}_6\text{SiCe}_5$
Ce2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5418		16-vertex Frank-Kasper $\text{Co}_9\text{Si}_3\text{Ce}_4$
Ce3	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper $\text{Co}_{18}\text{Ce}_2$
Co4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		icosahedron $\text{Co}_9\text{Ce}_3$
Co5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		icosahedron $\text{Co}_9\text{Ce}_3$
Si6	2 <i>a</i>	-3 <i>m</i> .	0	0	0		icosahedron $\text{Co}_6\text{Ce}_6$

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: powder, diffractometer, X-rays,  $R = 0.144$ Remarks: Atom coordinates from [2] ( $\text{CeNi}_3$ ), ordered arrangement of Co and Si confirmed.

References: [1] Bodak O.I. (1971), Visn. L'viv. Derzh. Univ., Ser. Khim. 12, 22-25. [2] Cromer D.T., Olsen C.E. (1959), Acta Crystallogr. 12, 689-694.

194  
*hP24*

$\text{Dy}_3\text{Ni}_7\text{B}_2$	<i>hP24</i>	(194) $P6_3/mmc - kfdcba$
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 **$\text{Dy}_3\text{Ni}_7\text{B}_2$**  [1];  $\text{CaAg}_{1.3}\text{Al}_{1.7}$  [2]Structural features: Intergrowth of binary Laves- and ternary  $\text{CaCu}_5$ -type ( $\text{CeCo}_3\text{B}_2$ ) slabs (common Kagomé-mesh layers) in the ratio 1:1, consecutive Laves-type slabs in h stacking. Ordering variant of  $\text{CeNi}_3$ .

Kuz'ma Y.B., Chaban N.F. (1980) [1]

 $\text{B}_2\text{Dy}_3\text{Ni}_7$  $a = 0.5078$ ,  $c = 1.4331$  nm,  $c/a = 2.822$ ,  $V = 0.3200$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	12 <i>k</i>	. <i>m</i> .	0.161	0.322	0.149		pseudo Frank-Kasper $\text{B}_2\text{Ni}_6\text{Dy}_5$
Dy2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.529		16-vertex Frank-Kasper $\text{Ni}_{12}\text{Dy}_4$
Dy3	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper $\text{Ni}_{12}\text{B}_6\text{Dy}_2$
B4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $\text{Ni}_6$
B5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism $\text{Ni}_6$
Ni6	2 <i>a</i>	-3 <i>m</i> .	0	0	0		14-vertex Frank-Kasper $\text{Ni}_6\text{Dy}_6\text{B}_2$

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: single crystal, photographs, X-rays,  $R = 0.122$ 

References: [1] Kuz'ma Y.B., Chaban N.F. (1980), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1980(1), 86-89. [2] Cordier G., Czech E., Dörsam G.R., Henseleit R., Röhr C., Mehner A., Thies S., Geibel C. (1991), J. Less-Common Met. 169, 55-72.

194  
*hP24*

$\text{YRh}_2\text{Si}$	<i>hP24</i>	(194) $P6_3/mmc - kfdcba$
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 **$\text{YRh}_2\text{Si}$**  [1]Structural features: Intergrowth of ternary Laves- and  $\text{CaCu}_5$ -type ( $\text{CeCo}_3\text{B}_2$ ) slabs (common Kagomé-mesh layers) in the ratio 1:1, consecutive Laves-type slabs in h stacking. Ordering variant of  $\text{CeNi}_3$ .

Paccard L., Paccard D. (1985) [1]

Rh<sub>2</sub>SiY

$a = 0.5495$ ,  $c = 1.503$  nm,  $c/a = 2.735$ ,  $V = 0.3930$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Rh1	12k	.m.	0.1666	0.3332	0.131		pseudo Frank-Kasper Si <sub>3</sub> Rh <sub>5</sub> Y <sub>5</sub>
Y2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5369		16-vertex Frank-Kasper Rh <sub>9</sub> Y <sub>4</sub> Si <sub>3</sub>
Y3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper Si <sub>6</sub> Y <sub>2</sub> Rh <sub>12</sub>
Si4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		icosahedron Rh <sub>6</sub> Si <sub>3</sub> Y <sub>3</sub>
Si5	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Rh <sub>6</sub>
Si6	2a	-3m.	0	0	0		octahedron Rh <sub>6</sub>

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

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

References: [1] Paccard L., Paccard D. (1985), J. Less-Common Met. 109, 229-232.

194  
hP24

K <sub>2</sub> [SO <sub>4</sub> ]	hP24	(194) P6 <sub>3</sub> /mmc – khdc
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**K<sub>2</sub>SO<sub>4</sub> α** [1]; Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> super α [2]

Structural features: K atoms and SO<sub>4</sub> tetrahedra (orientational disorder with one edge parallel to [001]) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Arnold H. et al. (1981) [1]

K<sub>2</sub>O<sub>4</sub>S

$a = 0.5886$ ,  $c = 0.8118$  nm,  $c/a = 1.379$ ,  $V = 0.2436$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.25	0.5	0.116	0.333	single atom O
O2	6h	mm2	0.1981	0.3962	$\frac{1}{4}$	0.667	non-colinear O <sub>2</sub>
K3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>
S4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism O <sub>9</sub>
K5	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, neutrons, R = 0.065, T = 847 K

Remarks: Phase stable at T > 853 K. We transformed the data from a non-conventional setting with an orthohexagonal cell. The authors of [1] state that this particular model for orientational disorder is more likely below ~1000 K.

References: [1] Arnold H., Kurtz W., Richter Zinnius A., Bethke J., Heger G. (1981), Acta Crystallogr. B 37, 1643-1651. [2] Knowles J.C., Gibson I.R., Abrahams I. (1999), Bioceram., Proc. Int. Symp. Ceram. Med. 1999, 341-344.

194  
hP24

NbSe <sub>2</sub>	hP24	(194) P6 <sub>3</sub> /mmc – khfb
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**NbSe<sub>2</sub> 2H It** [1]

Structural features: Close-packed Se layers in BBCC stacking; Nb in trigonal prismatic voids (BaB CaC). NbSe<sub>6</sub> trigonal prisms share edges to form infinite slabs. Deformation derivative of NbS<sub>2</sub> 2H with distortions in the Nb triangle mesh.

Marezio M. et al. (1972) [1]

NbSe<sub>2</sub>

$a = 0.688$ ,  $c = 1.2482$  nm,  $c/a = 1.814$ ,  $V = 0.5117$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Se1	12 <i>k</i>	. <i>m</i> .	0.1678	0.3356	0.616		non-coplanar triangle Nb <sub>3</sub>
Nb2	6 <i>h</i>	<i>mm</i> 2	0.5033	0.0066	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>
Se3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1178		non-coplanar triangle Nb <sub>3</sub>
Nb4	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.028$ ,  $T = 15$  K

Remarks: Phase stable at  $T < 40$  K. Models in space groups (186)  $P6_3mc$  and (194)  $P6_3/mmc$  with  $\frac{1}{4}$  cell volume were tested and rejected ( $R = 0.031$ ).

References: [1] Marezio M., Dernier P.D., Menth A., Hull G.W. Jr. (1972), J. Solid State Chem. 4, 425-429.

194  
*hP*24

PuAl <sub>3</sub>	<i>hP</i> 24	(194) $P6_3/mmc$ – khfb
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**PuAl<sub>3</sub>** [2]; VCo<sub>3</sub> rt [3]

Structural features: Close-packed PuAl<sub>3</sub> layers (Pu forms a triangle mesh) in  $hc_2$  stacking. Substitution derivative of Tb t.h.c.p. See Fig. III.30.

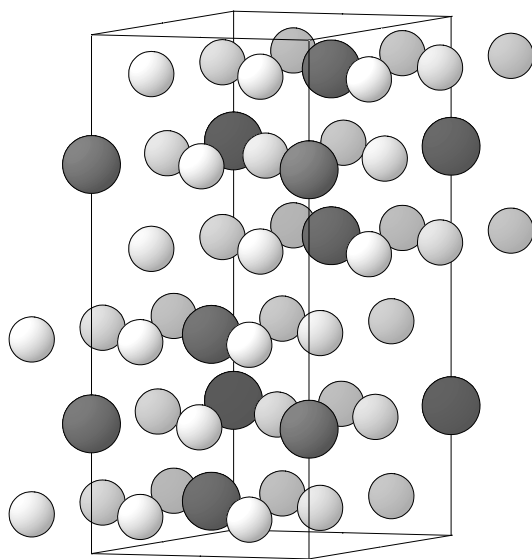


Fig. III.30. **PuAl<sub>3</sub>**

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

Larson A.C. et al. (1957) [1]

Al<sub>3</sub>Pu

$a = 0.610$ ,  $c = 1.447$  nm,  $c/a = 2.372$ ,  $V = 0.4663$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12 <i>k</i>	. <i>m</i> .	0.1663	0.3326	0.5815		cuboctahedron Al <sub>8</sub> Pu <sub>4</sub>
Al2	6 <i>h</i>	<i>mm</i> 2	0.5160	0.0320	$\frac{1}{4}$		anticuboctahedron Al <sub>8</sub> Pu <sub>4</sub>
Pu3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0892		cuboctahedron Al <sub>12</sub>

Pu4      2b   -6m2      0      0       $\frac{1}{4}$       anticuboctahedron Al<sub>12</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.109

Remarks: Space group (190) *P*-62*c* was tested and rejected. The description of rt-VCo<sub>3</sub> in space group (187) *P*-6*m*2 in [3] does not take into consideration all symmetry elements of the proposed structure (see [4]). The same is true for the description of PuAl<sub>3</sub> in [5] (stated by the authors).

References: [1] Larson A.C., Cromer D.T., Stambaugh C.K. (1957), Acta Crystallogr. 10, 443-446. [2] Coffinberry A.S., Ellinger F.H. (1955), Proc. Int. Conf. Peaceful Uses At. Energy, 1st, A/CONF/8/P/826, 21 pp.. [3] Saito S. (1959), Acta Crystallogr. 12, 500-502. [4] Cenzual K., Gelato L.M., Penzo M., Parthé E. (1991), Acta Crystallogr. B 47, 433-439. [5] Runnalls O.J.C. (1956), Can. J. Chem. 34, 133-145.

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hP24

Lu<sub>2</sub>CoGa<sub>3</sub>

hP24

(194) *P*6<sub>3</sub>/*mmc* – khfb

**Lu<sub>2</sub>CoGa<sub>3</sub>** [1]; Er<sub>2</sub>RhSi<sub>3</sub> [2]

Structural features: 3D-framework of fused CoLu<sub>6</sub> and GaLu<sub>6</sub> prisms. Puckered hexagon-mesh CoGa<sub>3</sub> layers with Ga<sub>6</sub> rings are interconnected via Co-Co bonds (Co<sub>2</sub> dumbbells parallel to [001]) to form a 3D-framework. Derivative of AlB<sub>2</sub>. See Fig. III.31.

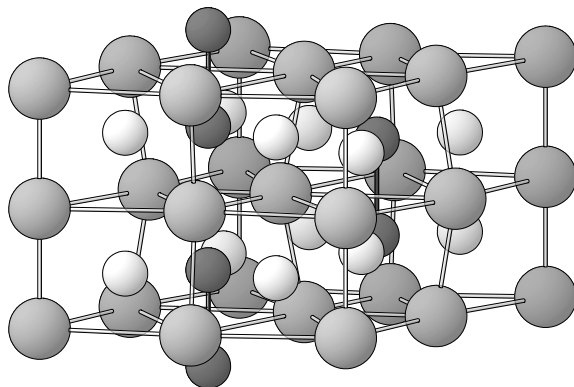


Fig. III.31. **Lu<sub>2</sub>CoGa<sub>3</sub>**

Arrangement of Lu<sub>6</sub> trigonal prisms (Lu atoms large), Co (dark) and Ga (light) atoms.

Gladyshevskii R.E., Chernyak B.I. (1986) [1]

CoGa<sub>3</sub>Lu<sub>2</sub>

*a* = 0.8659, *c* = 0.6823 nm, *c/a* = 0.788, *V* = 0.4430 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	12 <i>k</i>	. <i>m</i> .	0.1692	0.3384	0.0432		bicapped square prism CoGa <sub>3</sub> Lu <sub>6</sub>
Lu2	6 <i>h</i>	<i>mm</i> 2	0.5231	0.0462	$\frac{1}{4}$		16-vertex polyhedron Co <sub>4</sub> Ga <sub>8</sub> Lu <sub>4</sub>
Co3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.05		bicapped square prism Ga <sub>3</sub> CoLu <sub>6</sub>
Lu4	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		rhombic dodecahedron Ga <sub>12</sub> Lu <sub>2</sub>

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

Remarks: The same data are also reported in [2] and quoted in [3]. In [1] the *y*-coordinate of the Co site is misprinted as  $\frac{1}{3}$  instead of  $\frac{2}{3}$  (agreement with Wyckoff position 4*f*). A refinement of Er<sub>2</sub>RhSi<sub>3</sub> in space group (190) *P*-62*c* in [4] is superseded (see [2]); similar reliability factors were obtained for both space groups in [5], which indicates that the higher symmetry is probably correct.

References: [1] Gladyshevskii R.E., Chernyak B.I. (1986), Ukr. Resp. Konf. Neorg. Khim., 11th, L'vov 1986, Coll. Abstr. p. 49. [2] Gladyshevskii R.E., Cenzual K., Parthé E. (1992), J. Alloys Compd. 189,



221-228. [3] Barakatova Z.M., Aksel'rud L.G., Seropegin Y.D., Bodak O.I. (1995), Crystallogr. Rep. 40, 335-337 (Kristallografiya 40, 370-372). [4] Chevalier B., Lejay P., Etourneau J., Hagenmuller P. (1984), Solid State Commun. 49, 753-760. [5] Bazela W., Wawrzynska E., Penc B., Stüsser N., Szytula A., Zygmunt A. (2003), J. Alloys Compd. 360, 76-80.

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hP24

[N <sub>2</sub> ]	hP24	(194) <i>P6<sub>3</sub>/mmc</i> – 1
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N<sub>2</sub> β [2]; CO β [3]

Structural features: N<sub>2</sub> molecules in a Mg-type (h.c.p.) arrangement; each molecule forms an angle of 54° with [001] (6-fold orientational disorder).

Schiferl D. et al. (1983) [1]

N<sub>2</sub>

$a = 0.3595$ ,  $c = 0.5845$  nm,  $c/a = 1.626$ ,  $V = 0.0654$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
N1	24l	1	0.2096	0.5429	0.1947	0.167	

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.041$ ,  $T = 300$  K,  $p = 2.94$  GPa

Remarks: Phase stable at  $T > 35.5$  K at ambient pressure. Refinement with fixed bond length 0.110 nm. Short interatomic distances for partly occupied site(s). Models with spherical charge density or the molecular axis parallel to [001] were tested and rejected.

References: [1] Schiferl D., Cromer D.T., Ryan R.R., Larson A.C., Lesar R., Mills R.L. (1983), Acta Crystallogr. C 39, 1151-1153. [2] Streib W.E., Jordan T.H., Lipscomb W.N. (1962), J. Chem. Phys. 37, 2962-2965. [3] Cromer D.T., Schiferl D., Lesar R., Mills R.L. (1983), Acta Crystallogr. C 39, 1146-1150.

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hP26

(Zn <sub>0.8</sub> Fe <sub>0.2</sub> ) <sub>5</sub> LuO <sub>7</sub>	hP26	(194) <i>P6<sub>3</sub>/mmc</i> – f <sup>3</sup> e <sup>2</sup> cba
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LuFeO<sub>3</sub>(ZnO)<sub>4</sub> [1]

Structural features: Close-packed O layers in h<sub>5</sub>c<sub>2</sub> stacking; (Zn,Fe) in tetrahedral and trigonal bipyramidal voids, Lu in octahedral voids between c-stacked layers.

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

FeLuO<sub>7</sub>Zn<sub>4</sub>

$a = 0.33406$ ,  $c = 3.251$  nm,  $c/a = 9.732$ ,  $V = 0.3142$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.033		tetrahedron ZnLu <sub>3</sub>
M2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.09352		tetrahedron O <sub>4</sub>
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1827		tetrahedron Zn <sub>4</sub>
O4	4e	3m.	0	0	0.1088		tetrahedron Zn <sub>4</sub>
M5	4e	3m.	0	0	0.17203		trigonal bipyramid O <sub>5</sub>
M6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>
O7	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle Zn <sub>3</sub>
Lu8	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M2 = 0.8Zn + 0.2Fe; M5 = 0.8Zn + 0.2Fe; M6 = 0.8Zn + 0.2Fe

Experimental: single crystal, diffractometer, X-rays,  $R = 0.050$ ,  $T = 295$  K

References: [1] Isobe M., Kimizuka N., Nakamura M., Mohri T. (1994), Acta Crystallogr. C 50, 332-336.

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hP26

$\text{Cu}_{0.87}\text{Se}$	<i>hP26</i>	(194) $P6_3/mmc - h^2fedcb$
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**CuSe  $\alpha$**  [1], klockmannite

Structural features: Close-packed Se layers in AABAAC stacking with splitting of the sites in the B- and C-stacked layers; Cu in (distorted) tetrahedral voids, and inside B- and C-stacked Se layers (split sites). One Se-Se dumbbell for one single Se atom.

Effenberg H., Pertlik F. (1981) [1]

$\text{Cu}_{0.87}\text{Se}$

$a = 0.3939$ ,  $c = 1.725$  nm,  $c/a = 4.379$ ,  $V = 0.2318$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	6h	<i>mm2</i>	0.249	0.498	$\frac{1}{4}$	0.12	
Se2	6h	<i>mm2</i>	0.588	0.176	$\frac{1}{4}$	0.25	
Cu3	4f	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6117		
Se4	4e	<i>3m.</i>	0	0	0.0685		tetrahedron SeCu <sub>3</sub>
Se5	2d	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.25	
Cu6	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.15	
Cu7	2b	<i>-6m2</i>	0	0	$\frac{1}{4}$	0.10	coplanar triangle Cu <sub>3</sub>

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

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

Remarks: Short interatomic distances for partly occupied site(s). A structure proposal with the covellite type [2] is superseded (see [3]).

References: [1] Effenberg H., Pertlik F. (1981), Neues Jahrb. Mineral., Monatsh. 1981, 197-205. [2] Berry L.G. (1954), Am. Mineral. 39, 504-509. [3] Heyding R.D., Murray R.M. (1976), Can. J. Chem. 54, 841-848.

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hP26

$\text{Cs}_6\text{K}_7$	<i>hP26</i>	(194) $P6_3/mmc - kf^2cba$
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**Cs<sub>6</sub>K<sub>7</sub>** [1]

Structural features: Tetrahedrally close-packed structure (Frank-Kasper phase).

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

$\text{Cs}_6\text{K}_7$

$a = 0.9078$ ,  $c = 3.295$  nm,  $c/a = 3.630$ ,  $V = 2.3516$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	12k	<i>.m.</i>	0.16667	0.33334	0.1150		icosahedron K <sub>5</sub> Cs <sub>7</sub>
Cs2	4f	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.5231		16-vertex Frank-Kasper Cs <sub>4</sub> K <sub>12</sub>
Cs3	4f	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6792		14-vertex Frank-Kasper Cs <sub>8</sub> K <sub>6</sub>
Cs4	2c	<i>-6m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		15-vertex Frank-Kasper K <sub>6</sub> Cs <sub>9</sub>
Cs5	2b	<i>-6m2</i>	0	0	$\frac{1}{4}$		15-vertex Frank-Kasper K <sub>6</sub> Cs <sub>9</sub>
K6	2a	<i>-3m.</i>	0	0	0		icosahedron K <sub>6</sub> Cs <sub>6</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.129

References: [1] Simon A., Brämer W., Hillenkötter B., Kullmann H.J. (1976), Z. Anorg. Allg. Chem. 419, 253-274.

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hP26

$K_3Lu[Si_2O_7]$	<i>hP26</i>	(194) $P6_3/mmc - kF^2cba$
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### $K_3LuSi_2O_7$ [1]

Structural features: Units of two vertex-linked  $SiO_4$  tetrahedra (parallel to [001]) share vertices with  $LuO_6$  octahedra (arranged in layers) to form a 3D-framework.

Vidican I. et al. (2003) [1]

$K_3LuO_7Si_2$

$a = 0.57116$ ,  $c = 1.38883$  nm,  $c/a = 2.432$ ,  $V = 0.3924$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1798	0.3596	0.0961		single atom Si
Si2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1317		tetrahedron $O_4$
K3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5922		10-vertex polyhedron $O_9Si$
O4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear $Si_2$
K5	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism $O_6$
Lu6	2a	-3m.	0	0	0		octahedron $O_6$

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.043$ ,  $T = 293$  K

Remarks: In table 2 of [1] the Wyckoff positions are misprinted as those of space group (193)  $P6_3/mcm$  instead of (194)  $P6_3/mmc$ .

References: [1] Vidican I., Smith M.D., Zur Loye H.C. (2003), J. Solid State Chem. 170, 203-210.

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hP26

$(Zn_{0.68}Cr_{0.32})[SO_4]_{0.16}[OH]_2[H_2O]_{0.67}$	<i>hP26</i>	(194) $P6_3/mmc - kFe^2a$
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### $Zn_{0.68}Cr_{0.32}(OH)_2(SO_4)_{0.16} \cdot xH_2O$ [1]

Structural features: Slabs of edge-linked  $(Zn,Cr)(OH)_6$  octahedra alternate with layers containing a disordered arrangement of  $SO_4$  tetrahedra and  $H_2O$  molecules along [001].

Ennadi A. et al. (1994) [1]

$Cr_{0.32}H_{3.33}O_{3.33}S_{0.17}Zn_{0.68}$

$a = 0.31202$ ,  $c = 1.7844$  nm,  $c/a = 5.719$ ,  $V = 0.1504$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.2488	0.4976	0.2011	0.194	
(OH)2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0563		non-coplanar triangle $Zn_3$
O3	4e	3m.	0	0	0.1861	0.083	
S4	4e	3m.	0	0	0.2352	0.083	
M5	2a	-3m.	0	0	0		octahedron $(OH)_6$

$M1 = 0.572OH_2 + 0.428O$ ;  $M5 = 0.680Zn + 0.320Cr$

Experimental: powder, diffractometer, X-rays,  $R_B = 0.061$

Remarks: Referred to as LDH (lamellar double hydroxide). 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] Ennadi A., Khaldi M., De Roy A., Besse J.P. (1994), Mol. Cryst. Liq. Cryst. Sci. Technol. Sect. A 244, 373-378.

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hP26

K <sub>3</sub> Mo <sub>2</sub> BrO <sub>7</sub>			hP26			(194) P6 <sub>3</sub> /mmc – kfedcb	
<b>K<sub>3</sub>Mo<sub>2</sub>O<sub>7</sub>Br</b> [1]; KBa <sub>2</sub> V <sub>2</sub> O <sub>7</sub> Cl [2]							
Structural features: Units of two vertex-linked MoO <sub>4</sub> tetrahedra (parallel to [001]) arranged in layers; K and Br between units in the slabs, additional K between the slabs.							
Becher H.J., Fenske D. (1978) [1]							
BrK <sub>3</sub> Mo <sub>2</sub> O <sub>7</sub>							
<i>a</i> = 0.6017, <i>c</i> = 1.5624 nm, <i>c/a</i> = 2.597, <i>V</i> = 0.4899 nm <sup>3</sup> , <i>Z</i> = 2							
site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1546	0.3092	0.0923		single atom Mo
K2	4 <i>f</i>	3 <i>m</i> .	1/3	2/3	0.5421		10-vertex polyhedron O <sub>9</sub> Br
Mo3	4 <i>e</i>	3 <i>m</i> .	0	0	0.1305		tetrahedron O <sub>4</sub>
Br4	2 <i>d</i>	-6 <i>m</i> 2	1/3	2/3	3/4		8-vertex polyhedron K <sub>5</sub> O <sub>3</sub>
K5	2 <i>c</i>	-6 <i>m</i> 2	1/3	2/3	1/4		icosahedron O <sub>9</sub> Br <sub>3</sub>
O6	2 <i>b</i>	-6 <i>m</i> 2	0	0	1/4		colinear Mo <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: A partly ordered arrangement of K and Ba is reported for  $KBa_2V_2O_7Cl$ ,  $[(K,Ba)_2Ba]V_2O_7Cl$ .

References: [1] Becher H.J., Fenske D. (1978), J. Chem. Res., Synop. 1978, 167. [2] Martin F.D., Müller Buschbaum H. (1994), Z. Naturforsch. B 49, 1141-1144.

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hP26

$Mn_3Al_{10}$			hP26			(194) $P6_3/mmc - kh^2a$	
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**$Mn_3Al_{10}$**  [1]

Structural features: Infinite columns of face-sharing  $Al(Mn_6Al_6)$  icosahedra are interconnected via additional Al atoms to form a 3D-framework. See Fig. III.32.

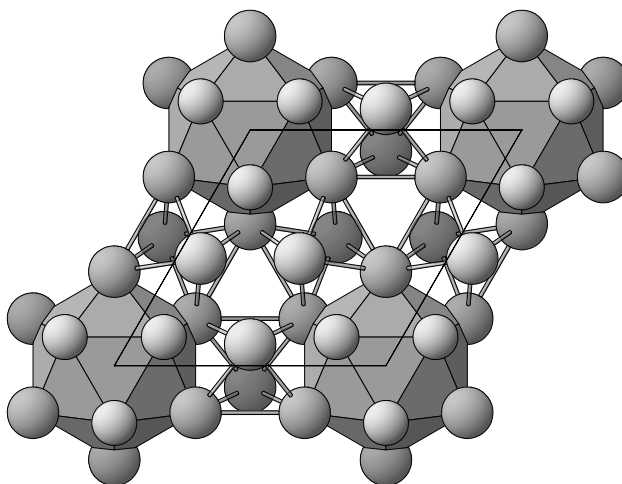


Fig. III.32.  **$Mn_3Al_{10}$**

Arrangement of  $Al(Mn_6Al_6)$  icosahedra (Mn atoms small, Al atoms large) and additional Al atoms viewed along [001].

Taylor M.A. (1959) [1]

$\text{Al}_{10}\text{Mn}_3$

$a = 0.7543$ ,  $c = 0.7898$  nm,  $c/a = 1.047$ ,  $V = 0.3892$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12 <i>k</i>	. <i>m</i> .	0.1995	0.3990	0.5630		pseudo Frank-Kasper $\text{Al}_{10}\text{Mn}_3$
Mn2	6 <i>h</i>	<i>mm</i> 2	0.1215	0.2430	$\frac{1}{4}$		icosahedron $\text{Al}_{10}\text{Mn}_2$
Al3	6 <i>h</i>	<i>mm</i> 2	0.4550	0.9100	$\frac{1}{4}$		12-vertex polyhedron $\text{Mn}_2\text{Al}_{10}$
Al4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		icosahedron $\text{Mn}_6\text{Al}_6$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.090$

References: [1] Taylor M.A. (1959), Acta Crystallogr. 12, 393-396.

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*hP26*

$\text{Mn}_3\text{Al}_9\text{Si}$	<i>hP26</i>	(194) $P6_3/mmc - kh^2a$
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**$\text{Mn}_3\text{Al}_9\text{Si}$**  [1], Strukturbericht notation E9<sub>c</sub>

Structural features: Infinite columns of face-sharing  $\text{Si}(\text{Mn}_6\text{Al}_6)$  icosahedra are interconnected via additional Al atoms to form a 3D-framework. Ordering variant of  $\text{Mn}_3\text{Al}_{10}$ .

Robinson K. (1952) [1]

$\text{Al}_9\text{Mn}_3\text{Si}$

$a = 0.7513$ ,  $c = 0.7745$  nm,  $c/a = 1.031$ ,  $V = 0.3786$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12 <i>k</i>	. <i>m</i> .	0.2007	0.4014	0.567		pseudo Frank-Kasper $\text{SiMn}_3\text{Al}_9$
Mn2	6 <i>h</i>	<i>mm</i> 2	0.1199	0.2398	$\frac{1}{4}$		icosahedron $\text{Al}_8\text{Si}_2\text{Mn}_2$
Al3	6 <i>h</i>	<i>mm</i> 2	0.4578	0.9156	$\frac{1}{4}$		12-vertex polyhedron $\text{Mn}_2\text{Al}_{10}$
Si4	2 <i>a</i>	-3 <i>m</i> .	0	0	0		icosahedron $\text{Mn}_6\text{Al}_6$

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

Remarks: According to [2] an ordered arrangement of Al and Si is doubtful.

References: [1] Robinson K. (1952), Acta Crystallogr. 5, 397-403. [2] Taylor M.A. (1959), Acta Crystallogr. 12, 393-396.

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*hP26*

$\text{Ca}[\text{CO}_3]$	<i>hP26</i>	(194) $P6_3/mmc - kh^2a$
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**$\text{CaCO}_3$**   $\mu$  [1], vaterite

Structural features: Ca atoms and  $\text{CO}_3$  trigonal units (parallel to [001], 3-fold orientational disorder) in a NiAs-type arrangement.

Kamhi S.R. (1963) [1]

$\text{CCaO}_3$

$a = 0.413$ ,  $c = 0.849$  nm,  $c/a = 2.056$ ,  $V = 0.1254$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.38	0.76	0.12	0.333	single atom C
O2	6 <i>h</i>	<i>mm</i> 2	0.12	0.24	$\frac{1}{4}$	0.333	
C3	6 <i>h</i>	<i>mm</i> 2	0.29	0.58	$\frac{1}{4}$	0.333	

Ca4      2a   -3m.      0      0      0

Experimental: single crystal, diffractometer and precession photographs, X-rays,  $R = 0.160$

Remarks: Short interatomic distances for partly occupied site(s). Average structure; additional reflections could be indexed with a 6-fold supercell (new axes  $2a+b$ ,  $-a+b$ ,  $2c$ ).

References: [1] Kamhi S.R. (1963), Acta Crystallogr. 16, 770-772.

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hP26

Nb<sub>4</sub>VSe<sub>8</sub>      hP26      (194)  $P6_3/mmc$  – khfba

**V<sub>0.25</sub>NbSe<sub>2</sub>** [1]; Co<sub>0.25</sub>NbSe<sub>2</sub> [1]; Mn<sub>0.25</sub>NbS<sub>2</sub> [2]

Structural features: Close-packed Se layers in BBCC stacking; Nb in trigonal prismatic, V in octahedral voids. NbSe<sub>6</sub> trigonal prisms share edges to form infinite slabs, which are interconnected via single VSe<sub>6</sub> octahedra to form a 3D-framework.

Voorhoeve Van Den Berg J.M., Robbins M. (1970) [1]

Nb<sub>4</sub>Se<sub>8</sub>V

$a = 0.6902$ ,  $c = 1.266$  nm,  $c/a = 1.834$ ,  $V = 0.5223$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	12k	.m.	0.1667	0.3334	0.125		4-vertex polyhedron Nb <sub>3</sub> V
Nb2	6h	mm2	0.5	0.0	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>
Se3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.625		non-coplanar triangle Nb <sub>3</sub>
Nb4	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Se <sub>6</sub>
V5	2a	-3m.	0	0	0		8-vertex polyhedron Se <sub>6</sub> Nb <sub>2</sub>

Transformation from published data ( $P6_3/mmc$  \*): origin shift  $0\ 0\ \frac{3}{4}$

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates. In [1] the origin of the cell is shifted by  $0\ 0\ \frac{1}{4}$  from the description in the International Tables for Crystallography. According to [3] the deviations from the ideal positions are significant for Mn<sub>0.25</sub>NbS<sub>2</sub> and the correct space group is (176)  $P6_3/m$ .

References: [1] Voorhoeve Van Den Berg J.M., Robbins M. (1970), J. Solid State Chem. 1, 134-137. [2] Van Laar B., Rietveld H.M., Ijdo D.J.W. (1971), J. Solid State Chem. 3, 154-160. [3] Anzenhofer K., De Boer J.J. (1971), Recl. Trav. Chim. Pays-Bas 90, 56-64.

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hP26

Ca<sub>3</sub>[SiO<sub>4</sub>]O      hP26      (194)  $P6_3/mmc$  – khfda

**Ca<sub>6</sub>Si<sub>2</sub>O<sub>10</sub>** [1], hatrurite high

Structural features: Single SiO<sub>4</sub> tetrahedra (2-fold orientational disorder) and infinite columns of face-linked OCa<sub>6</sub> octahedra.

Pérez Méndez M. et al. (1984) [1]

Ca<sub>3</sub>O<sub>5</sub>Si

$a = 0.7099$ ,  $c = 0.5687$  nm,  $c/a = 0.801$ ,  $V = 0.2482$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.2092	0.4184	0.656	0.5	
Ca2	6h	mm2	0.15685	0.3137	$\frac{1}{4}$		
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.03334	0.5	tetrahedron SiO <sub>3</sub>

Si4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	
O5	2a	-3m.	0	0	0	octahedron Ca <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.159

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Space group (186) *P6<sub>3</sub>mc* was tested and rejected (R = 0.15).

References: [1] Pérez Méndez M., Howie R.A., Glasser F.P. (1984), Cement Concr. Res. 14, 57-63.

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hP28

Ca <sub>4</sub> Cu <sub>3</sub> Zn <sub>2</sub> P <sub>5</sub>	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – f <sup>4</sup> e <sup>2</sup> dc
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### Ca<sub>4</sub>Cu<sub>3</sub>Zn<sub>2</sub>P<sub>5</sub> [1]

Structural features: Infinite slabs of edge-linked ZnP<sub>4</sub> tetrahedra and infinite triple slabs of fused CuCa<sub>6</sub> and PCa<sub>6</sub> trigonal prisms alternate along [001]. Intergrowth of CaAl<sub>2</sub>Si<sub>2</sub>- and ternary ZrBeSi-type slabs in the ratio 1:3.

Frik L., Mewis A. (1999) [1]

Ca<sub>4</sub>Cu<sub>3</sub>P<sub>5</sub>Zn<sub>2</sub>

*a* = 0.4041, *c* = 3.706 nm, *c/a* = 9.171, *V* = 0.5241 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0442		7-vertex polyhedron Zn <sub>4</sub> Ca <sub>3</sub>
Cu2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1439		non-coplanar triangle P <sub>3</sub>
Zn3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5243		tetrahedron P <sub>4</sub>
P4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6446		non-coplanar triangle Cu <sub>3</sub>
Ca5	4e	3m.	0	0	0.0911		19-vertex polyhedron P <sub>6</sub> Cu <sub>3</sub> Zn <sub>3</sub> Ca <sub>7</sub>
Ca6	4e	3m.	0	0	0.197		pseudo Frank-Kasper P <sub>6</sub> Cu <sub>6</sub> Ca <sub>8</sub>
Cu7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle P <sub>3</sub>
P8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Cu <sub>3</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.078

References: [1] Frik L., Mewis A. (1999), Z. Anorg. Allg. Chem. 625, 126-130.

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hP28

CsCrCl <sub>3</sub>	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> da
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### CsCrCl<sub>3</sub> α [1], perovskite 2H

Structural features: Close-packed CsCl<sub>3</sub> layers in h stacking; Cr in octahedral (Cl<sub>6</sub>) voids. CrCl<sub>6</sub> octahedra share faces to form infinite chains parallel to [001]. Variant of BaNiO<sub>3</sub> with complex splitting of the anion site leading to elongated octahedra.

Crama W.J., Zandbergen H.W. (1981) [1]

Cl<sub>3</sub>CrCs

*a* = 0.7257, *c* = 0.6238 nm, *c/a* = 0.860, *V* = 0.2845 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12k	.m.	0.1543	0.3086	0.2312	0.25	
Cl2	12k	.m.	0.1647	0.3294	0.2022	0.25	

Cs3	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$
Cr4	2a	-3m.	0	0	0

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

Remarks: Phase stable at T > 170 K. Short interatomic distances for partly occupied site(s). A similar model with splitting of site C11 into Wyckoff position 6h could not be excluded.

References: [1] Crama W.J., Zandbergen H.W. (1981), Acta Crystallogr. B 37, 1027-1031.

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hP28

CeNi <sub>5</sub> Sn	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – kF <sup>2</sup> dcba
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### CeNi<sub>5</sub>Sn [1]

Structural features: Intergrowth of CaCu<sub>5</sub>-type and CeNi<sub>5</sub>Sn<sub>2</sub> slabs along [001]. Interpenetrating Ni-centered icosahedra.

Skolozdra R.V. et al. (1981) [1]

CeNi<sub>5</sub>Sn

$a = 0.49049$ ,  $c = 1.9731$  nm,  $c/a = 4.023$ ,  $V = 0.4111$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12k	.m.	0.169	0.338	0.1458		icosahedron Ni <sub>7</sub> Sn <sub>2</sub> Ce <sub>3</sub>
Ni2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0425		pseudo Frank-Kasper Ni <sub>6</sub> Sn <sub>4</sub> Ce <sub>3</sub>
Sn3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5873		14-vertex Frank-Kasper Ni <sub>10</sub> Ce <sub>4</sub>
Ce4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper Ni <sub>18</sub> Sn <sub>2</sub>
Ni5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		icosahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ni6	2b	-6m2	0	0	$\frac{1}{4}$		icosahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ce7	2a	-3m.	0	0	0		18-vertex polyhedron Ni <sub>12</sub> Sn <sub>6</sub>

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

Experimental: single crystal, precession photographs, X-rays, R = 0.117

References: [1] Skolozdra R.V., Mandzyk V.M., Aksel'rud L.G. (1981), Sov. Phys. Crystallogr. 26, 272-274 (Kristallografiya 26, 480-483).

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hP28

NaBa <sub>3</sub> [Si <sub>2</sub> O <sub>7</sub> ][OH]	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – kF <sup>2</sup> dcba
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### NaBa<sub>3</sub>(Si<sub>2</sub>O<sub>7</sub>)(OH) [1]

Structural features: Units of two vertex-linked SiO<sub>4</sub> tetrahedra (parallel to [001]) share vertices with NaO<sub>6</sub> octahedra to form a 3D-framework; OH inside compressed Ba<sub>5</sub> trigonal bipyramids.

Filipenko O.S. et al. (1971) [1]

Ba<sub>3</sub>HNaO<sub>8</sub>Si<sub>2</sub>

$a = 0.5791$ ,  $c = 1.4748$  nm,  $c/a = 2.547$ ,  $V = 0.4283$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.185	0.37	0.1		single atom Si
Si2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.139		tetrahedron O <sub>4</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5782		single atom (OH)
(OH)4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Ba <sub>2</sub>
O5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Si <sub>2</sub>



Ba6	2b	-6m2	0	0	$\frac{1}{4}$	trigonal prism O <sub>6</sub>
Na7	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

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

References: [1] Filipenko O.S., Pobedinskaya E.A., Ponomarev V.J., Belov N.V. (1971), Dokl. Akad. Nauk SSSR 200, 591-593.

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hP28

Co <sub>2</sub> Al <sub>5</sub>	hP28	(194) P6 <sub>3</sub> /mmc – kh <sup>2</sup> ca
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**Co<sub>2</sub>Al<sub>5</sub>** [2], Strukturbericht notation D8<sub>11</sub>; Fe<sub>1.7</sub>Al<sub>4</sub>Si [3]

Structural features: Infinite columns of face-sharing Al(Co<sub>6</sub>Al<sub>6</sub>) icosahedra are interconnected via additional Al to form a 3D-framework; additional Co in trigonal prismatic voids.

Newkirk J.B. et al. (1961) [1]

Al<sub>5</sub>Co<sub>2</sub>

$a = 0.76560$ ,  $c = 0.75932$  nm,  $c/a = 0.992$ ,  $V = 0.3854$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.1946	0.3892	0.0580		14-vertex polyhedron Co <sub>4</sub> Al <sub>10</sub>
Al2	6h	mm2	0.5298	0.0596	$\frac{1}{4}$		tricapped pentagonal prism Co <sub>3</sub> Al <sub>10</sub>
Co3	6h	mm2	0.8732	0.7464	$\frac{1}{4}$		icosahedron Al <sub>10</sub> Co <sub>2</sub>
Co4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Al <sub>9</sub>
Al5	2a	-3m.	0	0	0		icosahedron Co <sub>6</sub> Al <sub>6</sub>

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

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

Remarks: Cell parameters from [2]. In [3] and [4] (Fe<sub>1.7</sub>Al<sub>4</sub>Si) the atom coordinates of Fe(1) are misprinted as  $\frac{1}{3}$   $\frac{2}{3}$   $\frac{1}{4}$  instead of  $\frac{1}{3}$   $\frac{2}{3}$   $\frac{3}{4}$  and the z-coordinate of (Al,Si)(3) as 0.4385 instead of -0.4385 (checked on interatomic distances).

References: [1] Newkirk J.B., Black P.J., Damjanovic A. (1961), Acta Crystallogr. 14, 532-533. [2] Bradley A.J., Cheng C.S. (1938), Z. Kristallogr. 99, 480-487. [3] German N.V., Bel'skii V.K., Yanson T.I., Zarechnyuk O.S. (1989), Sov. Phys. Crystallogr. 34, 437-438 (Kristallografiya 34, 735-737). [4] (1991), Structure Reports 56A, 29.

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hP28

Hf <sub>9</sub> Mo <sub>4</sub> B	hP28	(194) P6 <sub>3</sub> /mmc – kh <sup>2</sup> ca
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**Hf<sub>9</sub>Mo<sub>4</sub>B** [2], κ phase

Structural features: Infinite columns of face-sharing Mo(Hf<sub>6</sub>Mo<sub>6</sub>) icosahedra are interconnected via additional Hf to form a 3D-framework; B in trigonal prismatic voids. Ordering variant of Co<sub>2</sub>Al<sub>5</sub>, [Mo<sub>3</sub>B][Hf<sub>9</sub>Mo]. See Fig. III.33.

Rogl P. et al. (1973) [1]

BHf<sub>9</sub>Mo<sub>4</sub>

$a = 0.8565$ ,  $c = 0.8493$  nm,  $c/a = 0.992$ ,  $V = 0.5396$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hf1	12k	.m.	0.2032	0.4064	0.0471		14-vertex polyhedron BMo <sub>4</sub> Hf <sub>9</sub>
Hf2	6h	mm2	0.5403	0.0806	$\frac{1}{4}$		tricapped pentagonal prism Mo <sub>2</sub> BHf <sub>10</sub>
Mo3	6h	mm2	0.8905	0.781	$\frac{1}{4}$		icosahedron Mo <sub>4</sub> Hf <sub>8</sub>
B4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Hf <sub>9</sub>
Mo5	2a	-3m.	0	0	0		icosahedron Mo <sub>6</sub> Hf <sub>6</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.094

Remarks: Cell parameters from [2], where the atom distribution could not be fully determined.

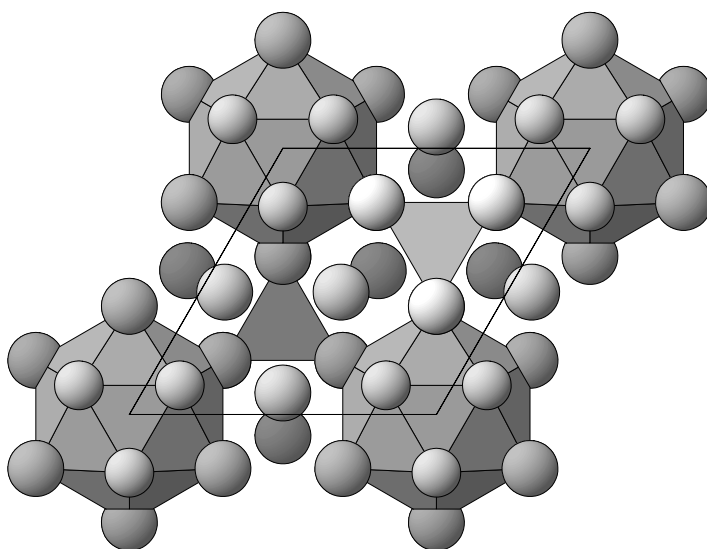


Fig. III.33. **Hf<sub>9</sub>Mo<sub>4</sub>B**

Arrangement of Mo(Hf<sub>6</sub>Mo<sub>6</sub>) icosahedra (Hf atoms large, Mo atoms small), BHf<sub>6</sub> trigonal prisms and additional Hf atoms viewed along [001].

References: [1] Rogl P., Nowotny H., Benesovsky F. (1973), Monatsh. Chem. 104, 182-193. [2] Rogl P., Nowotny H., Benesovsky F. (1971), Monatsh. Chem. 102, 971-984.

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hP28

Cs <sub>6</sub> K <sub>3</sub> GaSb <sub>4</sub>	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – kh <sup>2</sup> ca
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**Cs<sub>6</sub>K<sub>3</sub>Sb(GaSb<sub>3</sub>)** [1]; Cs<sub>6</sub>K<sub>3</sub>Sb(AlSb<sub>3</sub>) [2]

Structural features: GaSb<sub>3</sub> trigonal units and infinite chains of face-linked Sb(Cs<sub>6</sub>K<sub>6</sub>) icosahedra.

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

Cs<sub>6</sub>GaK<sub>3</sub>Sb<sub>4</sub>

*a* = 1.0972, *c* = 1.1501 nm, *c/a* = 1.048, *V* = 1.1991 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cs1	12k	.m.	0.20976	0.41952	0.54152		14-vertex Frank-Kasper K <sub>3</sub> Sb <sub>5</sub> Cs <sub>5</sub> Ga
K2	6h	mm2	0.1187	0.2374	$\frac{1}{4}$		pseudo Frank-Kasper Sb <sub>4</sub> Cs <sub>6</sub> K <sub>2</sub> Ga
Sb3	6h	mm2	0.47282	0.94564	$\frac{1}{4}$		single atom Ga
Ga4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Sb <sub>3</sub>
Sb5	2a	-3m.	0	0	0		icosahedron K <sub>6</sub> Cs <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.029, T = 293 K

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

References: [1] Somer M., Peters K., Von Schnering H.G. (1991), Z. Kristallogr. 195, 101-102. [2] Somer M., Peters K., Von Schnering H.G. (1991), Z. Kristallogr. 195, 316-317. [3] Somer M., Peters K., Popp T., Von Schnering H.G. (1991), Z. Anorg. Allg. Chem. 597, 201-208.

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hP28

$\text{Ca}_3\text{Au}_6(\text{Au}_{0.3}\text{Ga}_{0.7})_2\text{Ga}_3$	<i>hP28</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $\text{kh}^2\text{f}$
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### $\text{Ca}_3\text{Au}_{6.61}\text{Ga}_{4.39}$ [1]

Structural features: Slightly puckered hexagon-mesh  $(\text{Au,Ga})_8$  layers and  $\text{Ca}_3(\text{Ga}_3)$  layers (the Ca atoms and the centers of  $\text{Ga}_3$  triangles form a triangle mesh) alternate along [001]. Derivative of  $\text{AlB}_2$  where part of the large atoms have been replaced by small-atom triangles.

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

$\text{Au}_{6.60}\text{Ca}_3\text{Ga}_{4.40}$

$a = 0.9266$ ,  $c = 0.7331$  nm,  $c/a = 0.791$ ,  $V = 0.5451$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Au1	12 <i>k</i>	. <i>m</i> .	0.17504	0.35008	0.0548		icosahedron $\text{Ga}_5\text{Au}_3\text{Ca}_4$
Ca2	6 <i>h</i>	<i>mm</i> 2	0.5244	0.0488	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Au}_8\text{Ga}_6\text{Ca}_4$
Ga3	6 <i>h</i>	<i>mm</i> 2	0.9039	0.8078	$\frac{1}{4}$		10-vertex polyhedron $\text{Au}_6\text{Ga}_2\text{Ca}_2$
M4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0612		tetrahedron $\text{Au}_3\text{Ga}$

$\text{M4} = 0.70\text{Ga} + 0.30\text{Au}$

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

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

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

References: [1] Kussmann D., Hoffmann R.D., Pöttgen R. (2001), Z. Anorg. Allg. Chem. 627, 2053-2056.

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hP28

$\text{Cs}_3\text{Cr}_2\text{Cl}_9$	<i>hP28</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $\text{khf}^2\text{b}$
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### $\text{Cs}_3\text{Cr}_2\text{Cl}_9$ [2]

Structural features: Close-packed  $\text{CsCl}_3$  layers in  $hc_2$  stacking; Cr in octahedral ( $\text{Cl}_6$ ) voids, leaving the interlayers between c-stacked layers vacant. Units of two face-linked  $\text{CrCl}_6$  octahedra ( $\text{Cr}_2$  dumbbells), parallel to [001]. See Fig. III.34.

Sassmannshausen M., Lutz H.D. (2001) [1]

$\text{Cl}_9\text{Cr}_2\text{Cs}_3$

$a = 0.7217$ ,  $c = 1.791$  nm,  $c/a = 2.482$ ,  $V = 0.8079$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	12 <i>k</i>	. <i>m</i> .	0.17936	0.35872	0.59298		single atom Cr
Cl2	6 <i>h</i>	<i>mm</i> 2	0.51824	0.03648	$\frac{1}{4}$		non-colinear $\text{Cr}_2$
Cs3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0766		cuboctahedron $\text{Cl}_{12}$
Cr4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.66141		octahedron $\text{Cl}_6$
Cs5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron $\text{Cl}_{12}$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.020$ ,  $T = 293$  K

References: [1] Sassmannshausen M., Lutz H.D. (2001), Z. Anorg. Allg. Chem. 627, 1071-1076. [2] Wessel G.J., Ijdo D.J.W. (1957), Acta Crystallogr. 10, 466-468.

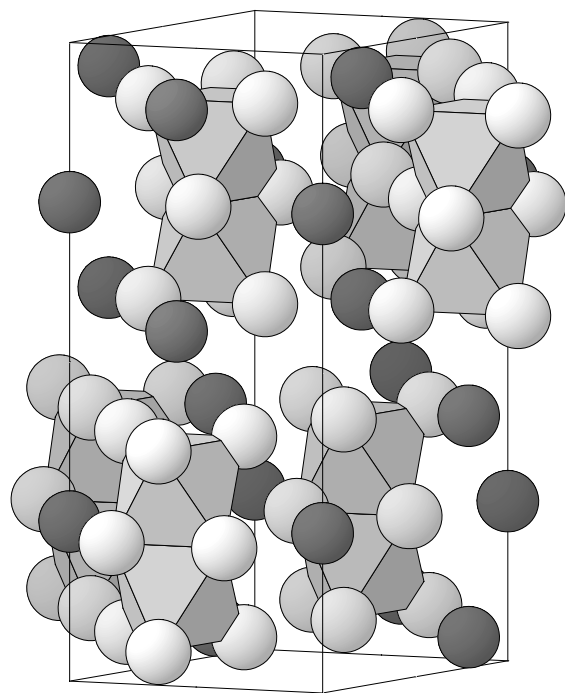
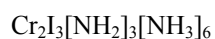


Fig. III.34.  $\text{Cs}_3\text{Cr}_2\text{Cl}_9$

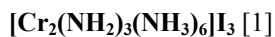
Arrangement of  $\text{CrCl}_6$  octahedra (Cl atoms light) and Cs atoms (dark).

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hP28



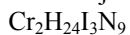
hP28

(194)  $P6_3/mmc - khf^2b$



Structural features: Single  $\text{Cr}_2(\text{NH}_2)_3(\text{NH}_3)_6$  units (two  $\text{Cr}[(\text{NH}_2)_3(\text{NH}_3)_3]$  octahedra sharing the  $(\text{NH}_2)_3$  face, parallel to  $[001]$ ) in a Mg-type (h.c.p.) arrangement.  $\text{Cr}_2$  dumbbells.

Zachwieja U., Jacobs H. (1993) [1]



$a = 0.767$ ,  $c = 1.8096$  nm,  $c/a = 2.359$ ,  $V = 0.9219$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12k	.m.	0.2048	0.4096	0.6082		single atom Cr
N2	6h	mm2	0.5512	0.1024	$\frac{1}{4}$		non-colinear $\text{Cr}_2$
I3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0818		9-vertex polyhedron $\text{N}_9$
Cr4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6768		octahedron $\text{N}_6$
I5	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron $\text{N}_{12}$
H6	24l	1	0.336	0.076	0.111		
H7	12k	.m.	0.207	0.414	0.559		
H8	12j	m..	0.434	0.022	$\frac{1}{4}$		

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

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

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In the abstract of [1] the number of formula units per cell  $Z$  is misprinted as 3 instead of 2.

References: [1] Zachwieja U., Jacobs H. (1993), *Z. Kristallogr.* 206, 247-254.

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*hP28*

$\text{Nb}_2\text{CrSe}_4$	<i>hP28</i>	(194) $P6_3/mmc$ – khfcb
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### $\text{Cr}_{0.5}\text{NbSe}_2$ [1]

Structural features: Close-packed Se layers in AAB $\bar{B}$  stacking; Nb in trigonal prismatic, Cr in trigonal prismatic and octahedral voids.

Meerschaut A. et al. (1970) [1]

$\text{CrNb}_2\text{Se}_4$

$a = 0.6908$ ,  $c = 1.2631$  nm,  $c/a = 1.828$ ,  $V = 0.5220$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Se1	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.125		5-vertex polyhedron $\text{Cr}_2\text{Nb}_3$
Nb2	6 <i>h</i>	<i>mm</i> 2	0.5	0.0	$\frac{1}{4}$		monocapped trigonal prism $\text{CrSe}_6$
Se3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.625		non-coplanar triangle $\text{Nb}_3$
Cr4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism $\text{Nb}_3\text{Se}_6$
Nb5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism $\text{Se}_6$
Cr6	2 <i>a</i>	-3. <i>m</i> .	0	0	0		8-vertex polyhedron $\text{Se}_6\text{Nb}_2$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.060$

Remarks: Short interatomic distances:  $d(\text{Nb2-Cr4}) = 0.199$  nm. The structure was later redetermined in space group (12)  $C2/m$  [2].

References: [1] Meerschaut A., Spiesser M., Rouxel J. (1970), *C. R. Seances Acad. Sci., Ser. C* 270, 45-48. [2] Meerschaut A., Spiesser M., Rouxel J., Gorochoy O. (1980), *J. Solid State Chem.* 31, 31-40.

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*hP28*

$[\text{NH}_4]_3\text{Si}[\text{NO}_3]\text{F}_6$	<i>hP28</i>	(194) $P6_3/mmc$ – khfdb
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### $(\text{NH}_4)_3\text{SiNO}_3\text{F}_6$ [1]

Structural features:  $\text{SiF}_6$  octahedra and  $\text{NO}_3$  trigonal units (perpendicular to [001]) in a NiAs-type arrangement.

Buchholz N., Mattes R. (1988) [1]

$\text{F}_6\text{H}_{12}\text{N}_4\text{O}_3\text{Si}$

$a = 0.586$ ,  $c = 1.4754$  nm,  $c/a = 2.518$ ,  $V = 0.4388$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
F1	12 <i>k</i>	. <i>m</i> .	0.1356	0.2712	0.5658		single atom Si
O2	6 <i>h</i>	<i>mm</i> 2	0.5427	0.0854	$\frac{1}{4}$		single atom N
( $\text{NH}_4$ )3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0916		cuboctahedron $\text{F}_9\text{O}_3$
N4	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle $\text{O}_3$
( $\text{NH}_4$ )5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron $\text{O}_6\text{F}_6$
Si6	2 <i>a</i>	-3. <i>m</i> .	0	0	0		octahedron $\text{F}_6$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.056$ ,  $T = 140$  K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Buchholz N., Mattes R. (1988), Mater. Res. Bull. 23, 755-758.

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hP28

Ba <sub>3</sub> Te <sub>2</sub> O <sub>9</sub>	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – khfed
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**Ba<sub>3</sub>Te<sub>2</sub>O<sub>9</sub>** [1]; Cs<sub>3</sub>Fe<sub>2</sub>F<sub>9</sub> (see remark)

Structural features: Close-packed BaO<sub>3</sub> layers in h stacking; Te in octahedral (O<sub>6</sub>) voids, leaving every third interlayer vacant. Units of two face-linked TeO<sub>6</sub> octahedra, parallel to [001].

Jacobson A.J. et al. (1981) [1]

Ba<sub>3</sub>O<sub>9</sub>Te<sub>2</sub>

$a = 0.58603$ ,  $c = 1.43037$  nm,  $c/a = 2.441$ ,  $V = 0.4254$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1639	0.3278	0.5906		single atom Te
O2	6h	mm2	0.1426	0.2852	$\frac{1}{4}$		non-colinear Te <sub>2</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.063		anticuboctahedron O <sub>12</sub>
Te4	4e	3m.	0	0	0.1493		octahedron O <sub>6</sub>
Ba5	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>

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

Remarks: Cs<sub>3</sub>Fe<sub>2</sub>F<sub>9</sub> was originally refined in space group (190) *P*-62c [3], however, this space group was superseded in [2].

References: [1] Jacobson A.J., Scanlon J.C., Poeppelmeier K.R., Longo J.M., Cox D.E. (1981), Mater. Res. Bull. 16, 359-367. [2] Dance J.M., Mur J., Darriet J., Hagenmuller P., Massa W., Kummer S., Babel D. (1986), J. Solid State Chem. 63, 446-451. [3] Wall F., Pausewang G., Babel D. (1971), J. Less-Common Met. 25, 257-270.

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hP28

Cs <sub>3</sub> V <sub>2</sub> (O <sub>0.33</sub> F <sub>0.67</sub> ) <sub>6</sub> F <sub>3</sub>	hP28	(194) <i>P6<sub>3</sub>/mmc</i> – khfed
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**Cs<sub>3</sub>V<sub>2</sub>O<sub>2</sub>F<sub>7</sub>** [1]; Cs<sub>3</sub>Mo<sub>2</sub>O<sub>6</sub>F<sub>3</sub> [2]

Structural features: Close-packed CsF<sub>3</sub> and Cs(F,O)<sub>3</sub> layers in h stacking; Te in octahedral voids, leaving every third interlayer vacant. Units of two Te(F<sub>3</sub>(F,O)<sub>3</sub>) octahedra sharing the F<sub>3</sub> face. Ordering variant of Ba<sub>3</sub>Te<sub>2</sub>O<sub>9</sub>.

Waltersson K. (1978) [1]

Cs<sub>3</sub>F<sub>7</sub>O<sub>2</sub>V<sub>2</sub>

$a = 0.63346$ ,  $c = 1.4871$  nm,  $c/a = 2.348$ ,  $V = 0.5168$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1456	0.2912	0.59614		single atom V
F2	6h	mm2	0.1298	0.2596	$\frac{1}{4}$		non-colinear V <sub>2</sub>
Cs3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.06839		9-vertex polyhedron F <sub>9</sub>
V4	4e	3m.	0	0	0.14931		octahedron F <sub>6</sub>
Cs5	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron F <sub>12</sub>

$$M1 = 0.667F + 0.333O$$

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

Remarks: Space group (190) *P*-62*c* was tested and rejected. A fully ordered structure is reported for Cs<sub>3</sub>Mo<sub>2</sub>O<sub>6</sub>F<sub>3</sub> in [2].

References: [1] Waltersson K. (1978), Cryst. Struct. Commun. 7, 507-511. [2] Mattes R., Mennemann K., Jäkel N., Rieskamp H., Brockmeyer H.J. (1980), J. Less-Common Met. 76, 199-212.

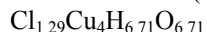
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hP28

Cu <sub>4</sub> Cl(Cl <sub>0.29</sub> [OH] <sub>0.71</sub> )[OH] <sub>6</sub>	hP28	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgcb
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**Cu<sub>4</sub>(OH)<sub>6.71</sub>Cl<sub>1.29</sub>** [1], claringbullite

Structural features: Cu(OH)<sub>4</sub> squares are interconnected to form a 3D-framework (disordered vacancies in units of three squares forming a trigonal prism).

Burns P.C. et al. (1995) [1]



$$a = 0.66733, c = 0.9185 \text{ nm}, c/a = 1.376, V = 0.3542 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.2017	0.4034	0.5918		
Cu2	6 <i>h</i>	<i>mm</i> 2	0.6289	0.2578	<sup>1</sup> / <sub>4</sub>	0.333	
Cu3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		coplanar square O <sub>4</sub>
Cl4	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		trigonal prism Cu <sub>6</sub>
M5	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>
H6	12 <i>k</i>	. <i>m</i> .	0.125	0.25	0.632		

$$M5 = 0.71OH + 0.29Cl$$

Experimental: single crystal, diffractometer, X-rays, wR = 0.032

Remarks: Natural specimen from Bisbee, Cochise County, Arizona. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (190) *P*-62*c* was tested and rejected.

References: [1] Burns P.C., Cooper M.A., Hawthorne F.C. (1995), Can. Mineral. 33, 633-639.

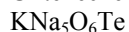
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hP28

KNa <sub>5</sub> [TeO <sub>6</sub> ]	hP28	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgda
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**KNa<sub>5</sub>TeO<sub>6</sub>** [1]

Structural features: TeO<sub>6</sub> octahedra and K atoms in a Mg-type (h.c.p.) arrangement.

Untenecker H., Hoppe R. (1987) [1]



$$a = 0.6568, c = 1.131 \text{ nm}, c/a = 1.722, V = 0.4225 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1392	0.2784	0.5989		single atom Te
Na2	6 <i>h</i>	<i>mm</i> 2	0.1452	0.2904	<sup>1</sup> / <sub>4</sub>		non-coplanar square O <sub>4</sub>
Na3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0	0.667	coplanar square O <sub>4</sub>
K4	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>
Te5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.056$

Remarks: In table 3 of [1] the Wyckoff position of the K site is misprinted as  $2c$  instead of  $2d$ .

References: [1] Untenecker H., Hoppe R. (1987), J. Less-Common Met. 132, 93-105.

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hP28

Sr[CN <sub>2</sub> ]	hP28	(194) $P6_3/mmc$ – khgdb
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**SrCN<sub>2</sub> hexagonal [1]**

Structural features: Single N=C=N linear units, some of them in complete rotational disorder (N not located).

Strid K.G., Vannerberg N.G. (1966) [1]

CN<sub>2</sub>Sr

$a = 1.0379$ ,  $c = 0.6633$  nm,  $c/a = 0.639$ ,  $V = 0.6188$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
N1	12k	.m.	0.569	0.138	0.55		single atom C
Sr2	6h	mm2	0.1965	0.393	$\frac{1}{4}$		non-coplanar square N <sub>4</sub>
C3	6g	.2/m.	$\frac{1}{2}$	0	0		colinear N <sub>2</sub>
Sr4	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		trigonal prism N <sub>6</sub>
(CN <sub>2</sub> )5	2b	-6m2	0	0	$\frac{1}{4}$		trigonal bipyramid (CN <sub>2</sub> ) <sub>2</sub> Sr <sub>3</sub>

Experimental: single crystal, Weissenberg and rotation photographs, X-rays,  $R = 0.137$

Remarks: Part of N not located.

References: [1] Strid K.G., Vannerberg N.G. (1966), Acta Chem. Scand. 20, 1064-1073.

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hP30

Ho <sub>2.5</sub> CoB <sub>3</sub>	hP30	(194) $P6_3/mmc$ – ihf <sup>2</sup> e
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**Ho<sub>2+x</sub>CoB<sub>3</sub> [1]**

Structural features: Planar hexagon-mesh B layers alternate with two directly superposed triangle-mesh Ho<sub>2</sub>Co layers (Co slightly out of the plane); additional Ho between directly superposed Co atoms (split site).

Gubich I.B. et al. (1992) [1]

B<sub>3</sub>CoHo<sub>2.51</sub>

$a = 0.54$ ,  $c = 1.5151$  nm,  $c/a = 2.806$ ,  $V = 0.3826$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
B1	12i	.2.	0.33	0	0		coplanar triangle B <sub>3</sub>
Ho2	6h	mm2	0.6466	0.2932	$\frac{1}{4}$	0.339	
Ho3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1296		non-coplanar hexagon B <sub>6</sub>
Co4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5734		non-coplanar hexagon B <sub>6</sub>
Ho5	4e	3m.	0	0	0.1294		non-coplanar hexagon B <sub>6</sub>

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

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

References: [1] Gubich I.B., Kuz'ma Y.B., Zavaliy P.Y., Pidgaetskaya G.M. (1992), Inorg. Mater. 28, 1104-1107 (Neorg. Mater. 28, 1397-1401).



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hP30

TiCo <sub>2</sub>	hP30	(194) $P6_3/mmc - jgf^2e$
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**TiCo<sub>2</sub> hexagonal [1]**

Structural features: Variant of MgNi<sub>2</sub> (Laves phase 4H) with splitting of the Co site forming the Kagomé-mesh layers.

Cruz Gandarilla F. et al. (2003) [1]

Co<sub>2</sub>Ti

$a = 0.4732$ ,  $c = 1.5409$  nm,  $c/a = 3.256$ ,  $V = 0.2988$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Co1	12j	$m..$	0.1444	0.3083	$1/4$	0.5	icosahedron Co <sub>6</sub> Ti <sub>6</sub>
Co2	6g	$.2/m.$	$1/2$	0	0		
Co3	4f	$3m.$	$1/3$	$2/3$	0.1389		
Ti4	4f	$3m.$	$1/3$	$2/3$	0.6368		
Ti5	4e	$3m.$	0	0	0.0902		

Experimental: powder, diffractometer, X-rays

Remarks: Nanocrystalline sample. Approximate composition, the authors state that contamination by Fe could not be excluded. Short interatomic distances for partly occupied site(s). Refinement of the occupancies of the Ti sites showed no significant deviation from unity; refinement of the occupancies of the Co sites gave  $\text{occ}(\text{Co}1) = 0.77$ ,  $\text{occ}(\text{Co}2) = 1.21$ ,  $\text{occ}(\text{Co}3) = 0.78$ . Ambiguous data: the space group is omitted in [1], we assume it is (194)  $P6_3/mmc$ , as given for the same phase in Co-rich samples. It is, however, not clear if the splitting of site Co1 is intentional or not (Wyckoff position  $6h$  stated in the text), or if a space group of lower symmetry was used.

References: [1] Cruz Gandarilla F., Gayosso Armenta R., Hesiquio Garduno M., Cabanas Moreno J.G., Martinez Sanchez R. (2003), Mater. Sci. Forum 442, 109-114.

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hP30

Na <sub>2</sub> [SO <sub>4</sub> ]	hP30	(194) $P6_3/mmc - k^2dca$
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**Na<sub>2</sub>SO<sub>4</sub> form I [1]**

Structural features: Na atoms and SO<sub>4</sub> tetrahedra (orientational disorder) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Naruse H. et al. (1987) [1]

Na<sub>2</sub>O<sub>4</sub>S

$a = 0.5444$ ,  $c = 0.7347$  nm,  $c/a = 1.35$ ,  $V = 0.1886$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	$.m.$	0.193	0.386	0.226	0.333	
O2	12k	$.m.$	0.271	0.542	0.05	0.333	
Na3	2d	$-6m2$	$1/3$	$2/3$	$3/4$		
S4	2c	$-6m2$	$1/3$	$2/3$	$1/4$		
Na5	2a	$-3m.$	0	0	0		

Experimental: single crystal, diffractometer, X-rays,  $R = 0.049$ ,  $T = 693$  K

Remarks: Phase stable at  $T > 510$  K. Short interatomic distances for partly occupied site(s).

References: [1] Naruse H., Tanaka K., Morikawa H., Marumo F., Mehrotra B.N. (1987), Acta Crystallogr. B 43, 143-146.

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hP30

BaAl <sub>5</sub> O <sub>8.5</sub> [H <sub>2</sub> O] <sub>0.5</sub>	hP30	(194) <i>P6<sub>3</sub>/mmc</i> – kgfecb
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### Ba<sub>2</sub>Al<sub>10</sub>O<sub>17</sub>·H<sub>2</sub>O [1]

Structural features: Infinite layers of edge-linked Al[O<sub>4</sub>(O,OH<sub>2</sub>)<sub>2</sub>] octahedra are interconnected via common vertices with units of two vertex-linked AlO<sub>4</sub> octahedra to form a 3D-framework; Ba in channels parallel to <110>. Vacancy derivative of β-alumina.

Cruickshank M.C. et al. (1985) [1]

Al<sub>3</sub>BaHO<sub>9</sub>

$a = 0.5635$ ,  $c = 1.3489$  nm,  $c/a = 2.394$ ,  $V = 0.3709$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.173	0.346	0.0786		non-coplanar triangle Al <sub>3</sub>
Al2	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		octahedron O <sub>6</sub>
M3	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5709		non-coplanar triangle Al <sub>3</sub>
Al4	4 <i>e</i>	3 <i>m</i> .	0	0	0.1201		tetrahedron O <sub>4</sub>
Ba5	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>
O6	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		colinear Al <sub>2</sub>

M3 = 0.75O + 0.25OH<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.069, T = 298 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (186) *P6<sub>3</sub>mc* was tested and rejected.

References: [1] Cruickshank M.C., Dent Glasser L.S., Howie R.A. (1985), Acta Crystallogr. C 41, 159-161.

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hP30

Li <sub>4</sub> Ba	hP30	(194) <i>P6<sub>3</sub>/mmc</i> – kh <sup>2</sup> fa
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### BaLi<sub>4</sub> [1]

Structural features: Ba<sub>3</sub>(Li<sub>3</sub>) layers (the Ba atoms and the centers of Li<sub>3</sub> triangles form a triangle mesh) and puckered Li<sub>9</sub> layers (a hexagon mesh with every fourth hexagon centered by an additional Li) alternate along [001]. Ba<sub>3</sub> trigonal clusters perpendicular to [001] are interconnected via Ba-Ba distances of similar length to form a 3D-framework.

Wang F.E. et al. (1965) [1]

BaLi<sub>4</sub>

$a = 1.1026$ ,  $c = 0.8891$  nm,  $c/a = 0.806$ ,  $V = 0.9361$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	12 <i>k</i>	. <i>m</i> .	0.1621	0.3242	0.0615		icosahedron Li <sub>8</sub> Ba <sub>4</sub>
Ba2	6 <i>h</i>	<i>mm</i> 2	0.528	0.056	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Li <sub>14</sub> Ba <sub>4</sub>
Li3	6 <i>h</i>	<i>mm</i> 2	0.8973	0.7946	<sup>1</sup> / <sub>4</sub>		icosahedron Li <sub>10</sub> Ba <sub>2</sub>
Li4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0808		bicapped square prism Li <sub>4</sub> Ba <sub>6</sub>
Li5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		icosahedron Li <sub>12</sub>

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

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

Remarks: Preliminary data in [2].

References: [1] Wang F.E., Kanda F.A., Miskell C.F., King A.J. (1965), Acta Crystallogr. 18, 24-31. [2] Keller D.V. (1958), Thesis, Syracuse, New York.

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hP30

$\text{YCo}_2(\text{Co}_{0.5}\text{Sn}_{0.5})_2$	<i>hP30</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $\text{kh}^2\text{fa}$
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### **YCo<sub>3</sub>Sn [1]**

Structural features:  $\text{Y}_3(\text{Co}_3)$  layers (the Y atoms and the centers of  $\text{Co}_3$  triangles form a triangle mesh) and partly ordered puckered  $(\text{Co},\text{Sn})_9$  layers (hexagon mesh with every fourth hexagon centered by an additional Co) alternate along [001]. Ordering variant of  $\text{Li}_4\text{Ba}$ .

Skolozdra R.V. (1983) [1]

$\text{Co}_3\text{SnY}$

$a = 0.8844$ ,  $c = 0.7446$  nm,  $c/a = 0.842$ ,  $V = 0.5044$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.073		icosahedron $\text{Co}_8\text{Y}_4$
Y2	6 <i>h</i>	<i>mm</i> 2	0.524	0.048	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Co}_{14}\text{Y}_4$
Co3	6 <i>h</i>	<i>mm</i> 2	0.903	0.806	$\frac{1}{4}$		icosahedron $\text{Co}_{10}\text{Y}_2$
Co4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.039		bicapped square prism $\text{Co}_4\text{Y}_6$
Co5	2 <i>a</i>	-3. <i>m</i> .	0	0	0		icosahedron $\text{Co}_{12}$

$\text{M1} = 0.5\text{Co} + 0.5\text{Sn}$

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

References: [1] Skolozdra R.V. (1983), Vses. Konf. Kristalloghim. Intermet. Soeden., 4th, L'vov 1983, Coll. Abstr. pp. 44-45.

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hP30

$\text{BaNi}_9\text{P}_5$	<i>hP30</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $\text{kh}^2\text{fa}$
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### **BaNi<sub>9</sub>P<sub>5</sub> [2]**

Structural features:  $\text{NiP}_4$  tetrahedra share edges and vertices to form a 3D-framework; Ba in  $\text{Ni}_{18}\text{P}_{12}$  cages. See Fig. III.35.

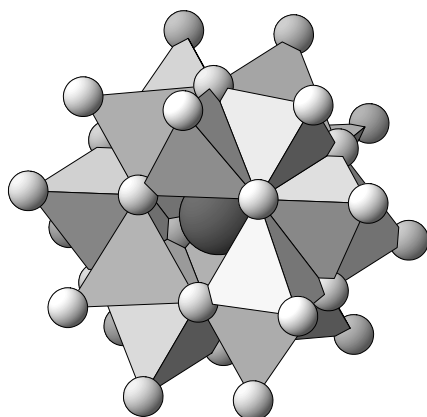
Probst H., Mewis A. (1991) [1]

$\text{BaNi}_9\text{P}_5$

$a = 0.6534$ ,  $c = 1.0847$  nm,  $c/a = 1.660$ ,  $V = 0.4010$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ni1	12 <i>k</i>	. <i>m</i> .	0.5356	0.0712	0.1077		9-vertex polyhedron $\text{P}_4\text{Ni}_5$
Ni2	6 <i>h</i>	<i>mm</i> 2	0.2039	0.4078	$\frac{1}{4}$		10-vertex polyhedron $\text{P}_4\text{Ni}_6$
P3	6 <i>h</i>	<i>mm</i> 2	0.8259	0.6518	$\frac{1}{4}$		trigonal prism $\text{Ni}_6$
P4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0611		9-vertex polyhedron $\text{Ni}_9$
Ba5	2 <i>a</i>	-3. <i>m</i> .	0	0	0		30-vertex polyhedron $\text{P}_{12}\text{Ni}_{18}$

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.041$

Fig. III.35. **BaNi<sub>9</sub>P<sub>5</sub>**

Arrangement of NiP<sub>4</sub> tetrahedra (P atoms small) around a Ba atom (large).

References: [1] Probst H., Mewis A. (1991), Z. Anorg. Allg. Chem. 597, 173-182. [2] Badding J.V., Stacy A.M. (1990), J. Solid State Chem. 87, 10-14.

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hP30

<b>Yb<sub>0.98</sub>Al<sub>2.8</sub>Si<sub>0.2</sub></b>	<b>hP30</b>	<b>(194) <i>P6<sub>3</sub>/mmc</i> – kh<sup>2</sup>fb</b>
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**Yb<sub>1-x</sub>Al<sub>2.8</sub>Si<sub>0.2</sub>** [1]; Yb<sub>1-x</sub>Al<sub>2.8</sub>Ge<sub>0.2</sub> [1]

Structural features: Close-packed Yb(Al,Si)<sub>3</sub> layers (Yb forms a triangle mesh) in hc<sub>2</sub> stacking (in part distinct positions for Al and Si). Variant of PuAl<sub>3</sub> with site splitting.

Zhao J.T. et al. (2002) [1]

Al<sub>2.80</sub>Si<sub>0.20</sub>Yb<sub>0.98</sub>

*a* = 0.6009, *c* = 1.4199 nm, *c/a* = 2.363, *V* = 0.4440 nm<sup>3</sup>, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.1675	0.335	0.5812		
Al2	6 <i>h</i>	<i>mm</i> 2	0.5188	0.0376	<sup>1</sup> / <sub>4</sub>	0.83	
Si3	6 <i>h</i>	<i>mm</i> 2	0.537	0.074	<sup>1</sup> / <sub>4</sub>	0.17	
Yb4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.09213	0.963	
Yb5	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		

M1 = 0.985Al + 0.015Si

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.049

Remarks: The occupancies of the Al and Si sites were fixed in agreement with a refinement on the isotypic alumogermanide. Short interatomic distances for partly occupied site(s).

References: [1] Zhao J.T., Schnelle W., Grin Y. (2002), J. Solid State Chem. 163, 113-120.

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hP30

<b>BaTiO<sub>3</sub></b>	<b>hP30</b>	<b>(194) <i>P6<sub>3</sub>/mmc</i> – khf<sup>2</sup>ba</b>
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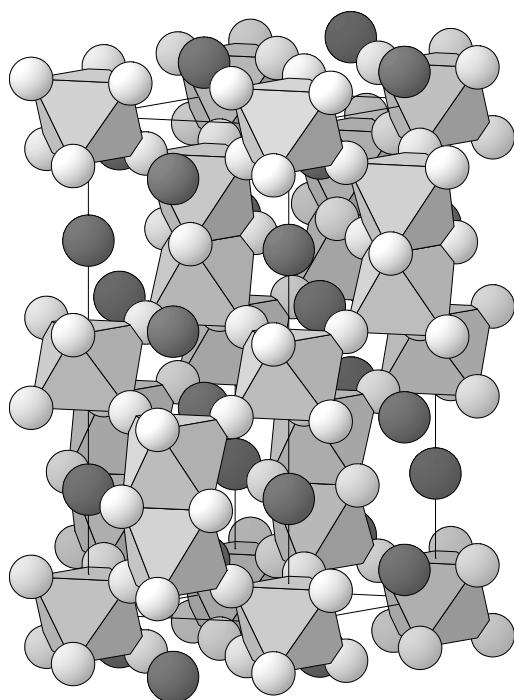
**BaTiO<sub>3</sub> hexagonal** [2], perovskite 6H; RbMgH<sub>3</sub> [4]

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Ti in octahedral (O<sub>6</sub>) voids. Pairs of face-linked and single TiO<sub>6</sub> octahedra (Ti<sub>2</sub> dumbbells and single Ti) share vertices to form a 3D-framework. See Fig. III.36.

Akimoto J. et al. (1994) [1]

 $\text{BaO}_3\text{Ti}$  $a = 0.57238$ ,  $c = 1.39649$  nm,  $c/a = 2.440$ ,  $V = 0.3962$  nm<sup>3</sup>,  $Z = 6$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1651	0.3302	0.5802		non-colinear Ti <sub>2</sub>
O2	6 <i>h</i>	<i>mm</i> 2	0.5185	0.037	$\frac{1}{4}$		non-colinear Ti <sub>2</sub>
Ba3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.09671		cuboctahedron O <sub>12</sub>
Ti4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.65367		octahedron O <sub>6</sub>
Ba5	2 <i>b</i>	-6. <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Ti6	2 <i>a</i>	-3. <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.036$ ,  $T = 296$  KRemarks: The crystal studied in [2] was later shown to contain small amounts of Pt introduced by interaction with the crucible (see [1]). The structure of oxygen-deficient  $\text{BaTiO}_3$  is studied in [3].Fig. III.36. **BaTiO<sub>3</sub> hexagonal**Arrangement of TiO<sub>6</sub> octahedra (O atoms light) and Ba atoms (dark).

References: [1] Akimoto J., Gotoh Y., Oosawa Y. (1994), Acta Crystallogr. C 50, 160-161. [2] Burbank R.D., Evans H.T. Jr. (1948), Acta Crystallogr. 1, 330-336. [3] Sinclair D.C., Skakle J.M.S., Morrison F.D., Smith R.I., Beales T.P. (1999), J. Mater. Chem. 9, 1327-1331. [4] Gingl F., Vogt T., Akiba E., Yvon K. (1999), J. Alloys Compd. 282, 125-129.

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*hP30* $\text{K}_4\text{I}_2\text{O}_9$ *hP30*(194)  $P6_3/mmc - khf^2ba$ **K<sub>4</sub>I<sub>2</sub>O<sub>9</sub>** [1]

Structural features: Close-packed KO<sub>3</sub> layers in *hc*<sub>2</sub> stacking; I and additional K in octahedral (O<sub>6</sub>) voids. Pairs of face-linked IO<sub>6</sub> octahedra. Ordering variant of hexagonal BaTiO<sub>3</sub>, K<sub>3</sub>[KI<sub>2</sub>]O<sub>9</sub>.

Brehler B. et al. (1968) [1]

 $\text{I}_2\text{K}_4\text{O}_9$  $a = 0.621$ ,  $c = 1.536$  nm,  $c/a = 2.473$ ,  $V = 0.5130$  nm<sup>3</sup>,  $Z = 2$ 

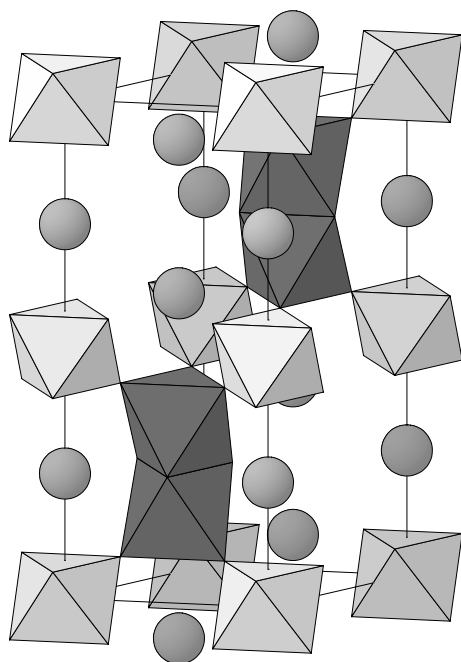
site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1897	0.3794	0.6016		single atom I
O2	6 <i>h</i>	<i>mm</i> 2	0.5384	0.0768	$\frac{1}{4}$		non-colinear I <sub>2</sub>
K3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0886		cuboctahedron O <sub>12</sub>
I4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.655		octahedron O <sub>6</sub>
K5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
K6	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.054$ Remarks: In table 1 of [1] the Wyckoff letter of former O(I) is misprinted as *b* instead of *h*.

References: [1] Brehler B., Jacobi H., Siebert H. (1968), Z. Anorg. Allg. Chem. 362, 301-311.

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*hP*30

$\text{Ba}_3(\text{W}_{0.5}\text{Fe}_{0.5})_2\text{FeO}_9$	<i>hP</i> 30	(194) $P6_3/mmc - \text{kfh}^2\text{ba}$
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**Ba<sub>3</sub>WFe<sub>2</sub>O<sub>9</sub>** [2], perovskite 6H; Ba<sub>3</sub>Fe<sub>2</sub>TeO<sub>9</sub> [4]; Ba<sub>3</sub>NiSb<sub>2</sub>O<sub>9</sub> [7]; Ba<sub>3</sub>YIr<sub>2</sub>O<sub>9</sub> [3]; Ba<sub>3</sub>YRu<sub>2</sub>O<sub>9</sub> [6]Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Fe and (Fe,W) in octahedral (O<sub>6</sub>) voids. Pairs of face-linked (Fe,W)O<sub>6</sub> octahedra ((Fe,W)<sub>2</sub> dumbbells) share vertices with single FeO<sub>6</sub> octahedra to form a 3D-framework. See Fig. III.37.Fig. III.37. **Ba<sub>3</sub>WFe<sub>2</sub>O<sub>9</sub>**Arrangement of (W,Fe)O<sub>6</sub> (dark) and FeO<sub>6</sub> (light) octahedra and Ba atoms.

Ivanov S.A. et al. (2004) [1]

 $\text{Ba}_3\text{Fe}_2\text{O}_{8.70}\text{W}$  $a = 0.57584$ ,  $c = 1.41019$  nm,  $c/a = 2.449$ ,  $V = 0.4050$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1678	0.3356	0.5832	0.96	non-colinear Fe <sub>2</sub>
O2	6h	mm2	0.5159	0.0318	1/4	0.98	non-colinear Fe <sub>2</sub>
Ba3	4f	3m.	1/3	2/3	0.0928		cuboctahedron O <sub>12</sub>
M4	4f	3m.	1/3	2/3	0.6478		octahedron O <sub>6</sub>
Ba5	2b	-6m2	0	0	1/4		anticuboctahedron O <sub>12</sub>
Fe6	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M4 = 0.5Fe + 0.5W

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.041, T = 300 K

Remarks: Antiferroelectric below 573 K, weakly ferromagnetic below 330 K. Fully ordered structures are reported for Ba<sub>3</sub>NiSb<sub>2</sub>O<sub>9</sub>, Ba<sub>3</sub>YIr<sub>2</sub>O<sub>9</sub> and Ba<sub>3</sub>YRu<sub>2</sub>O<sub>9</sub>. Ba<sub>3</sub>WFe<sub>2</sub>O<sub>9</sub> and Ba<sub>3</sub>Fe<sub>2</sub>TeO<sub>9</sub> were refined in space group (182) *P*6<sub>3</sub>22 in [5]. In table 2 of [6] the *y*-coordinate of former O(1) is misprinted as 0.0255 instead of -0.0255 (site splitting is assumed to be not intentional). In table 1 of the same reference the *a*-parameter is misprinted as 0.5595 nm instead of 0.5895 nm (given in the abstract, where, however, the cell parameters of compounds I and II are interchanged).

References: [1] Ivanov S.A., Eriksson S.G., Eriksson J., Tellgren R., Rundlof H. (2004), Mater. Res. Bull. 39, 615-628. [2] Sévêque F., Delamoye P., Poix P., Michel A. (1969), C. R. Seances Acad. Sci., Ser. C 269, 1536-1538. [3] Thumm I., Treiber U., Kemmler Sack S. (1980), J. Solid State Chem. 35, 156-166. [4] Harari D., Bernier J.C., Poix P. (1972), J. Solid State Chem. 5, 382-390. [5] Gagulin V.V., Fadeeva N.V., Belous A.G., Titov A.V., Mitrofanov K.P., Plotnikova M.V., Soloviev S.P., Venevtsev Y.N. (1978), Phys. Status Solidi A 48, 183-189. [6] Rath M., Müller Buschbaum H. (1994), J. Alloys Compd. 210, 119-123. [7] Jacobson A.J., Calvert A.J. (1978), J. Inorg. Nucl. Chem. 40, 447-449.

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hP30

Ti <sub>2</sub> In <sub>3</sub> Br <sub>9</sub>	hP30	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khf <sup>2</sup> e
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### In<sub>3</sub>Ti<sub>2</sub>Br<sub>9</sub> [1]

Structural features: Close-packed InBr<sub>3</sub> layers in hc<sub>2</sub> stacking; Ti in octahedral (Br<sub>6</sub>) voids next to h-stacked layers, leaving every third interlayer vacant. Units of two face-linked TiBr<sub>6</sub> octahedra (Ti<sub>2</sub> dumbbells) parallel to [001]. Variant of Cs<sub>3</sub>Cr<sub>2</sub>Cl<sub>9</sub> with splitting of one In site.

Dronskowski R. (1995) [1]

Br<sub>9</sub>In<sub>3</sub>Ti<sub>2</sub>

*a* = 0.7382, *c* = 1.8139 nm, *c/a* = 2.457, *V* = 0.8560 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Br1	12k	.m.	0.1698	0.3396	0.58704		single atom Ti
Br2	6h	mm2	0.5029	0.0058	1/4		non-colinear Ti <sub>2</sub>
In3	4f	3m.	1/3	2/3	0.0604		non-coplanar triangle Br <sub>3</sub>
Ti4	4f	3m.	1/3	2/3	0.6633		octahedron Br <sub>6</sub>
In5	4e	3m.	0	0	0.2318	0.5	

Experimental: single crystal, diffractometer, X-rays, R = 0.048, T = 293 K

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

References: [1] Dronskowski R. (1995), Chem. Eur. J. 1, 118-123.

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hP30

Na <sub>1.88</sub> Y <sub>0.04</sub> [SO <sub>4</sub> ]	hP30	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kjdca
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**Na<sub>2</sub>SO<sub>4</sub> form I:Y** [1]; Na<sub>2</sub>SO<sub>4</sub> form I [2]

Structural features: (Na,Y) atoms and SO<sub>4</sub> tetrahedra (orientational disorder) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement.

Eysel W. et al. (1985) [1]

Na<sub>1.88</sub>O<sub>4</sub>SY<sub>0.04</sub>

$a = 0.5326$ ,  $c = 0.7126$  nm,  $c/a = 1.338$ ,  $V = 0.1751$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.242	0.484	0.082	0.333	anticuboctahedron O <sub>12</sub>
O2	12 <i>j</i>	<i>m</i> ..	0.147	0.346	$\frac{1}{4}$	0.333	
M3	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.96	
S4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
M5	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.96	

M3 = 0.98Na + 0.02Y; M5 = 0.98Na + 0.02Y

Experimental: single crystal, diffractometer, X-rays, R = 0.093, T = 293 K

Remarks: Phase stable at T > ~510 K, homogeneity range (Na<sub>2</sub>SO<sub>4</sub>)<sub>100-x</sub>(Y<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>)<sub>x</sub>, 0 < x < 19 at 1058 K. Short interatomic distances for partly occupied site(s).

References: [1] Eysel W., Höfer H.H., Keester K.L., Hahn T. (1985), Acta Crystallogr. B 41, 5-11. [2] Rasmussen S.E., Jorgensen J., Lundtoft B. (1996), J. Appl. Crystallogr. 29, 42-47.

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hP32

CoCl <sub>3</sub> [NH <sub>3</sub> ] <sub>3</sub> [H <sub>2</sub> O]	hP32	(194) P6 <sub>3</sub> /mmc – j <sup>2</sup> fca
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**[Co(NH<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)Cl<sub>2</sub>]Cl** [1]

Structural features: Cl anions and Co[(NH<sub>3</sub>,OH<sub>2</sub>)<sub>4</sub>Cl<sub>2</sub>] octahedral units (rotational disorder about the axis defined by the Cl atoms) in a NiAs-type arrangement.

Tanito Y. et al. (1952) [1]

Cl<sub>3</sub>CoH<sub>10.99</sub>N<sub>3</sub>O

$a = 0.737$ ,  $c = 0.875$  nm,  $c/a = 1.187$ ,  $V = 0.4116$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	12 <i>j</i>	<i>m</i> ..	0.038	0.451	$\frac{1}{4}$	0.333	single atom Co
M2	12 <i>j</i>	<i>m</i> ..	0.117	0.372	$\frac{1}{4}$	0.333	
Cl3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.516		
Co4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Cl5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

M1 = 0.75NH<sub>3</sub> + 0.25OH<sub>2</sub>; M2 = 0.75NH<sub>3</sub> + 0.25OH<sub>2</sub>

Experimental: single crystal, oscillation photographs, X-rays

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

References: [1] Tanito Y., Saito Y., Kuroya H. (1952), Bull. Chem. Soc. Jpn. 25, 328-331.

194  
hP32

Ca <sub>2</sub> [SiO <sub>4</sub> ]	hP32	(194) P6 <sub>3</sub> /mmc – k <sup>2</sup> fca
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**Ca<sub>2</sub>SiO<sub>4</sub> α** [1]



Structural features: Ca atoms and SiO<sub>4</sub> tetrahedra (rotational disorder) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement (part of Ca displaced from the ideal positions).

Mumme W. et al. (1996) [1]

Ca<sub>2</sub>O<sub>4</sub>Si

$a = 0.5532$ ,  $c = 0.7327$  nm,  $c/a = 1.324$ ,  $V = 0.1942$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1741	0.3482	0.2018	0.333	
O2	12 <i>k</i>	. <i>m</i> .	0.2721	0.5442	0.0405	0.333	
Ca3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.7373	0.5	
Si4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Ca5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.065$ ,  $T = 1818$  K

Remarks: Phase stable at  $T > 1698$  K. Short interatomic distances for partly occupied site(s). A similar model with site O1 on the 3-fold axis is also reported.

References: [1] Mumme W., Cranswick L., Chakoumakos B. (1996), Neues Jahrb. Mineral., Abh. 170, 171-188.

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*hP32*

Cu <sub>2</sub> S	<i>hP32</i>	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> fc <b>b</b>
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**Cu<sub>2</sub>S chalcocite ht** [1], chalcocite high

Structural features: Close-packed S layers in h stacking; Cu in tetrahedral, trigonal and linear voids (disorder).

Sadanaga R. et al. (1965) [1]

Cu<sub>2</sub>S

$a = 0.3961$ ,  $c = 0.6722$  nm,  $c/a = 1.697$ ,  $V = 0.0913$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	12 <i>k</i>	. <i>m</i> .	0.21667	0.43333	0.570	0.133	
Cu2	12 <i>k</i>	. <i>m</i> .	0.58333	0.16667	0.033	0.067	
Cu3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.600	0.1	
S4	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Cu5	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$	0.6	trigonal prism Cu <sub>6</sub>

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

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.170$ ,  $T = 417$  K

Remarks: Phase stable at  $377 < T < 708$  K. Natural specimen from St. Ives, Cornwall, United Kingdom. Cell parameters from [2]. Short interatomic distances for partly occupied site(s). The structure proposal is criticized in [3].

References: [1] Sadanaga R., Ohmasa M., Morimoto N. (1965), Mineral. J. 4, 275-290. [2] Djurle S. (1958), Acta Chem. Scand. 12, 1415-1426. [3] Cava R.J., Reidinger F., Wuensch B.J. (1981), Solid State Ionics 5, 501-504.

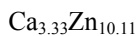
194  
*hP32*

Ca <sub>3.33</sub> Zn <sub>10.11</sub>	<i>hP32</i>	(194) <i>P6<sub>3</sub>/mmc</i> – kh <sup>2</sup> fb <b>a</b>
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**CaZn<sub>3</sub>** [1]

Structural features: Derivative of AlB<sub>2</sub> with part of the Ca atoms replaced by Zn<sub>3</sub> triangles perpendicular to [001] (partial disorder); additional Zn at the centers of hexagons in the puckered hexagon-mesh Zn layers.

Fornasini M.L., Merlo F. (1980) [1]



$a = 0.9168$ ,  $c = 0.7327$  nm,  $c/a = 0.799$ ,  $V = 0.5333$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	12 <i>k</i>	. <i>m</i> .	0.1692	0.3384	0.0556		8-vertex polyhedron Zn <sub>8</sub>
Ca2	6 <i>h</i>	<i>mm</i> 2	0.5260	0.0520	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>14</sub> Ca <sub>4</sub>
Zn3	6 <i>h</i>	<i>mm</i> 2	0.9022	0.8044	<sup>1</sup> / <sub>4</sub>	0.66	
Zn4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0715		tetrahedron Zn <sub>4</sub>
Ca5	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.33	
Zn6	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.13	colinear Ca <sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Identical to the phase called Ca<sub>7</sub>Zn<sub>20</sub> in [2]. Short interatomic distances for partly occupied site(s).

References: [1] Fornasini M.L., Merlo F. (1980), Acta Crystallogr. B 36, 1739-1744. [2] Messing A.F., Adams M.D., Steunenberg R.K. (1963), ASM Trans. Q. 56, 345-350.

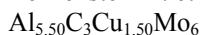
194  
hP32

(Cu <sub>0.5</sub> Al <sub>0.5</sub> ) <sub>3</sub> (Mo <sub>0.67</sub> Al <sub>0.33</sub> ) <sub>9</sub> AlC <sub>3</sub>	hP32	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kh <sup>2</sup> ga
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**Mo<sub>12</sub>Cu<sub>3</sub>Al<sub>11</sub>C<sub>6</sub>** [1], κ phase; Ti<sub>9</sub>Fe<sub>3</sub>(Ti<sub>0.7</sub>Fe<sub>0.3</sub>)O<sub>3</sub> [2]

Structural features: Infinite columns of face-sharing Al[(Mo,Al)<sub>6</sub>(Al,Cu)<sub>6</sub>] icosahedra are interconnected via additional (Mo,Al) atoms to form a 3D-framework; C in octahedral voids.

Reiffenstein E. et al. (1966) [1]



$a = 0.7952$ ,  $c = 0.7865$  nm,  $c/a = 0.989$ ,  $V = 0.4307$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.215	0.43	0.562		non-colinear C <sub>2</sub>
M2	6 <i>h</i>	<i>mm</i> 2	0.11	0.22	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>4</sub> Mo <sub>8</sub>
M3	6 <i>h</i>	<i>mm</i> 2	0.45	0.9	<sup>1</sup> / <sub>4</sub>		non-colinear C <sub>2</sub>
C4	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		octahedron Mo <sub>6</sub>
Al5	2 <i>a</i>	-3 <i>m</i> .	0	0	0		icosahedron Al <sub>6</sub> Mo <sub>6</sub>

M1 = 0.667Mo + 0.333Al; M2 = 0.5Al + 0.5Cu; M3 = 0.667Mo + 0.333Al

Experimental: powder, film, X-rays

References: [1] Reiffenstein E., Nowotny H., Benesovsky F. (1966), Monatsh. Chem. 97, 499-505. [2] Rogl P., Rupp B., Wiesinger G., Schefer J., Fischer P. (1985), J. Less-Common Met. 113, 103-111.

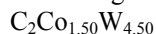
194  
hP32

W <sub>3</sub> (W <sub>0.5</sub> Co <sub>0.5</sub> ) <sub>3</sub> C <sub>2</sub>	hP32	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kh <sup>2</sup> gc
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**W<sub>9</sub>Co<sub>3</sub>C<sub>4</sub>** [1],  $\kappa$  phase

Structural features: Infinite columns of face-sharing empty [(W,Co)<sub>6</sub>W<sub>6</sub>] icosahedra are interconnected via additional (W,Co) atoms to form a 3D-framework; C in octahedral and trigonal prismatic voids.

Schönberg N. (1954) [1]



$a = 0.7826$ ,  $c = 0.7826$  nm,  $c/a = 1.000$ ,  $V = 0.4151$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
W1	12 <i>k</i>	. <i>m</i> .	0.205	0.41	0.075		non-coplanar triangle C <sub>3</sub>
M2	6 <i>h</i>	<i>mm</i> 2	0.555	0.11	$\frac{1}{4}$		non-colinear C <sub>2</sub>
M3	6 <i>h</i>	<i>mm</i> 2	0.89	0.78	$\frac{1}{4}$		10-vertex polyhedron Co <sub>4</sub> W <sub>6</sub>
C4	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		octahedron Co <sub>2</sub> W <sub>4</sub>
C5	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism W <sub>6</sub>

M2 = 0.5Co + 0.5W; M3 = 0.5Co + 0.5W

Experimental: powder, film, X-rays

Remarks: An ordered arrangement of W and Co and additional W in Wyckoff position 2*a* were later found [2].

References: [1] Schönberg N. (1954), Acta Metall. 2, 837-840. [2] Harsta A., Johansson T., Rundqvist S., Thomas J.O. (1977), Acta Chem. Scand. A 31, 260-264.

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*hP*34

(Zn <sub>0.86</sub> Fe <sub>0.14</sub> ) <sub>7</sub> LuO <sub>9</sub>	<i>hP</i> 34	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – f <sup>4</sup> e <sup>3</sup> cba
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**LuFeO<sub>3</sub>(ZnO)<sub>6</sub>** [1]

Structural features: Close-packed O layers in  $h_7c_2$  stacking; (Zn,Fe) in tetrahedral and trigonal bipyramidal voids, Lu in octahedral voids between c-stacked layers.

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



$a = 0.3322$ ,  $c = 4.291$  nm,  $c/a = 12.917$ ,  $V = 0.4101$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0234		tetrahedron ZnLu <sub>3</sub>
M2	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.07105		tetrahedron O <sub>4</sub>
O3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1407		tetrahedron Zn <sub>4</sub>
M4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.19028		tetrahedron O <sub>4</sub>
O5	4 <i>e</i>	3 <i>m</i> .	0	0	0.0832		tetrahedron Zn <sub>4</sub>
M6	4 <i>e</i>	3 <i>m</i> .	0	0	0.13094		tetrahedron O <sub>4</sub>
O7	4 <i>e</i>	3 <i>m</i> .	0	0	0.1976		tetrahedron Zn <sub>4</sub>
O8	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Zn <sub>3</sub>
M9	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>
Lu10	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M2 = 0.857Zn + 0.143Fe; M4 = 0.857Zn + 0.143Fe; M6 = 0.857Zn + 0.143Fe; M9 = 0.857Zn + 0.143Fe

Experimental: single crystal, diffractometer, X-rays,  $R = 0.066$ ,  $T = 295$  K

References: [1] Isobe M., Kimizuka N., Nakamura M., Mohri T. (1994), Acta Crystallogr. C 50, 332-336.

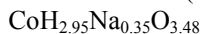
194  
hP34

$\text{Na}_{0.35}\text{CoO}_2[\text{H}_2\text{O}]_{1.3}$	<i>hP34</i>	(194) $P6_3/mmc - k^2fcba$
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 **$\text{Na}_{0.35}\text{CoO}_2 \cdot 1.3\text{H}_2\text{O}$  [1]**

Structural features: Infinite layers of edge-linked  $\text{CoO}_6$  octahedra (h stacking) and double  $\text{H}_2\text{O}$  layers (partial disorder) alternate along [001]; Na between the  $\text{H}_2\text{O}$  layers (partial disorder).

Takada K. et al. (2003) [1]


 $a = 0.2823$ ,  $c = 1.96207$  nm,  $c/a = 6.95$ ,  $V = 0.1354$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH <sub>2</sub> )1	12k	.m.	0.174	0.348	0.6793	0.07	
(OH <sub>2</sub> )2	12k	.m.	0.185	0.37	0.1793	0.176	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5451		non-coplanar triangle Co <sub>3</sub>
Na4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.159	
Na5	2b	-6m2	0	0	$\frac{1}{4}$	0.192	
Co6	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: powder, diffractometer, X-rays,  $R_B = 0.028$ 

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] Takada K., Sakurai H., Takayama Muromachi E., Izumi F., Dilanian R.A., Sasaki T. (2003), Nature (London) 422, 53-55.

194  
hP34

$\text{W}_{10}\text{Co}_3\text{C}_{3.4}$	<i>hP34</i>	(194) $P6_3/mmc - kh^2gca$
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 **$\text{W}_{10}\text{Co}_3\text{C}_{3.4}$  [1],  $\kappa$  phase; (CFeW)  $\kappa$  [2]**

Structural features: Infinite columns of face-sharing  $\text{W}(\text{W}_6\text{Co}_6)$  icosahedra are interconnected via additional W atoms to form a 3D-framework; C in octahedral and trigonal prismatic voids.

Harsta A. et al. (1977) [1]


 $a = 0.78304$ ,  $c = 0.78361$  nm,  $c/a = 1.001$ ,  $V = 0.4161$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
W1	12k	.m.	0.2038	0.4076	0.0682		non-coplanar triangle C <sub>3</sub>
W2	6h	mm2	0.5497	0.0994	$\frac{1}{4}$		non-colinear C <sub>2</sub>
Co3	6h	mm2	0.8868	0.7736	$\frac{1}{4}$		icosahedron $\text{W}_{10}\text{Co}_2$
C4	6g	.2/m.	$\frac{1}{2}$	0	0		octahedron W <sub>6</sub>
C5	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.415	trigonal prism W <sub>6</sub>
W6	2a	-3m.	0	0	0		icosahedron $\text{Co}_6\text{W}_6$

Experimental: powder, diffractometer, neutrons,  $R_B = 0.078$ , T = 298 K

Remarks: Supersedes a structure proposal with Wyckoff position 2a vacant and full occupation of position 2c [3].

References: [1] Harsta A., Johansson T., Rundqvist S., Thomas J.O. (1977), Acta Chem. Scand. A 31, 260-264. [2] Harsta A., Rundqvist S., Thomas J.O. (1983), J. Solid State Chem. 49, 118-122. [3] Schönberg N. (1954), Acta Metall. 2, 837-840.

194  
hP34

$\text{Hf}_{9.25}\text{Mo}_{3.75}\text{Ge}_{0.88}\text{O}_{1.5}$	<i>hP34</i>	(194) $P6_3/mmc - \text{kh}^2\text{gca}$
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### $\text{Hf}_{9+x}\text{Mo}_{4-x}\text{Ge}_y\text{O}_{1.5}$ [1], $\kappa$ phase

Structural features: Infinite columns of face-sharing  $(\text{Mo}, \text{Hf})[(\text{Mo}, \text{Hf})_6\text{Hf}_6]$  icosahedra are interconnected via additional Hf atoms to form a 3D-framework; O in octahedral, Ge in trigonal prismatic voids. Ordering variant of  $\text{W}_{10}\text{Co}_3\text{C}_{3.4}$ .

Harsta A. (1985) [1]

$\text{Ge}_{0.88}\text{Hf}_{9.25}\text{Mo}_{3.75}\text{O}_{1.47}$

$a = 0.86394$ ,  $c = 0.86827$  nm,  $c/a = 1.005$ ,  $V = 0.5612$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Hf1	12 <i>k</i>	<i>m.</i>	0.19912	0.39824	0.04652		non-colinear O <sub>2</sub>
Hf2	6 <i>h</i>	<i>mm2</i>	0.54074	0.08148	<sup>1</sup> / <sub>4</sub>		non-colinear O <sub>2</sub>
M3	6 <i>h</i>	<i>mm2</i>	0.89093	0.78186	<sup>1</sup> / <sub>4</sub>		icosahedron Mo <sub>4</sub> Hf <sub>8</sub>
O4	6 <i>g</i>	<i>.2/m.</i>	<sup>1</sup> / <sub>2</sub>	0	0	0.49	octahedron Hf <sub>6</sub>
Ge5	2 <i>c</i>	<i>-6m2</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.88	trigonal prism Hf <sub>6</sub>
M6	2 <i>a</i>	<i>-3m.</i>	0	0	0		icosahedron Mo <sub>6</sub> Hf <sub>6</sub>

M3 = 0.94Mo + 0.06Hf; M6 = 0.93Mo + 0.07Hf

Experimental: single crystal, diffractometer, X-rays, R = 0.066

References: [1] Harsta A. (1985), J. Solid State Chem. 57, 373-378.

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hP34

$\text{Ba}_5\text{Ru}_2\text{O}_{10}$	<i>hP34</i>	(194) $P6_3/mmc - \text{khf}^2\text{eda}$
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### $\text{Ba}_5\text{Ru}_2\text{O}_{10}$ [1]

Structural features: Double perovskite-type slabs (three close-packed BaO<sub>3</sub> layers, Ru in octahedral voids) alternate with triangle-mesh Ba<sub>2</sub>O layers along [001]. Units of two face-linked RuO<sub>6</sub> octahedra (Ru<sub>2</sub> dumbbells).

Dussarrat C. et al. (1994) [1]

$\text{Ba}_5\text{O}_{10}\text{Ru}_2$

$a = 0.5958$ ,  $c = 1.8045$  nm,  $c/a = 3.029$ ,  $V = 0.5547$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	<i>m.</i>	0.5166	0.0332	0.6176		single atom Ru
O2	6 <i>h</i>	<i>mm2</i>	0.1863	0.3726	<sup>1</sup> / <sub>4</sub>		non-colinear Ru <sub>2</sub>
Ru3	4 <i>f</i>	3 <i>m.</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1742		octahedron O <sub>6</sub>
Ba4	4 <i>f</i>	3 <i>m.</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5158		trigonal prism O <sub>6</sub>
Ba5	4 <i>e</i>	3 <i>m.</i>	0	0	0.1382		10-vertex polyhedron O <sub>10</sub>
Ba6	2 <i>d</i>	<i>-6m2</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>
O7	2 <i>a</i>	<i>-3m.</i>	0	0	0		colinear Ba <sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.048

Remarks: Identical to the phases called Ba<sub>4</sub>RuO<sub>6</sub> in [2] and Ba<sub>3</sub>RuO<sub>5</sub> in [3]. Space groups (186) *P6<sub>3</sub>mc* and (190) *P-62c* were tested and rejected.

References: [1] Dussarrat C., Fompeyrine J., Darriet J. (1994), Eur. J. Solid State Inorg. Chem. 31, 289-300. [2] Prosychev I.I., Shaplygin I.S. (1980), Russ. J. Inorg. Chem. 25, 489 (Zh. Neorg. Khim. 25, 876-877). [3] Popova T.L., Kisel N.G., Krivobok V.I., Karlov V.P. (1983), Sov. Prog. Chem. (Engl. Transl.) 48, 8.

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Na <sub>0.95</sub> Ba <sub>3</sub> Ru <sub>1.74</sub> [CO <sub>3</sub> ] <sub>0.31</sub> O <sub>7.76</sub>	hP34	(194) <i>P6<sub>3</sub>/mmc</i> – khf <sup>3</sup> ba
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**Ba<sub>3</sub>(Ru<sub>1.69</sub>C<sub>0.31</sub>)(Na<sub>0.95</sub>Ru<sub>0.05</sub>)O<sub>8.69</sub>** [1], perovskite 6H carbonate

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Ru and (Na,Ru) in octahedral voids. Derivative of Ba<sub>3</sub>(W<sub>0.5</sub>Fe<sub>0.5</sub>)<sub>2</sub>FeO<sub>9</sub>, Ba<sub>3</sub>Ru<sub>2</sub>(Na,Ru)O<sub>9</sub>, with part of the units of two face-linked RuO<sub>6</sub> octahedra (Ru<sub>2</sub> dumbbells) replaced by a RuO<sub>5</sub> square pyramid and a CO<sub>3</sub> trigonal unit.

Quarez E. et al. (2003) [1]

Ba<sub>3</sub>C<sub>0.30</sub>Na<sub>0.94</sub>O<sub>8.70</sub>Ru<sub>1.76</sub>

*a* = 0.58313, *c* = 1.44535 nm, *c/a* = 2.479, *V* = 0.4256 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1792	0.3584	0.5912		
O2	6 <i>h</i>	<i>mm</i> 2	0.513	0.026	<sup>1</sup> / <sub>4</sub>	0.9	non-colinear Ru <sub>2</sub>
Ba3	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0898		13-vertex polyhedron CO <sub>12</sub>
C4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.612	0.15	
Ru5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6564	0.85	
Ba6	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>
M7	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M7 = 0.94Na + 0.06Ru

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, R = 0.030, T = 300 K

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

References: [1] Quarez E., Huvé M., Abraham F., Mentré O. (2003), Solid State Sci. 5, 951-963.

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K <sub>2</sub> Co <sub>2</sub> [SeO <sub>3</sub> ] <sub>3</sub>	hP34	(194) <i>P6<sub>3</sub>/mmc</i> – khf <sup>3</sup> e
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**K<sub>2</sub>Co<sub>2</sub>(SeO<sub>3</sub>)<sub>3</sub>** [1]

Structural features: Units of two face-linked CoO<sub>6</sub> octahedra (Co<sub>2</sub> dumbbells) share vertices with single :SeO<sub>3</sub> ψ-tetrahedra to form infinite double slabs.

Wildner M. (1994) [1]

Co<sub>2</sub>K<sub>2</sub>O<sub>9</sub>Se<sub>3</sub>

*a* = 0.5486, *c* = 1.7574 nm, *c/a* = 3.203, *V* = 0.4580 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1599	0.3198	0.0958		non-colinear SeCo
O2	6 <i>h</i>	<i>mm</i> 2	0.5031	0.0062	<sup>1</sup> / <sub>4</sub>		non-colinear Se <sub>2</sub>
Co3	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.16586		octahedron O <sub>6</sub>
K4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.53494		10-vertex polyhedron O <sub>9</sub> Se

Se5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7148	0.5	
Se6	4e	3m.	0	0	0.13913		non-coplanar triangle O <sub>3</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.034, T = 295 K

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

References: [1] Wildner M. (1994), Acta Crystallogr. C 50, 336-338.

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hP34

CsTi <sub>4.3</sub> I <sub>11</sub>	hP34	(194) P6 <sub>3</sub> /mmc – khgf <sup>2</sup> b
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### CsTi<sub>4.3</sub>I<sub>11</sub> [1]

Structural features: Close-packed CsI<sub>3</sub> and I<sub>4</sub> layers in hc<sub>2</sub> stacking; Ti in octahedral (I<sub>6</sub>) voids. Infinite layers of edge-linked TiI<sub>6</sub> octahedra (partial vacancies ignored) share additional edges with units of two face-linked octahedra (Ti<sub>2</sub> dumbbells) to form a 3D-framework.

Zhang J. et al. (1991) [1]

CsI<sub>11</sub>Ti<sub>4.31</sub>

$a = 0.82058$ ,  $c = 1.9723$  nm,  $c/a = 2.404$ ,  $V = 1.1501$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	12k	.m.	0.1693	0.3386	0.58447		non-coplanar triangle Ti <sub>3</sub>
I2	6h	mm2	0.504	0.008	$\frac{1}{4}$		non-colinear Ti <sub>2</sub>
Ti3	6g	.2/m.	$\frac{1}{2}$	0	0	0.77	octahedron I <sub>6</sub>
I4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0819		non-coplanar triangle Ti <sub>3</sub>
Ti5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6676		octahedron I <sub>6</sub>
Cs6	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron I <sub>12</sub>

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

References: [1] Zhang J., Qi R.Y., Corbett J.D. (1991), Inorg. Chem. 30, 4794-4798.

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hP34

BaRuO <sub>3</sub> [OH] <sub>2</sub>	hP34	(194) P6 <sub>3</sub> /mmc – kjhca
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### BaRuO<sub>3</sub>(OH)<sub>2</sub> [1]

Structural features: Ba atoms and Ru[O<sub>3</sub>(OH)<sub>2</sub>] trigonal bipyramids (orientational disorder) in a NiAs-type arrangement.

Nowogrocki G. et al. (1976) [1]

BaH<sub>2</sub>O<sub>4.99</sub>Ru

$a = 0.5787$ ,  $c = 0.8491$  nm,  $c/a = 1.467$ ,  $V = 0.2463$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.562	0.124	0.59	0.333	
(OH)2	12j	m..	0.315	0.009	$\frac{1}{4}$	0.333	
O3	6h	mm2	0.168	0.336	$\frac{1}{4}$	0.333	
Ru4	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism O <sub>9</sub>
Ba5	2a	-3m.	0	0	0		

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

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Average structure; the superstructure was refined in space group (167)  $R\bar{3}c$  (new axes  $2a+b, -a+b, 3c$ ).

References: [1] Nowogrocki G., Abraham F., Trehoux J., Thomas D. (1976), Acta Crystallogr. B 32, 2413-2419.

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hP36

Ti <sub>0.77</sub> S	hP36	(194) $P6_3/mmc - f^6e^3ca$
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### Ti<sub>6.9</sub>S<sub>9</sub> [1]

Structural features: Close-packed S layers in h<sub>2</sub>c(hc)<sub>3</sub> stacking; Ti in octahedral voids (partial order).

Onoda M., Wada H. (1987) [1]

STi<sub>0.76</sub>

$a = 0.34365$ ,  $c = 5.165$  nm,  $c/a = 15.030$ ,  $V = 0.5282$  nm<sup>3</sup>,  $Z = 18$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	4f	3m.	1/3	2/3	0.029		trigonal prism Ti <sub>6</sub>
Ti2	4f	3m.	1/3	2/3	0.110		octahedron S <sub>6</sub>
Ti3	4f	3m.	1/3	2/3	0.166	0.65	octahedron S <sub>6</sub>
S4	4f	3m.	1/3	2/3	0.584		octahedron Ti <sub>6</sub>
S5	4f	3m.	1/3	2/3	0.694		octahedron Ti <sub>6</sub>
Ti6	4e	3m.	0	0	0.059	0.47	octahedron S <sub>6</sub>
S7	4e	3m.	0	0	0.137		trigonal prism Ti <sub>6</sub>
Ti8	4e	3m.	0	0	0.219	0.83	octahedron S <sub>6</sub>
S9	2c	-6m2	1/3	2/3	1/4		trigonal prism Ti <sub>6</sub>
Ti10	2a	-3m.	0	0	0	0.98	octahedron S <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.160

Remarks: The structure was studied jointly on X-ray and electron diffraction data.

References: [1] Onoda M., Wada H. (1987), J. Less-Common Met. 132, 195-207.

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hP36

Li <sub>2</sub> UCl <sub>6</sub>	hP36	(194) $P6_3/mmc - ih^3fa$
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### Li<sub>2</sub>UCl<sub>6</sub> [1]

Structural features: Close-packed Cl layers in h stacking; Li and U in octahedral voids (disordered vacancies).

Bendall P.J. et al. (1983) [1]

Cl<sub>6</sub>Li<sub>2</sub>U

$a = 1.11915$ ,  $c = 0.60356$  nm,  $c/a = 0.539$ ,  $V = 0.6547$  nm<sup>3</sup>,  $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	12i	.2.	0.338	0	0	0.5	8-vertex polyhedron Cl <sub>6</sub> Li <sub>2</sub>
Cl2	6h	mm2	0.2185	0.437	1/4		trigonal prism Li <sub>4</sub> U <sub>2</sub>
Cl3	6h	mm2	0.5545	0.109	1/4		trigonal prism Li <sub>4</sub> U <sub>2</sub>
Cl4	6h	mm2	0.8924	0.7848	1/4		trigonal prism U <sub>2</sub> Li <sub>4</sub>
U5	4f	3m.	1/3	2/3	0.004	0.5	8-vertex polyhedron Cl <sub>6</sub> U <sub>2</sub>



U6      2a   -3m.      0      0      0      0.5      8-vertex polyhedron Cl<sub>6</sub>U<sub>2</sub>

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

Experimental: powder, diffractometer, neutrons,  $R_B = 0.077$

Remarks: Space groups (176)  $P6_3/m$  and (163)  $P-31c$  were tested and rejected ( $wR_p = 0.101$  for both). In table 3 of [1] the Wyckoff position of former U(2) is misprinted as 5f instead of 4f.

References: [1] Bendall P.J., Fitch A.N., Fender B.E.F. (1983), J. Appl. Crystallogr. 16, 164-170.

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hP36

ThTi <sub>2</sub> H <sub>6</sub>	hP36	(194) $P6_3/mmc - k^2hfa$
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### ThTi<sub>2</sub>H<sub>6</sub> [1]

Structural features: Filled-up derivative of MgZn<sub>2</sub> with H in tetrahedral (Th<sub>2</sub>Ti<sub>2</sub>) and trigonal (ThTi<sub>2</sub>) voids.

Van Houten R., Bartram S. (1971) [1]

H<sub>6</sub>ThTi<sub>2</sub>

$a = 0.6176$ ,  $c = 1.0085$  nm,  $c/a = 1.633$ ,  $V = 0.3331$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
H1	12k	.m.	0.17	0.34	0.06		non-colinear H <sub>2</sub>
H2	12k	.m.	0.55	0.1	0.65		non-colinear H <sub>2</sub>
Ti3	6h	mm2	0.16667	0.33333	$\frac{1}{4}$		6-vertex polyhedron H <sub>6</sub>
Th4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5625		non-coplanar triangle H <sub>3</sub>
Ti5	2a	-3m.	0	0	0		octahedron H <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays

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

References: [1] Van Houten R., Bartram S. (1971), Metall. Trans. 2, 527-530.

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hP36

Cs <sub>2</sub> NaAu <sub>3</sub> [CN] <sub>6</sub>	hP36	(194) $P6_3/mmc - k^2hfa$
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### Cs<sub>2</sub>Na[Au(CN)<sub>2</sub>]<sub>3</sub> [1]

Structural features: NC-Au-CN linear units parallel to [001]; the centering Au atoms form a Kagomé mesh.

Blom N. et al. (1984) [1]

Au<sub>3</sub>C<sub>6</sub>Cs<sub>2</sub>N<sub>6</sub>Na

$a = 0.70679$ ,  $c = 1.82566$  nm,  $c/a = 2.583$ ,  $V = 0.7898$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12k	.m.	0.1646	0.3292	0.0811		single atom C
C2	12k	.m.	0.1683	0.3366	0.1436		single atom N
Au3	6h	mm2	0.1707	0.3414	$\frac{1}{4}$		non-colinear C <sub>2</sub>
Cs4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5604		9-vertex polyhedron N <sub>9</sub>
Na5	2a	-3m.	0	0	0		octahedron N <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.032$ ,  $T = 298$  K

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

References: [1] Blom N., Ludi A., Burgi H.B. (1984), Acta Crystallogr. C 40, 1770-1772.

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hP36

$\text{Ba}_2\text{InAlO}_5$	<i>hP36</i>	(194) $P6_3/mmc - \text{kgf}^2\text{ecba}$
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### $\text{Ba}_2\text{InAlO}_5$ [1]

Structural features: Double layers of vertex-linked  $\text{InO}_6$  octahedra are interconnected via common vertices with units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Müller Buschbaum H., Abed M. (1990) [1]

$\text{AlBa}_2\text{InO}_5$

$a = 0.57809$ ,  $c = 1.96248$  nm,  $c/a = 3.395$ ,  $V = 0.5680$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.166	0.332	0.133		non-colinear AlIn
O2	6g	.2/m.	$\frac{1}{2}$	0	0		colinear $\text{In}_2$
In3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0672		octahedron $\text{O}_6$
Ba4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6096		9-vertex polyhedron $\text{O}_9$
Al5	4e	3m.	0	0	0.1597		tetrahedron $\text{O}_4$
Ba6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $\text{O}_6$
O7	2b	-6m2	0	0	$\frac{1}{4}$		colinear $\text{Al}_2$
Ba8	2a	-3m.	0	0	0		14-vertex polyhedron $\text{O}_{12}\text{Al}_2$

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.076$

Remarks: In table 1 of [1] the Wyckoff position of former Al is misprinted as 4c instead of 4e.

References: [1] Müller Buschbaum H., Abed M. (1990), Z. Anorg. Allg. Chem. 591, 174-180.

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hP36

$\text{Zn}_5\text{Er}$	<i>hP36</i>	(194) $P6_3/mmc - \text{kh}^2\text{gfa}$
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### $\text{ErZn}_5$ [1]; "EuMg<sub>5</sub>" [2]

Structural features: Puckered triangle-mesh  $\text{Zn}_{12}$  layers and  $\text{Er}_3\text{Zn}_3$  layers ( $\text{Er}_3$  trigonal clusters and smaller  $\text{Zn}_3$  triangles) alternate along [001].

Fornasini M.L. (1971) [1]

$\text{ErZn}_5$

$a = 0.8848$ ,  $c = 0.9164$  nm,  $c/a = 1.036$ ,  $V = 0.6213$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Zn1	12k	.m.	0.1605	0.3210	0.5904		icosahedron $\text{Zn}_9\text{Er}_3$
Er2	6h	mm2	0.1951	0.3902	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Zn}_{16}\text{Er}_2$
Zn3	6h	mm2	0.5682	0.1364	$\frac{1}{4}$		icosahedron $\text{Zn}_{10}\text{Er}_2$
Zn4	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron $\text{Zn}_8\text{Er}_4$
Zn5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0054		icosahedron $\text{Zn}_9\text{Er}_3$
Zn6	2a	-3m.	0	0	0		octahedron $\text{Zn}_6$

Experimental: single crystal, precession photographs, X-rays,  $R = 0.116$

Remarks: The author states that the Er/Zn ratio probably deviates from 1:5. Additional reflections could be indexed with an 18-fold supercell (new axes  $2a+b$ ,  $-a+b$ ,  $6c$ ); additional reflections from other crystals could be indexed with a rhombohedral supercell. A similar structure proposal for  $\text{EuMg}_5$  in [2] is superseded (see [3], where the composition was corrected to  $\text{EuMg}_{5.2}$ ).

References: [1] Fornasini M.L. (1971), J. Less-Common Met. 25, 329-332. [2] Mühlpfordt W. (1970), Z. Anorg. Allg. Chem. 374, 174-185. [3] Erassme J., Lueken H. (1987), Acta Crystallogr. B 43, 244-250.

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*hP36*

$\text{Na}_2\text{ZrSi}_3\text{O}_9[\text{H}_2\text{O}]_2$	<i>hP36</i>	(194) $P6_3/mmc - kh^2gfa$
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**$\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$**  [1], catapleiite high, Strukturbericht notation  $S3_4$

Structural features:  $\text{ZrO}_6$  octahedra and rings of three vertex-linked  $\text{SiO}_4$  tetrahedra share vertices to form a 3D-framework (additional O coordinated only to Na).

Brunowsky B. (1936) [1]

$\text{H}_4\text{Na}_2\text{O}_{11}\text{Si}_3\text{Zr}$

$a = 0.739$ ,  $c = 1.006$  nm,  $c/a = 1.361$ ,  $V = 0.4758$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.135	0.27	0.125		single atom Si
Si2	6 <i>h</i>	<i>mm</i> 2	0.2	0.4	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O3	6 <i>h</i>	<i>mm</i> 2	0.47	0.94	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )4	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0	0.667	colinear Na <sub>2</sub>
Na5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.08		12-vertex polyhedron (OH <sub>2</sub> ) <sub>3</sub> Si <sub>3</sub> O <sub>6</sub>
Zr6	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, Laue photographs, X-rays

Remarks: Natural specimen from Khibiny tundra, Kola Peninsula. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Brunowsky B. (1936), Acta Physicochim. URSS 5, 863-892.

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*hP36*

$\text{Sc}_3\text{Ni}_{11}\text{Si}_4$	<i>hP36</i>	(194) $P6_3/mmc - kh^2gfb$
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**$\text{Sc}_3\text{Ni}_{11}\text{Si}_4$**  [1];  $\text{MgYZn}_3$  [2]

Structural features: Puckered triangle-mesh  $\text{Ni}_8\text{Si}_3$  layers and  $\text{Sc}_3\text{Ni}_3\text{Si}$  layers ( $\text{Sc}_3$  trigonal clusters and smaller  $\text{Ni}_3$  triangles) alternate along [001].

Kotur B.Y. et al. (1983) [1]

$\text{Ni}_{11}\text{Sc}_3\text{Si}_4$

$a = 0.8024$ ,  $c = 0.8429$  nm,  $c/a = 1.050$ ,  $V = 0.4700$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Ni1	12 <i>k</i>	. <i>m</i> .	0.1614	0.3228	0.5857		icosahedron Si <sub>3</sub> Ni <sub>6</sub> Sc <sub>3</sub>
Sc2	6 <i>h</i>	<i>mm</i> 2	0.192	0.384	$\frac{1}{4}$		7-capped pentagonal prism Si <sub>5</sub> Ni <sub>10</sub> Sc <sub>2</sub>
Ni3	6 <i>h</i>	<i>mm</i> 2	0.5618	0.1236	$\frac{1}{4}$		icosahedron Si <sub>2</sub> Ni <sub>8</sub> Sc <sub>2</sub>
Si4	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		icosahedron Ni <sub>8</sub> Sc <sub>4</sub>
Ni5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0086		icosahedron Si <sub>3</sub> Ni <sub>6</sub> Sc <sub>3</sub>

Si6      2b   -6m2      0      0       $\frac{1}{4}$       tricapped trigonal prism Ni<sub>6</sub>Sc<sub>3</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.079

Remarks: Different atom distribution is reported for MgYZn<sub>3</sub>, Y<sub>3</sub>[(Mg,Zn)<sub>6</sub>Zn<sub>5</sub>][Zn<sub>3</sub>(Y,Mg)].

References: [1] Kotur B.Y., Sikiritsa M., Bodak O.I., Gladyshevskii E.I. (1983), Sov. Phys. Crystallogr. 28, 387-389 (Kristallografiya 28, 658-661). [2] Deng D.W., Kuo K.H., Luo Z.P., Miller D.J., Kramer M.J., Dennis K.W. (2004), J. Alloys Compd. 373, 156-160.

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hP36

Na<sub>0.8</sub>(Na<sub>0.9</sub>La<sub>0.05</sub>Yb<sub>0.05</sub>)[SO<sub>4</sub>]      hP36      (194) *P*6<sub>3</sub>/*mmc* – khf<sup>3</sup>dca

### Na<sub>2</sub>SO<sub>4</sub> form I:La,Yb [1]

Structural features: (Na,La,Yb) and Na atoms and SO<sub>4</sub> tetrahedra (rotational disorder) in a ZrBeSi-type arrangement (Na in part displaced from the prism centers).

Armbruster T. et al. (1999) [1]

La<sub>0.05</sub>Na<sub>1.75</sub>O<sub>4.04</sub>SYb<sub>0.05</sub>

$a = 0.5331$ ,  $c = 0.7188$  nm,  $c/a = 1.348$ ,  $V = 0.1769$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.235	0.47	0.093	0.18	
O2	6 <i>h</i>	<i>mm</i> 2	0.1831	0.3662	$\frac{1}{4}$	0.8	
O3	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.014	0.28	
S4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.201	0.28	
Na5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.677	0.19	
Na6	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.47	
S7	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.44	
M8	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M8 = 0.898Na + 0.051La + 0.051Yb

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

Remarks: Phase stable at high temperature. We assigned an approximate value to the La/Yb ratio of site M8. Short interatomic distances for partly occupied site(s).

References: [1] Armbruster T., Basler R., Mikhail P., Hulliger J. (1999), J. Solid State Chem. 145, 309-316.

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hP36

Mg(Cu<sub>0.55</sub>Ni<sub>0.45</sub>)<sub>2</sub>      hP36      (194) *P*6<sub>3</sub>/*mmc* – khf<sup>3</sup>ea

### Mg(Ni<sub>0.45</sub>Cu<sub>0.55</sub>)<sub>2</sub> 6H [1], Laves phase 6H

Structural features: Mg[Mg<sub>4</sub>(Cu,Ni)<sub>12</sub>] Friauf polyhedra share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. (Cu,Ni)<sub>4</sub> tetrahedra share faces and vertices to form a 3D-framework. Kagomé-mesh (Cu,Ni)<sub>3</sub> layers and puckered triangle-mesh Mg<sub>2</sub>(Cu,Ni) layers alternate along [001]. Laves-type slabs in hc<sub>2</sub> stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Komura Y. et al. (1972) [1]

Cu<sub>1.10</sub>MgNi<sub>0.90</sub>

$a = 0.4917$ ,  $c = 2.4040$  nm,  $c/a = 4.889$ ,  $V = 0.5033$  nm<sup>3</sup>,  $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1670	0.3341	0.0835		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M2	6h	mm2	0.5022	0.0044	<sup>1</sup> / <sub>4</sub>		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M3	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1672		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
Mg4	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5233		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6448		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg6	4e	3m.	0	0	0.1906		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
M7	2a	-3m.	0	0	0		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>

M1 = 0.55Cu + 0.45Ni; M2 = 0.55Cu + 0.45Ni; M3 = 0.55Cu + 0.45Ni; M7 = 0.55Cu + 0.45Ni

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.114

Remarks: We assigned an approximate value to the Cu/Ni ratio of sites M based on the nominal composition.

References: [1] Komura Y., Nakaue A., Mitarai M. (1972), Acta Crystallogr. B 28, 727-732.

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hP36

Ce <sub>2</sub> Ni <sub>7</sub>	hP36	(194) P6 <sub>3</sub> /mmc – khf <sup>3</sup> ea
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### Ce<sub>2</sub>Ni<sub>7</sub> [1]

Structural features: Intergrowth of Laves- and CaCu<sub>5</sub>-type slabs (common Kagomé-mesh layers) in the ratio 1:2, consecutive Laves-type slabs in h stacking. See Fig. III.38.

Cromer D.T., Larson A.C. (1959) [1]

Ce<sub>2</sub>Ni<sub>7</sub>

a = 0.498, c = 2.452 nm, c/a = 4.924, V = 0.5266 nm<sup>3</sup>, Z = 4

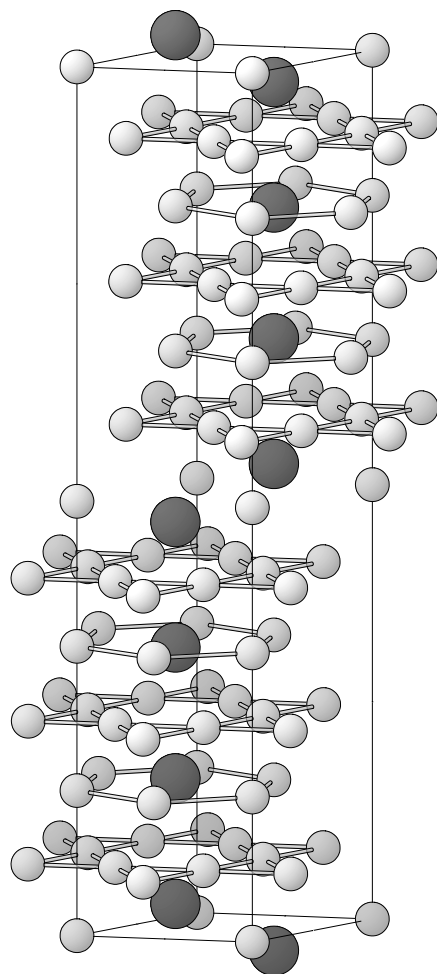
site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12k	.m.	0.1662	0.3324	0.0854		icosahedron Ni <sub>7</sub> Ce <sub>5</sub>
Ni2	6h	mm2	0.1649	0.3298	<sup>1</sup> / <sub>4</sub>		icosahedron Ni <sub>8</sub> Ce <sub>4</sub>
Ni3	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1666		anticuboctahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ce4	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5302		16-vertex Frank-Kasper Ni <sub>12</sub> Ce <sub>4</sub>
Ce5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6747		pseudo Frank-Kasper Ni <sub>18</sub> Ce <sub>2</sub>
Ni6	4e	3m.	0	0	0.1670		anticuboctahedron Ni <sub>9</sub> Ce <sub>3</sub>
Ni7	2a	-3m.	0	0	0		icosahedron Ni <sub>6</sub> Ce <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.099

Remarks: Identical to the unknown phase reported in [2] and probably also to so-called CeNi<sub>4</sub> in [3].

References: [1] Cromer D.T., Larson A.C. (1959), Acta Crystallogr. 12, 855-859. [2] Cromer D.T., Olsen C.E. (1959), Acta Crystallogr. 12, 689-694. [3] Vogel R., Fülling W. (1947), Z. Metallkd. 38, 97-103.

Fig. III.38.  $\text{Ce}_2\text{Ni}_7$ 

Arrangement of Ce (dark) and Ni (light) atoms.

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$\text{Ce}_2\text{Co}_5\text{B}_2$

hP36

(194)  $P6_3/mmc - khf^3ea$

### $\text{Ce}_2\text{Co}_5\text{B}_2$ [1]

Structural features:  $\text{BCo}_6$  trigonal prisms share triangular faces and edges to form infinite double slabs; no B-B contact. Intergrowth of Laves- and ternary  $\text{CaCu}_5$ -type ( $\text{CeCo}_3\text{B}_2$ ) slabs (common Kagomé-mesh layers) in the ratio 1:2, consecutive Laves-type slabs in h stacking.

Kuz'ma Y.B. (1979) [1]

$\text{B}_2\text{Ce}_2\text{Co}_5$

$a = 0.506$ ,  $c = 2.043$  nm,  $c/a = 4.038$ ,  $V = 0.4530$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Co1	12k	.m.	0.176	0.352	0.103		pseudo Frank-Kasper $\text{B}_2\text{Co}_6\text{Ce}_5$
Co2	6h	mm2	0.189	0.378	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{B}_4\text{Co}_6\text{Ce}_4$
B3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.177		trigonal prism $\text{Co}_6$
Ce4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.522		16-vertex Frank-Kasper $\text{Co}_{12}\text{Ce}_4$
Ce5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67		pseudo Frank-Kasper $\text{Co}_{12}\text{B}_6\text{Ce}_2$
B6	4e	3m.	0	0	0.177		trigonal prism $\text{Co}_6$

Co7      2a   -3m.      0      0      0      icosahedron Co<sub>6</sub>Ce<sub>6</sub>

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

Experimental: powder, film, X-rays

References: [1] Kuz'ma Y.B. (1979), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1979, 146-151.

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Y <sub>4</sub> Ir <sub>9</sub> Si <sub>5</sub>	hP36	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khf <sup>3</sup> ea
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### Y<sub>4</sub>Ir<sub>9</sub>Si<sub>5</sub> [1]

Structural features: Intergrowth of ternary Laves- and CaCu<sub>5</sub>-type (CeCo<sub>3</sub>B<sub>2</sub>) slabs (common Kagomé-mesh layers) in the ratio 1:2, consecutive Laves-type slabs in h stacking.

Cenzual K. et al. (1988) [1]

Ir<sub>9.12</sub>Si<sub>4.88</sub>Y<sub>4</sub>

$a = 0.54894$  nm,  $c/a = 4.118$ ,  $V = 0.5899$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ir1	12 <i>k</i>	. <i>m</i> .	0.1674	0.3348	0.088		pseudo Frank-Kasper Si <sub>3</sub> Ir <sub>5</sub> Y <sub>5</sub>
Ir2	6 <i>h</i>	<i>mm</i> 2	0.1663	0.3326	$\frac{1}{4}$		14-vertex Frank-Kasper Si <sub>4</sub> Ir <sub>6</sub> Y <sub>4</sub>
Si3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1681		trigonal prism Ir <sub>6</sub>
Y4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5277		16-vertex Frank-Kasper Ir <sub>9</sub> Si <sub>3</sub> Y <sub>4</sub>
Y5	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6737		pseudo Frank-Kasper Si <sub>6</sub> Ir <sub>12</sub> Y <sub>2</sub>
Si6	4 <i>e</i>	3. <i>m</i> .	0	0	0.167		trigonal prism Ir <sub>6</sub>
M7	2 <i>a</i>	-3. <i>m</i> .	0	0	0		octahedron Ir <sub>6</sub>

M7 = 0.88Si + 0.12Ir

Experimental: single crystal, diffractometer, X-rays, wR = 0.061, T = 293 K

References: [1] Cenzual K., Chabot B., Parthé E. (1988), Acta Crystallogr. C 44, 400-405.

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Ba <sub>5</sub> (W <sub>0.2</sub> Ru <sub>0.8</sub> ) <sub>2</sub> Cl <sub>2</sub> O <sub>9</sub>	hP36	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khf <sup>3</sup> ed
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### Ba<sub>5</sub>Ru<sub>1.6</sub>W<sub>0.4</sub>O<sub>9</sub>Cl<sub>2</sub> [1]

Structural features: Double perovskite-type slabs (three close-packed BaO<sub>3</sub> layers, (Ru,W) in octahedral voids) alternate with two hexagon-mesh BaCl layers along [001]. Units of two face-linked (Ru,W)O<sub>6</sub> octahedra ((Ru,W)<sub>2</sub> dumbbells).

Hong S.T., Sleight A.W. (1997) [1]

Ba<sub>5</sub>Cl<sub>2</sub>O<sub>9</sub>Ru<sub>1.60</sub>W<sub>0.40</sub>

$a = 0.5817$  nm,  $c/a = 4.270$ ,  $V = 0.7279$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.16	0.32	0.6563		single atom Ru
O2	6 <i>h</i>	<i>mm</i> 2	0.151	0.302	$\frac{1}{4}$		non-colinear Ru <sub>2</sub>
Cl3	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0497		colinear Ba <sub>2</sub>
Ba4	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.16964		10-vertex polyhedron O <sub>9</sub> Cl
Ba5	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.57456		monocapped trigonal prism O <sub>3</sub> Cl <sub>4</sub>
M6	4 <i>e</i>	3. <i>m</i> .	0	0	0.19219		octahedron O <sub>6</sub>

Ba7      2d   -6m2       $\frac{1}{3}$        $\frac{2}{3}$        $\frac{3}{4}$       anticuboctahedron O<sub>12</sub>

M6 = 0.80Ru + 0.20W

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

Experimental: single crystal, diffractometer, X-rays, R = 0.038, T = 296 K

References: [1] Hong S.T., Sleight A.W. (1997), J. Solid State Chem. 132, 407-410.

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hP36

Cs<sub>3</sub>V<sub>2</sub>(O<sub>0.44</sub>F<sub>0.56</sub>)<sub>9</sub>

hP36

(194) P6<sub>3</sub>/mmc – khfe<sup>3</sup>d

**Cs<sub>3</sub>V<sub>2</sub>O<sub>4</sub>F<sub>5</sub>** [1]

Structural features: Close-packed Cs(F,O)<sub>3</sub> layers in h stacking; V in octahedral voids (disorder, displaced from the octahedron centers). Variant of Ba<sub>3</sub>Te<sub>2</sub>O<sub>9</sub> with the V sites split along [001].

Mattes R., Förster H. (1982) [1]

Cs<sub>3</sub>F<sub>5</sub>O<sub>4</sub>V<sub>2.06</sub>

a = 0.6319, c = 1.485 nm, c/a = 2.35, V = 0.5135 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1475	0.295	0.5648		single atom V
M2	6h	mm2	0.137	0.274	$\frac{1}{4}$		non-colinear V <sub>2</sub>
Cs3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0865		anticuboctahedron F <sub>12</sub>
V4	4e	3m.	0	0	0.0163	0.28	
V5	4e	3m.	0	0	0.1468	0.4	
V6	4e	3m.	0	0	0.1894	0.35	
Cs7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron F <sub>12</sub>

M1 = 0.556F + 0.444O; M2 = 0.556F + 0.444O

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

Remarks: We assigned an approximate value to the F/O ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 2 of [1] the z-coordinate of former V(1) is misprinted as 0.0894 instead of 0.1894 (checked on interatomic distances).

References: [1] Mattes R., Förster H. (1982), J. Less-Common Met. 87, 237-247.

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Ba(Ti<sub>0.33</sub>Fe<sub>0.67</sub>)<sub>6</sub>O<sub>11</sub>

hP36

(194) P6<sub>3</sub>/mmc – khgfedc

**BaFe<sub>4</sub>Ti<sub>2</sub>O<sub>11</sub>** [2], ferrite R-type

Structural features: Close-packed BaO<sub>3</sub> and O<sub>4</sub> layers in h stacking; (Fe,Ti) in octahedral and trigonal bipyramidal voids. Infinite layers of edge-linked (Fe,Ti)O<sub>6</sub> octahedra share vertices with slabs where units of two face-linked (Fe,Ti)O<sub>6</sub> octahedra share vertices with (Fe,Ti)O<sub>5</sub> trigonal bipyramids to form a 3D-framework. See Fig. III.39.

Sosnowska I. et al. (1996) [1]

BaFe<sub>4</sub>O<sub>11</sub>Ti<sub>2</sub>

a = 0.58213, c = 1.357 nm, c/a = 2.331, V = 0.3982 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.171	0.342	0.5809		non-coplanar triangle Fe <sub>3</sub>
O2	6h	mm2	0.1496	0.2992	$\frac{1}{4}$		coplanar triangle Fe <sub>3</sub>



M3	6g	.2/m.	$\frac{1}{2}$	0	0	octahedron O <sub>6</sub>
O4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.08	tetrahedron Fe <sub>4</sub>
M5	4e	3m.	0	0	0.142	octahedron O <sub>6</sub>
Ba6	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	anticuboctahedron O <sub>12</sub>
M7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	trigonal bipyramid O <sub>5</sub>

M3 = 0.667Fe + 0.333Ti; M5 = 0.667Fe + 0.333Ti; M7 = 0.667Fe + 0.333Ti

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

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.039, T = 240 K

Remarks: We assigned an approximate value to the Ti/Fe ratio of sites M based on the nominal composition.

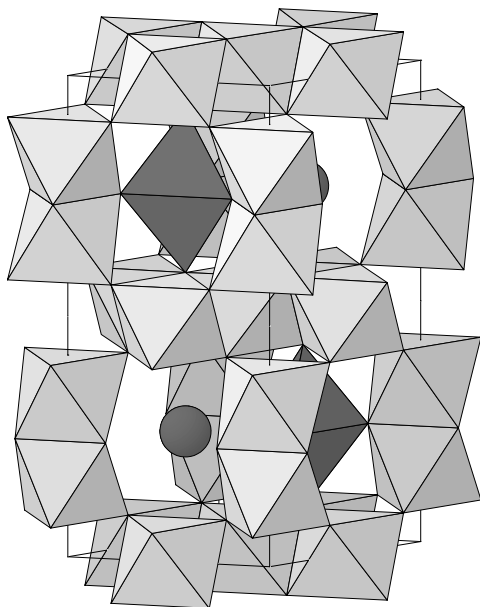


Fig. III.39. **BaFe<sub>4</sub>Ti<sub>2</sub>O<sub>11</sub>**

Arrangement of (Fe,Ti)O<sub>5</sub> trigonal bipyramids (dark), (Fe,Ti)O<sub>6</sub> octahedra (light) and Ba atoms.

References: [1] Sosnowska I., Przenioslo R., Shiojiri M., Fischer P. (1996), J. Magn. Magn. Mater. 160, 382-383. [2] Haberey F., Velicescu M. (1974), Acta Crystallogr. B 30, 1507-1510.

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Na <sub>0.31</sub> CoO <sub>2</sub> [H <sub>2</sub> O] <sub>1.25</sub>	hP36	(194) P6 <sub>3</sub> /mmc – lhfa
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#### Na<sub>0.31</sub>CoO<sub>2</sub>·1.25H<sub>2</sub>O [1]

Structural features: Infinite layers of edge-linked CoO<sub>6</sub> octahedra (h stacking) and double H<sub>2</sub>O layers (partial disorder) alternate along [001]; Na between the H<sub>2</sub>O layers (partial disorder).

Jorgensen J.D. et al. (2003) [1]

CoD<sub>2.86</sub>Na<sub>0.36</sub>O<sub>3.43</sub>

*a* = 0.28217, *c* = 1.97681 nm, *c/a* = 7.006, *V* = 0.1363 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24l	1	0.263	0.073	0.1706	0.119	
Na2	6h	mm2	0.2625	0.525	$\frac{1}{4}$	0.12	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5469		non-coplanar triangle Co <sub>3</sub>
Co4	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

D5	24/	1	0.112	0.437	0.1801	0.119
D6	24/	1	0.421	0.159	0.124	0.119

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

Experimental: powder, diffractometer, neutrons, time-of-flight, T = 295 K

Remarks: Referred to as BLH (bilayer hydrate). A model for short-range order with an orthorhombic supercell (new axes 3a,a+2b,3c) is proposed. 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] Jorgensen J.D., Avdeev M., Hinks D.G., Burley J.C., Short S. (2003), Phys. Rev. B: Condens. Matter 68, 214517: 1-10.

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hP38

$\text{Pd}_7\text{Sn}_2\text{Se}_{9.85}$	<i>hP38</i>	(194) $P6_3/mmc - k^2hfca$
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### **$\text{Pd}_7\text{Sn}_2\text{Se}_{9.85}$ [1]**

Structural features:  $\text{PdSe}_6$  octahedra and  $\text{SnSe}_3$   $\psi$ -tetrahedra share vertices to form infinite slabs, which are interconnected via edge- and vertex-linked  $\text{PdSe}_4$  squares to form a 3D-framework; additional Se in anticuboctahedral ( $\text{Se}_{12}$ ) voids.

Pocha R., Johrendt D. (2004) [1]

$\text{Pd}_7\text{Se}_{9.85}\text{Sn}_2$

$a = 0.7297$ ,  $c = 1.6314$  nm,  $c/a = 2.236$ ,  $V = 0.7523$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	12k	.m.	0.1711	0.3422	0.0829		tetrahedron $\text{Pd}_3\text{Sn}$
Pd2	12k	.m.	0.5205	0.041	0.1572		non-coplanar square $\text{Se}_4$
Se3	6h	$mm2$	0.835	0.67	$\frac{1}{4}$		non-coplanar square $\text{Pd}_4$
Sn4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5275		octahedron $\text{Se}_3\text{Pd}_3$
Se5	2c	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.851	trigonal prism $\text{Pd}_6$
Pd6	2a	$-3m.$	0	0	0		octahedron $\text{Se}_6$

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

Remarks: Homogeneity range  $\text{Pd}_8\text{Sn}_2\text{Se}_{9+x}$ ,  $0.5 < x < 0.85$ . Refinement of the site occupancies showed no significant deviation from unity, except for site Se5.

References: [1] Pocha R., Johrendt D. (2004), Z. Anorg. Allg. Chem. 630, 2468-2472.

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hP38

$\text{LaFe}[\text{CN}]_6[\text{H}_2\text{O}]_4$	<i>hP38</i>	(194) $P6_3/mmc - k^2hfca$
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### **$\text{La}[\text{Fe}(\text{CN})_6] \cdot 4\text{H}_2\text{O}$ [1]**

Structural features:  $\text{Fe}(\text{CN})_6$  octahedral units (approximately linear Fe-C-N segments) and La atoms in a NiAs-type arrangement;  $\text{H}_2\text{O}$  in voids (partial disorder).

Herbstein F.H., Marsh R.E. (1982) [1]

$\text{C}_6\text{FeH}_8\text{LaN}_6\text{O}_4$

$a = 0.7541$ ,  $c = 1.3955$  nm,  $c/a = 1.851$ ,  $V = 0.6873$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	12k	.m.	0.12	0.24	0.079		single atom N

N2	12k	.m.	0.196	0.392	0.119	single atom C
(OH <sub>2</sub> ) <sub>3</sub>	6h	mm2	0.525	0.05	<sup>1</sup> / <sub>4</sub>	0.667 single atom La
(OH <sub>2</sub> ) <sub>4</sub>	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.596	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
La5	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	tricapped trigonal prism (OH <sub>2</sub> ) <sub>3</sub> N <sub>6</sub>
Fe6	2a	-3m.	0	0	0	octahedron C <sub>6</sub>

Remarks: The authors state that the description in space group (176)  $P6_3/m$  in [2] (refinement on single crystal, diffractometer, X-rays) does not take into consideration all symmetry elements of the proposed structure. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Herbstein F.H., Marsh R.E. (1982), Acta Crystallogr. B 38, 1051-1055. [2] Mullica D.F., Milligan W.O., Garner R.L. (1980), Acta Crystallogr. B 36, 2561-2564.

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hP38

Sc <sub>3</sub> Ni <sub>11</sub> Ge <sub>4</sub>	hP38	(194) $P6_3/mmc - kh^2gfb$
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### Sc<sub>3</sub>Ni<sub>11</sub>Ge<sub>4</sub> [1]

Structural features: Puckered triangle-mesh Ni<sub>8</sub>Ge<sub>3</sub>(Ge,□) layers and Sc<sub>3</sub>Ni<sub>3</sub>(Ge,□) layers (Sc<sub>3</sub> trigonal clusters and smaller Ni<sub>3</sub> triangles) alternate along [001]. Variant of Sc<sub>3</sub>Ni<sub>11</sub>Si<sub>4</sub> with a partly disordered atom arrangement along 0 0 z.

Andrusyak R.I. (1988) [1]

Ge<sub>4</sub>Ni<sub>11</sub>Sc<sub>3</sub>

$a = 0.813$ ,  $c = 0.8505$  nm,  $c/a = 1.046$ ,  $V = 0.4868$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12k	.m.	0.162	0.324	0.581		pseudo Frank-Kasper Ge <sub>4</sub> Ni <sub>6</sub> Sc <sub>3</sub>
Sc2	6h	mm2	0.19	0.38	<sup>1</sup> / <sub>4</sub>		15-vertex polyhedron Ge <sub>5</sub> Ni <sub>10</sub>
Ni3	6h	mm2	0.555	0.11	<sup>1</sup> / <sub>4</sub>		icosahedron Ge <sub>2</sub> Ni <sub>8</sub> Sc <sub>2</sub>
Ge4	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		icosahedron Ni <sub>8</sub> Sc <sub>4</sub>
Ni5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.008		icosahedron Ge <sub>3</sub> Ni <sub>6</sub> Sc <sub>3</sub>
Ge6	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>	0.72	pentacapped trigonal prism Ge <sub>2</sub> Sc <sub>3</sub> Ni <sub>6</sub>
Ge7	2a	-3m.	0	0	0	0.28	square prism (cube) Ge <sub>2</sub> Ni <sub>6</sub>

Experimental: powder, diffractometer, X-rays,  $R_B = 0.126$

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

References: [1] Andrusyak R.I. (1988), Sov. Phys. Crystallogr. 33, 599-600 (Kristallografiya 33, 1012-1014).

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hP38

Gd <sub>3</sub> Ru <sub>4</sub> Al <sub>12</sub>	hP38	(194) $P6_3/mmc - kh^2gfb$
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### Gd<sub>3</sub>Ru<sub>4</sub>Al<sub>12</sub> [1]

Structural features: Puckered triangle-mesh Ru<sub>4</sub>Al<sub>8</sub> layers and Gd<sub>3</sub>Al<sub>4</sub> layers (Gd<sub>3</sub> trigonal clusters) alternate along [001]. Ordering variant of Sc<sub>3</sub>Ni<sub>11</sub>Ge<sub>4</sub> (Sc<sub>3</sub>Ni<sub>11</sub>Ge<sub>5-x</sub>), Gd<sub>3</sub>Al<sub>11</sub>[AlRu<sub>4</sub>].

Gladyshevskii R.E. et al. (1993) [1]

Al<sub>11.87</sub>Gd<sub>3</sub>Ru<sub>4.13</sub>

$a = 0.88142$ ,  $c = 0.95692$  nm,  $c/a = 1.086$ ,  $V = 0.6438$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.1622	0.3244	0.5762		pseudo Frank-Kasper Ru <sub>3</sub> Al <sub>7</sub> Gd <sub>3</sub>
Gd2	6h	mm2	0.19285	0.3857	<sup>1</sup> / <sub>4</sub>		7-capped pentagonal prism Al <sub>11</sub> Ru <sub>4</sub> Gd <sub>2</sub>
M3	6h	mm2	0.5637	0.1274	<sup>1</sup> / <sub>4</sub>		icosahedron Ru <sub>2</sub> Al <sub>8</sub> Gd <sub>2</sub>
Ru4	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		icosahedron Al <sub>8</sub> Gd <sub>4</sub>
Al5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0116		icosahedron Ru <sub>3</sub> Al <sub>6</sub> Gd <sub>3</sub>
Al6	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Ru <sub>2</sub> Gd <sub>3</sub> Al <sub>6</sub>
Ru7	2a	-3m.	0	0	0		square prism (cube) Al <sub>8</sub>

M3 = 0.956Al + 0.044Ru

Experimental: single crystal, diffractometer, X-rays, wR = 0.023, T = 293 K

References: [1] Gladyshevskii R.E., Strusievicz O.R., Cenxual K., Parthé E. (1993), Acta Crystallogr. B 49, 474-478.

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hP38

H <sub>3</sub> K <sub>6</sub> BiCl <sub>8</sub> F <sub>4</sub>	hP38	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kh <sup>2</sup> gfda
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### **K<sub>6</sub>H<sub>3</sub>BiCl<sub>8</sub>F<sub>4</sub> rt [1]**

Structural features: BiCl<sub>6</sub> octahedra and planar F(HF)<sub>3</sub> trigonal units (perpendicular to [001]) in a NiAs-type arrangement; additional Cl in K<sub>6</sub> octahedra.

Udovichenko A.A. et al. (1987) [1]

BiCl<sub>8</sub>F<sub>4</sub>H<sub>3</sub>K<sub>6</sub>

*a* = 0.91453, *c* = 1.4466 nm, *c/a* = 1.582, *V* = 1.0478 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12k	.m.	0.1393	0.2786	0.6072		single atom Bi
K2	6h	mm2	0.1791	0.3582	<sup>1</sup> / <sub>4</sub>		square antiprism F <sub>2</sub> Cl <sub>6</sub>
F3	6h	mm2	0.5186	0.0372	<sup>1</sup> / <sub>4</sub>		coplanar triangle FK <sub>2</sub>
K4	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		square prism (cube) Cl <sub>6</sub> F <sub>2</sub>
Cl5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1068		octahedron K <sub>6</sub>
F6	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		coplanar triangle F <sub>3</sub>
Bi7	2a	-3m.	0	0	0		octahedron Cl <sub>6</sub>
H8	6h	mm2	0.573	0.146	<sup>1</sup> / <sub>4</sub>		

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

Remarks: Phase stable at T > 130 K. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space groups (186) *P*6<sub>3</sub>*mc* and (190) *P*-62*c* were tested and rejected (R = 0.030 and 0.032, respectively).

References: [1] Udovichenko A.A., Davidovich R.L., Medkov M.A., Gerr R.G., Struchkov Y.T. (1987), Koord. Khim. 13, 274-278.

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hP38

Ba(Ti <sub>0.4</sub> Fe <sub>0.6</sub> ) <sub>5</sub> FeO <sub>11</sub>	hP38	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgf <sup>2</sup> ed
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### **BaFe<sub>4</sub>Ti<sub>2</sub>O<sub>11</sub> [2], ferrite R-type**

Structural features: Close-packed BaO<sub>3</sub> and O<sub>4</sub> layers in h stacking; (Fe,Ti) in octahedral, Fe in tetrahedral voids. Infinite layers of edge-linked (Fe,Ti)O<sub>6</sub> octahedra share vertices with slabs where units

of two face-linked (Fe,Ti)O<sub>6</sub> octahedra ((Fe,Ti)<sub>2</sub> dumbbells) share vertices with FeO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra).

Cadee M.C., Ijdo D.J.W. (1984) [1]

BaFe<sub>3.99</sub>O<sub>11</sub>Ti<sub>2.01</sub>

$a = 0.5847$ ,  $c = 1.36116$  nm,  $c/a = 2.328$ ,  $V = 0.4030$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1714	0.3428	0.581		non-coplanar triangle Fe <sub>3</sub>
O2	6 <i>h</i>	<i>mm</i> 2	0.1505	0.301	$\frac{1}{4}$		
M3	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		octahedron O <sub>6</sub>
O4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0783		tetrahedron Fe <sub>4</sub>
Fe5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2322	0.5	
M6	4 <i>e</i>	3 <i>m</i> .	0	0	0.1435		octahedron O <sub>6</sub>
Ba7	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>

M3 = 0.65Fe + 0.35Ti; M6 = 0.52Fe + 0.48Ti

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

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.038, T = 300 K

Remarks: Short interatomic distances for partly occupied site(s). In table II of [1] the  $y$ -coordinate of former O(3) is misprinted as 0.4328 instead of 0.3428 (agreement with Wyckoff position 12*k*; checked on interatomic distances) and the Wyckoff position of site Ba as 2*a* instead of 2*c*.

References: [1] Cadee M.C., Ijdo D.J.W. (1984), J. Solid State Chem. 52, 302-312. [2] Obradors X., Collomb A., Pannetier J., Isalgue A., Tejada J., Joubert J.C. (1983), Mater. Res. Bull. 18, 1543-1553.

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hP38

Th <sub>2</sub> Ni <sub>17</sub>	hP38	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kjgfc
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Th<sub>2</sub>Ni<sub>17</sub> [1]; Ce<sub>2</sub>Ni<sub>15</sub>Si<sub>2</sub> [2]

Structural features: Kagomé-mesh Ni<sub>9</sub> layers and Th<sub>2</sub>(Ni<sub>2</sub>)Ni<sub>6</sub> layers (a Ni hexagon mesh, the hexagons of which are centered by a Th atom or a Ni<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks in the ratio 2:1. See Fig. III.40.

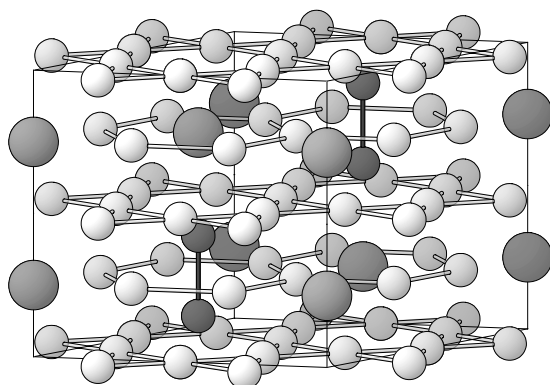


Fig. III.40. Th<sub>2</sub>Ni<sub>17</sub>

Arrangement of Th (large) and Ni (small, Ni<sub>2</sub> dumbbells dark) atoms.

Florio J.V. et al. (1956) [1]

Ni<sub>17</sub>Th<sub>2</sub>

$a = 0.837$ ,  $c = 0.814$  nm,  $c/a = 0.973$ ,  $V = 0.4939$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12k	.m.	0.1667	0.3334	0.0		icosahedron Ni <sub>9</sub> Th <sub>3</sub>
Ni2	12j	m..	0.0	0.3333	1/4		pseudo Frank-Kasper Ni <sub>11</sub> Th <sub>2</sub>
Ni3	6g	.2/m.	1/2	0	0		icosahedron Ni <sub>10</sub> Th <sub>2</sub>
Ni4	4f	3m.	1/3	2/3	0.61		14-vertex Frank-Kasper Ni <sub>13</sub> Th
Th5	2c	-6m2	1/3	2/3	1/4		pseudo Frank-Kasper Ni <sub>20</sub>
Th6	2b	-6m2	0	0	1/4		sixcapped hexagonal prism Ni <sub>18</sub>

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

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

Remarks: Idealized coordinates.

References: [1] Florio J.V., Baenziger N.C., Rundle R.E. (1956), Acta Crystallogr. 9, 367-372. [2] Gladyshevs'kii E.I., Krypyakevych P.I., Bodak O.I. (1967), Visn. L'viv. Derzh. Univ., Ser. Khim. 9, 34-39.

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hP40

LiMg <sub>4</sub> Os <sub>2</sub> H <sub>13</sub>	hP40	(194) $P6_3/mmc - k^2f^2ecb$
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### LiMg<sub>4</sub>Os<sub>2</sub>H<sub>13</sub> [1]

Structural features: Single OsH<sub>6</sub> octahedra arranged in double layers; additional H in linear (Mg<sub>2</sub>) voids.

Huang B. et al. (1996) [1]

D<sub>13</sub>LiMg<sub>4</sub>Os<sub>2</sub>

$a = 0.47214$ ,  $c = 1.84437$  nm,  $c/a = 3.906$ ,  $V = 0.3561$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12k	.m.	0.1637	0.3274	0.0514		single atom Os
D2	12k	.m.	0.5035	0.007	0.6602		single atom Os
Os3	4f	3m.	1/3	2/3	0.1043		octahedron D <sub>6</sub>
Mg4	4f	3m.	1/3	2/3	0.552		cuboctahedron D <sub>12</sub>
Mg5	4e	3m.	0	0	0.1486		10-vertex polyhedron D <sub>10</sub>
Li6	2c	-6m2	1/3	2/3	1/4		trigonal prism D <sub>6</sub>
D7	2b	-6m2	0	0	1/4		colinear Mg <sub>2</sub>

Experimental: powder, diffractometer, neutrons,  $R_p = 0.031$ ,  $T = 295$  K

References: [1] Huang B., Fischer P., Yvon K. (1996), J. Alloys Compd. 245, L24-L27.

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hP40

Ta(Rh <sub>0.33</sub> Pd <sub>0.67</sub> ) <sub>3</sub>	hP40	(194) $P6_3/mmc - k^2hf^2b$
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### TaRhPd<sub>2</sub> γ [1]

Structural features: Close-packed Ta(Pd,Rh)<sub>3</sub> layers (Ta forms a triangle mesh) in h<sub>2</sub>chc stacking.

Giessen B.C., Grant N.J. (1965) [1]

Pd<sub>2.01</sub>Rh<sub>0.99</sub>Ta

$a = 0.5520$ ,  $c = 2.243$  nm,  $c/a = 4.063$ ,  $V = 0.5919$  nm<sup>3</sup>,  $Z = 10$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.16667	0.33333	0.15		cuboctahedron Ta <sub>4</sub> Pd <sub>8</sub>

M2	12 <i>k</i>	. <i>m</i> .	0.16667	0.33333	0.55	anticuboctahedron Pd <sub>8</sub> Ta <sub>4</sub>
M3	6 <i>h</i>	<i>mm</i> 2	0.5	0.0	<sup>1</sup> / <sub>4</sub>	anticuboctahedron Pd <sub>8</sub> Ta <sub>4</sub>
Ta4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.05	anticuboctahedron Pd <sub>12</sub>
Ta5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.65	cuboctahedron Pd <sub>12</sub>
Ta6	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	anticuboctahedron Pd <sub>12</sub>

M1 = 0.67Pd + 0.33Rh; M2 = 0.67Pd + 0.33Rh; M3 = 0.67Pd + 0.33Rh

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates. In [1] the *x*-coordinate of the second mixed site in Wyckoff position 12*k* is misprinted as <sup>1</sup>/<sub>6</sub> instead of -<sup>1</sup>/<sub>6</sub> (from the description of the structure). In [2] the *x*-coordinates of both mixed sites in Wyckoff position 12*k* are misprinted as <sup>1</sup>/<sub>6</sub> instead of -<sup>1</sup>/<sub>6</sub>.

References: [1] Giessen B.C., Grant N.J. (1965), Acta Crystallogr. 18, 1080-1081. [2] (1975), Structure Reports 30A, 64.

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hP40

(Li <sub>0.5</sub> Nb <sub>0.5</sub> )Ba <sub>2</sub> NbO <sub>6</sub>	hP40	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgf <sup>2</sup> eda
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**Ba<sub>4</sub>Nb<sub>3</sub>LiO<sub>12</sub>** [1], perovskite 8H; Ba<sub>4</sub>Ta<sub>3</sub>LiO<sub>12</sub> [2]

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>3</sub> stacking; Nb and (Li,Nb) in octahedral voids. Double layers of vertex-linked NbO<sub>6</sub> octahedra are interconnected via common vertices with units of two face-linked (Li,Nb)O<sub>6</sub> octahedra to form a 3D-framework.

Jendrek E.F. Jr. et al. (1974) [1]

Ba<sub>2</sub>Li<sub>0.50</sub>Nb<sub>1.50</sub>O<sub>6</sub>

*a* = 0.5777, *c* = 1.895 nm, *c/a* = 3.28, *V* = 0.5477 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1716	0.3432	0.6188		non-colinear NbLi
O2	6 <i>h</i>	<i>mm</i> 2	0.1593	0.3187	<sup>1</sup> / <sub>4</sub>		non-colinear Li <sub>2</sub>
O3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		colinear Nb <sub>2</sub>
Ba4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.135		cuboctahedron O <sub>12</sub>
Nb5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5638		octahedron O <sub>6</sub>
M6	4 <i>e</i>	3 <i>m</i> .	0	0	0.1905		7-vertex polyhedron O <sub>6</sub> Li
Ba7	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>
Ba8	2 <i>a</i>	-3 <i>m</i> .	0	0	0		cuboctahedron O <sub>12</sub>

M6 = 0.5Li + 0.5Nb

Experimental: single crystal, diffractometer, X-rays, R = 0.076

Remarks: In table 1 of [1] the Wyckoff position of former Ba(2) is misprinted as 2*b* instead of 2*d*.

References: [1] Jendrek E.F. Jr., Potoff A.D., Katz L. (1974), J. Solid State Chem. 9, 375-379. [2] Collins B.M., Jacobson A.J., Fender B.E.F. (1974), J. Solid State Chem. 10, 29-35.

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hP40

Sr(V <sub>0.83</sub> Fe <sub>0.17</sub> ) <sub>6</sub> O <sub>11</sub>	hP40	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgf <sup>2</sup> edc
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**SrFeV<sub>5</sub>O<sub>11</sub>** [1], ferrite R-type

Structural features: Close-packed SrO<sub>3</sub> and O<sub>4</sub> layers in h stacking; V and (V,Fe) in octahedral, Fe in tetrahedral and additional V in trigonal bipyramidal voids. Infinite layers of edge-linked VO<sub>6</sub> octahedra share vertices with slabs where units of two face-linked (V,Fe)O<sub>6</sub> octahedra share vertices with FeO<sub>4</sub>

tetrahedra and VO<sub>5</sub> trigonal bipyramids (statistical occupation of two face-sharing tetrahedra forming a trigonal bipyramid).

Kanke Y. et al. (1991) [1]

Fe<sub>1.04</sub>O<sub>11</sub>SrV<sub>4.96</sub>

$a = 0.57592$ ,  $c = 1.3217$  nm,  $c/a = 2.295$ ,  $V = 0.3797$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1729	0.3458	0.5841		non-coplanar triangle V <sub>3</sub>
O2	6 <i>h</i>	<i>mm</i> 2	0.1527	0.3054	<sup>1</sup> / <sub>4</sub>		
V3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		octahedron O <sub>6</sub>
O4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0909		
Fe5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2322	0.282	
M6	4 <i>e</i>	3 <i>m</i> .	0	0	0.1399		octahedron O <sub>6</sub>
Sr7	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>
V8	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.436	

M6 = 0.762V + 0.238Fe

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, time-of-flight, R<sub>B</sub> = 0.028

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

References: [1] Kanke Y., Izumi F., Takayama Muromachi E., Kato K., Kamiyama T., Asano H. (1991), J. Solid State Chem. 92, 261-272.

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hP40

BaMnO <sub>3</sub>	hP40	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – khgf <sup>3</sup> ba
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**BaMnO<sub>3</sub> 8H** [2], perovskite 8H

Structural features: Close-packed BaO<sub>3</sub> layers in h<sub>3</sub>c stacking; Mn in octahedral voids. Units of four face-linked MnO<sub>6</sub> octahedra (linear Mn<sub>4</sub> chains) share vertices to form a 3D-framework.

Potoff A.D. et al. (1973) [1]

BaMnO<sub>3</sub>

$a = 0.5667$ ,  $c = 1.8738$  nm,  $c/a = 3.307$ ,  $V = 0.5211$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1874	0.3748	0.6197		non-colinear Mn <sub>2</sub>
O2	6 <i>h</i>	<i>mm</i> 2	0.5202	0.0404	<sup>1</sup> / <sub>4</sub>		non-colinear Mn <sub>2</sub>
O3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		colinear Mn <sub>2</sub>
Ba4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1285		anticuboctahedron O <sub>12</sub>
Mn5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5517		octahedron O <sub>6</sub>
Mn6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6857		octahedron O <sub>6</sub>
Ba7	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>
Ba8	2 <i>a</i>	-3 <i>m</i> .	0	0	0		cuboctahedron O <sub>12</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.079

References: [1] Potoff A.D., Chamberland B.L., Katz L. (1973), J. Solid State Chem. 8, 234-237. [2] Negas T., Roth R.S. (1971), J. Solid State Chem. 3, 323-339.



$(\text{K}_{0.67}\text{Ca}_{0.33})_3[\text{CO}_3]_2$	<i>hP40</i>	(194) <i>P6<sub>3</sub>/mmc</i> – kihfdb
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**K<sub>2</sub>Ca(CO<sub>3</sub>)<sub>2</sub>** [1], fairchildite

Structural features: CO<sub>3</sub> trigonal units in a Mg-type (h.c.p.) arrangement; part of them perpendicular to [001], the others in rotational disorder.

Pertlik F. (1981) [1]

C<sub>2</sub>CaK<sub>2</sub>O<sub>6</sub>

$a = 0.5294$ ,  $c = 1.3355$  nm,  $c/a = 2.523$ ,  $V = 0.3241$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.0865	0.173	0.5776	0.33	single atom C
O2	12 <i>i</i>	.2.	0.238	0	0	0.17	
O3	6 <i>h</i>	<i>mm</i> 2	0.52649	0.05297	<sup>1</sup> / <sub>4</sub>		
M4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0996		coplanar triangle O <sub>3</sub>
C5	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		
M6	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		coplanar hexagon O <sub>6</sub>
C7	2 <i>a</i>	-3 <i>m</i> .	0	0	0		

M4 = 0.667K + 0.333Ca; M6 = 0.667K + 0.333Ca

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

Remarks: Space groups (186) *P6<sub>3</sub>mc* and (190) *P-62c* were tested and rejected.

References: [1] Pertlik F. (1981), Z. Kristallogr. 157, 199-205.

$\text{Sm}_{1.2}\text{Zr}_{0.85}\text{Co}_{16.9}$	<i>hP40</i>	(194) <i>P6<sub>3</sub>/mmc</i> – kjgfdcb
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**Sm<sub>7</sub>Zr<sub>4</sub>Co<sub>89</sub>** [1]

Structural features: Kagomé-mesh Co<sub>9</sub> layers and (Sm,Zr)<sub>2</sub>Zr<sub>x</sub>(Co<sub>2</sub>)<sub>1-x</sub>Co<sub>6</sub> layers (a Co hexagon mesh, the hexagons of which are centered by a Sm or Zr atom or a Co<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder).

Lefevre A. et al. (1997) [1]

Co<sub>16.86</sub>Sm<sub>1.29</sub>Zr<sub>0.78</sub>

$a = 0.83403$ ,  $c = 0.81526$  nm,  $c/a = 0.977$ ,  $V = 0.4911$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	12 <i>k</i>	. <i>m</i> .	0.1672	0.3344	0.0185		9-vertex polyhedron Co <sub>9</sub>
Co2	12 <i>j</i>	. <i>m</i> ..	0.3697	0.0443	<sup>1</sup> / <sub>4</sub>		
Co3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		10-vertex polyhedron Co <sub>10</sub>
Co4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6175	0.93	
Zr5	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.07	pseudo Frank-Kasper Co <sub>20</sub> sixcapped hexagonal prism Co <sub>18</sub>
M6	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		
M7	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		

M6 = 0.78Sm + 0.22Zr; M7 = 0.51Sm + 0.49Zr

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.073

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

References: [1] Lefevre A., Cohen Adad M.T., Mentzen B.F. (1997), J. Alloys Compd. 256, 207-212.

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hP40

$\text{Na}_2[\text{MoO}_4]$	<i>hP40</i>	(194) $P6_3/mmc - \text{I}f^3e$
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**$\text{Na}_2\text{MoO}_4$   $\alpha_2$  [1]**

Structural features: Na atoms and  $\text{MoO}_4$  tetrahedra (orientational disorder) in a  $\text{Ni}_2\text{In}$ -type ( $\text{ht-Co}_2\text{Ge}$ ) arrangement (all atoms displaced from the ideal positions).

Bottelberghs P.H., Van Buren F.R. (1975) [1]

$\text{MoNa}_2\text{O}_4$

$a = 0.5934$ ,  $c = 0.7549$  nm,  $c/a = 1.272$ ,  $V = 0.2302$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24l	1	0.162	0.354	0.167	0.25	
O2	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.032	0.5	
Mo3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.242	0.5	
Na4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.692	0.5	
Na5	4e	3m.	0	0	0.033	0.5	

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

Experimental: powder, film, X-rays, T = 937 K

Remarks: Phase stable at T > 913 K. Short interatomic distances for partly occupied site(s).

References: [1] Bottelberghs P.H., Van Buren F.R. (1975), J. Solid State Chem. 13, 182-191.

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hP42

$\text{NaBaCe}_2[\text{CO}_3]_4\text{F}$	<i>hP42</i>	(194) $P6_3/mmc - k^2f^2edca$
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**$\text{NaBaCe}_2(\text{CO}_3)_4\text{F}$  [2], cordylite-(Ce)**

Structural features:  $\text{CO}_3$  trigonal units arranged in approximately planar layers where C forms a triangle mesh (stacking sequence BAABCAAC).  $\text{Ce}(\text{O}_9\text{F})$  polyhedra (an  $\text{O}_{12}$  anticuboctahedron with one triangle replaced by a single F) share vertices to form infinite slabs; C in trigonal, Na in trigonal prismatic voids in the slabs, Ba between the slabs. See Fig. III.41.

Giester G. et al. (1998) [1]

$\text{BaC}_4\text{Ce}_2\text{FNaO}_{12}$

$a = 0.50913$ ,  $c = 2.307$  nm,  $c/a = 4.531$ ,  $V = 0.5179$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.1448	0.2896	0.1761		single atom C
O2	12k	.m.	0.521	0.042	0.565		single atom C
C3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0674		non-coplanar triangle $\text{O}_3$
Ce4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.64649		10-vertex polyhedron $\text{FO}_9$
C5	4e	3m.	0	0	0.1802		non-coplanar triangle $\text{O}_3$
F6	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear $\text{Ce}_2$
Na7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism $\text{O}_6$
Ba8	2a	-3m.	0	0	0		hexagonal prism $\text{O}_{12}$

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

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

Remarks: Natural specimen from Narssarssuk, Greenland. Composition  $\text{Na}_{1.79}\text{Ca}_{0.19}\text{Ba}_{1.75}\text{Sr}_{0.13}\text{Ce}_{2.31}\text{La}_{1.25}\text{Nd}_{0.34}\text{Pr}_{0.22}\}(\text{CO}_3)_{6.75}\text{F}_{1.74}$  from chemical analysis.

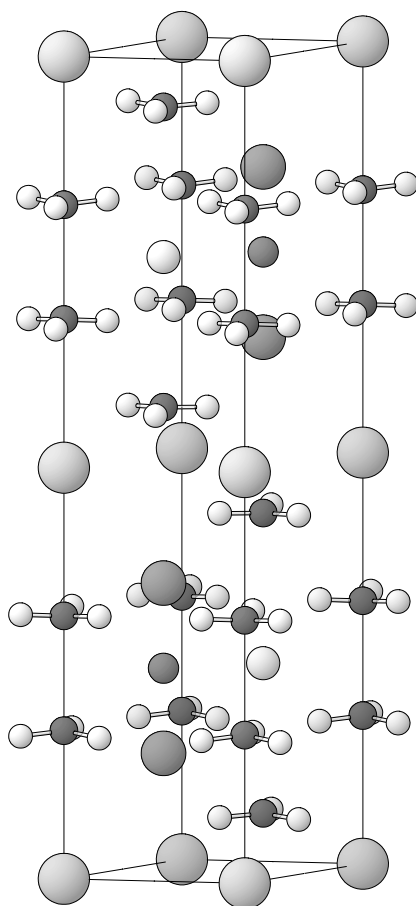


Fig. III.41.  $\text{NaBaCe}_2(\text{CO}_3)_4\text{F}$

Arrangement of  $\text{CO}_3$  triangles (C atoms small dark, O atoms small light), Na (medium light), Ba (large light), Ce (large dark) and F (medium dark) atoms.

References: [1] Giester G., Ni Y., Jarosch D., Hughes J.M., Ronsbo J., Yang Z., Zemmann J. (1998), Am. Mineral. 83, 178-184. [2] Fu P.Q., Kong Y.H., Gong G., Shao M., Qian J. (1987), Kuangwu Xuebao 7, 298-304.

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hP42

$\text{Hg}_4[\text{SO}_4]_{0.5}\text{N}_2\text{Cl}[\text{H}_2\text{O}]$	hP42	(194) $P6_3/mmc - \text{kh}^2\text{gfdcba}$
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**$(\text{Hg}_2\text{N})(\text{Cl},\text{SO}_4) \cdot x\text{H}_2\text{O}$  [1], kleinite**

Structural features: N-Hg-N linear units share vertices to form a tetrahedral framework;  $\text{SO}_4$  tetrahedra, Cl and  $\text{H}_2\text{O}$  in voids (disorder).

Giester G. et al. (1996) [1]

$\text{ClH}_2\text{Hg}_4\text{N}_2\text{OS}_{0.50}$

$a = 0.6762$ ,  $c = 1.1068$  nm,  $c/a = 1.637$ ,  $V = 0.4383$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH <sub>2</sub> )1	12k	.m.	0.1659	0.3318	0.0	0.1	coplanar hexagon (OH <sub>2</sub> ) <sub>2</sub> ClHg <sub>2</sub> N
S2	6h	mm2	0.0364	0.0728	1/4	0.083	
(OH <sub>2</sub> )3	6h	mm2	0.1969	0.3938	1/4	0.1	colinear (OH <sub>2</sub> )S

Hg4	6g	.2/m.	$\frac{1}{2}$	0	0		coplanar hexagon (OH <sub>2</sub> ) <sub>4</sub> N <sub>2</sub>
N5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5625		7-vertex polyhedron Hg <sub>4</sub> (OH <sub>2</sub> ) <sub>3</sub>
Hg6	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear N <sub>2</sub>
(OH <sub>2</sub> )7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.1	coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
S8	2b	-6m2	0	0	$\frac{1}{4}$	0.25	
Cl9	2a	-3m.	0	0	0		coplanar hexagon (OH <sub>2</sub> ) <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.066, T = 286 K

Remarks: Natural specimen from Terlingua, Brewster County, Texas. ~3 wt.% SO<sub>4</sub> and ~1 wt.% H<sub>2</sub>O from chemical analysis (on a different sample). O of SO<sub>4</sub> units 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] Giester G., Mikenda W., Pertlik F. (1996), Neues Jahrb. Mineral., Monatsh. 1996, 49-56.

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hP42

Mg<sub>5.2</sub>Eu

hP42

(194) *P*6<sub>3</sub>/*mmc* – kh<sup>2</sup>gfeba

### EuMg<sub>5.2</sub> [1]

Structural features: Puckered triangle-mesh Mg<sub>11</sub>(Mg, □) layers and Eu<sub>3</sub>Mg<sub>3</sub>(Mg, □) layers (Eu<sub>3</sub> trigonal clusters) alternate along [001]; partly disordered atom arrangement along 0 0 *z*. See Fig. III.42.

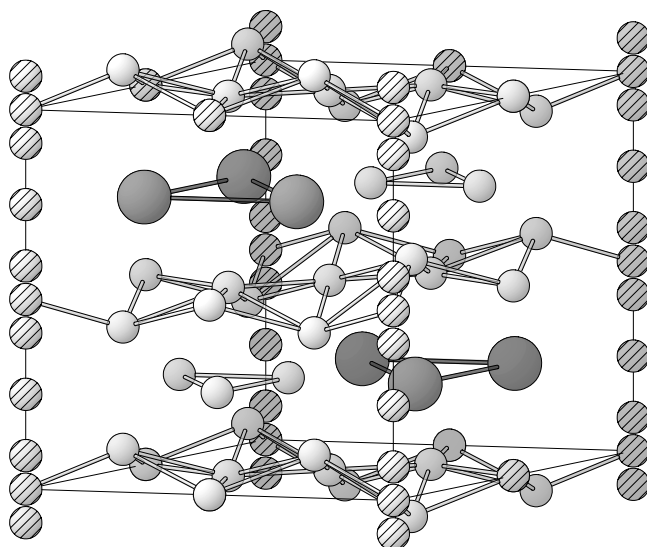


Fig. III.42. EuMg<sub>5.2</sub>

Arrangement of Eu<sub>3</sub> triangles (Eu atoms large) and Mg atoms (small; atoms in partly occupied sites are hatched).

Erassme J., Lueken H. (1987) [1]

EuMg<sub>5.23</sub>

*a* = 1.0395, *c* = 1.0746 nm, *c/a* = 1.034, *V* = 1.0056 nm<sup>3</sup>, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mg1	12k	.m.	0.1599	0.3198	0.5888		
Eu2	6h	<i>mm</i> 2	0.19510	0.39021	$\frac{1}{4}$		
Mg3	6h	<i>mm</i> 2	0.5680	0.1360	$\frac{1}{4}$		icosahedron Mg <sub>10</sub> Eu <sub>2</sub>
Mg4	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Mg <sub>8</sub> Eu <sub>4</sub>
Mg5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5019		icosahedron Mg <sub>9</sub> Eu <sub>3</sub>

Mg6	4e	3m.	0	0	0.0883	0.26
Mg7	2b	-6m2	0	0	$\frac{1}{4}$	0.77
Mg8	2a	-3m.	0	0	0	0.4

Experimental: single crystal, diffractometer, X-rays, R = 0.026, T = 294 K

Remarks: Short interatomic distances for partly occupied site(s). Supersedes structure proposals for composition  $\text{EuMg}_5$  with full occupation of Wyckoff position 2a or partial occupation of Wyckoff positions 2a and 4e [2].

References: [1] Erassme J., Lueken H. (1987), Acta Crystallogr. B 43, 244-250. [2] Mühlpfordt W. (1970), Z. Anorg. Allg. Chem. 374, 174-185.

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hP42

$\text{Ag}_{0.2}(\text{Ag}_{0.55}\text{Al}_{0.45})_4\text{DyAl}_{0.8}$	hP42	(194) $P6_3/mmc$ – kh <sup>2</sup> gfeba
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### DyAg<sub>2.4</sub>Al<sub>2.6</sub> [1]

Structural features: Puckered triangle-mesh (Al,Ag)<sub>9</sub>(Al,□)<sub>3</sub> layers and Dy<sub>3</sub>(Al,Ag)<sub>3</sub>(Ag,□) layers (Dy<sub>3</sub> trigonal clusters) alternate along [001]; partly disordered atom arrangement along 0 0 z. Ordering variant of  $\text{EuMg}_{5.22}$ .

Stel'makhovich B.M., Kuz'ma Y.B. (1992) [1]

$\text{Ag}_{2.41}\text{Al}_{2.64}\text{Dy}$

$a = 0.9132$ ,  $c = 0.9414$  nm,  $c/a = 1.031$ ,  $V = 0.6799$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1574	0.3148	0.5921		
Dy2	6h	mm2	0.19583	0.39166	$\frac{1}{4}$		
M3	6h	mm2	0.5679	0.1358	$\frac{1}{4}$		icosahedron $\text{Ag}_6\text{Al}_4\text{Dy}_2$
M4	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron $\text{Al}_4\text{Ag}_4\text{Dy}_4$
Al5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0132		icosahedron $\text{Ag}_6\text{Al}_3\text{Dy}_3$
Ag6	4e	3m.	0	0	0.213	0.164	
Ag7	2b	-6m2	0	0	$\frac{1}{4}$	0.27	
Al8	2a	-3m.	0	0	0	0.54	

$\text{M1} = 0.734\text{Ag} + 0.266\text{Al}$ ;  $\text{M3} = 0.870\text{Al} + 0.130\text{Ag}$ ;  $\text{M4} = 0.613\text{Ag} + 0.387\text{Al}$

Experimental: single crystal, diffractometer, X-rays, R = 0.060

Remarks: Homogeneity range  $\text{DyAg}_{5-x}\text{Al}_x$ ,  $2.4 < x < 2.8$ . Short interatomic distances for partly occupied site(s).

References: [1] Stel'makhovich B.M., Kuz'ma Y.B. (1992), Sov. Phys. Crystallogr. 37, 719-721 (Kristallografiya 37, 1334-1337).

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hP42

$\text{Ag}_{0.3}(\text{Ag}_{0.46}\text{Al}_{0.54})_{17}\text{Dy}_{1.7}$	hP42	(194) $P6_3/mmc$ – kjgfeeb
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### Dy<sub>1.75</sub>Ag<sub>8.1</sub>Al<sub>9.2</sub> [1]

Structural features: Kagomé-mesh (Al,Ag)<sub>9</sub> layers and Dy<sub>2-x</sub>[(Ag,Al)<sub>2</sub>](Ag<sub>2</sub>)<sub>x</sub>(Ag,Al)<sub>6</sub> layers (an(Ag,Al) hexagon mesh, the hexagons of which are centered by a Dy atom or an (Ag,Al)<sub>2</sub> or Ag<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder).

Stel'makhovich B.M., Kuz'ma Y.B. (1991) [1]

$\text{Ag}_{8.03}\text{Al}_{9.20}\text{Dy}_{1.74}$

$a = 0.9285$ ,  $c = 0.9098$  nm,  $c/a = 0.98$ ,  $V = 0.6793$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1637	0.3274	0.0236		11-vertex polyhedron $\text{Ag}_9\text{Al}_2$
M2	12j	m..	0.363	0.0332	$\frac{1}{4}$		
M3	6g	2/m.	$\frac{1}{2}$	0	0		icosahedron $\text{Ag}_{10}\text{Dy}_2$
M4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5979		14-vertex Frank-Kasper $\text{Ag}_{10}\text{Al}_3\text{Dy}$
Ag5	4e	3m.	0	0	0.101	0.114	
Dy6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Ag}_{14}\text{Al}_6$
Dy7	2b	-6m2	0	0	$\frac{1}{4}$	0.736	

$\text{M1} = 0.50\text{Ag} + 0.50\text{Al}$ ;  $\text{M2} = 0.50\text{Ag} + 0.50\text{Al}$ ;  $\text{M3} = 0.80\text{Al} + 0.20\text{Ag}$ ;  $\text{M4} = 0.60\text{Ag} + 0.40\text{Al}$

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

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

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

References: [1] Stel'makhovich B.M., Kuz'ma Y.B. (1991), Dokl. Akad. Nauk Ukr. SSR 1991(7), 135-137.

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hP42

$\text{Zr}(\text{Mo}_{0.5}\text{Fe}_{0.5})_2\text{H}_{2.6}$

hP42

(194)  $P6_3/mmc - 1h^2fa$

**ZrMoFeH<sub>2.6</sub>** [1]

Structural features: Filled-up derivative of  $\text{MgZn}_2$  with H in tetrahedral ( $\text{Zr}_2(\text{Fe},\text{Mo})_2$ ) voids.

Yartys' V.A. et al. (1982) [1]

$\text{D}_{2.60}\text{FeMoZr}$

$a = 0.542$ ,  $c = 0.8826$  nm,  $c/a = 1.628$ ,  $V = 0.2245$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	24l	1	0.058	0.35	0.036	0.275	non-colinear $\text{D}_2$
M2	6h	mm2	0.163	0.326	$\frac{1}{4}$		non-colinear $\text{D}_2$
D3	6h	mm2	0.537	0.074	$\frac{1}{4}$	0.633	non-colinear $\text{Fe}_2$
Zr4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.569		non-coplanar hexagon $\text{D}_6$
M5	2a	-3m.	0	0	0		hexagonal prism $\text{D}_{12}$

$\text{M2} = 0.5\text{Fe} + 0.5\text{Mo}$ ;  $\text{M5} = 0.5\text{Fe} + 0.5\text{Mo}$

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

Experimental: powder, diffractometer, neutrons,  $R_B = 0.083$

Remarks: We assigned an approximate value to the Mo/Fe ratio of sites M based on the nominal composition. Space groups (173)  $P6_3/m$ , (182)  $P6_322$ , (186)  $P6_3mc$  and (190)  $P-62c$  were tested and rejected.

References: [1] Yartys' V.A., Burnasheva V.V., Fadeeva N.V., Solov'ev S.P., Semenenko K.N. (1982), Sov. Phys. Crystallogr. 27, 540-543 (Kristallografiya 27, 900-904).

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hP42

$\text{NaBa}_3\text{Ru}_2\text{O}_9$

hP42

(194)  $P6_3/mmc - 1hf^2ba$

**NaBa<sub>3</sub>Ru<sub>2</sub>O<sub>9</sub>** [1], perovskite 6H

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Ru and Na in octahedral (O<sub>6</sub>) voids. Pairs of face-linked RuO<sub>6</sub> octahedra (Ru<sub>2</sub> dumbbells) share vertices with single NaO<sub>6</sub> octahedra to form a 3D-framework. Variant of Ba<sub>3</sub>WFe<sub>2</sub>O<sub>9</sub> with splitting of one O site.

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

Ba<sub>3</sub>NaO<sub>9</sub>Ru<sub>2</sub>

$a = 0.5865$ ,  $c = 1.4421$  nm,  $c/a = 2.459$ ,  $V = 0.4296$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24l	1	0.312	0.144	0.095	0.5	non-collinear Ru <sub>2</sub>
O2	6h	mm2	0.508	0.016	<sup>1</sup> / <sub>4</sub>		
Ba3	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.093		
Ru4	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.657		
Ba5	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>		
Na6	2a	-3m.	0	0	0		

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.044

Remarks: Ambiguous data: it is not clear if the splitting of site O1 is intentional, standard uncertainties not reported. Short interatomic distances for partly occupied site(s). In table 1 of [1] the Wyckoff positions of former Ru and O(2) are misprinted as 2a and 12k instead of 4f and 24l, respectively.

References: [1] Samata H., Kai M., Uchida T., Ohtsuka M., Tanaka G., Sawada S., Taniguchi T., Nagata Y. (2003), J. Alloys Compd. 350, 77-85.

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hP44

Lu <sub>4</sub> (Mn <sub>0.2</sub> Fe <sub>0.8</sub> ) <sub>5</sub> O <sub>13</sub>	hP44	(194) $P6_3/mmc - f^7e^3dc$
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**Lu<sub>4</sub>MnFe<sub>4</sub>O<sub>13</sub>** [1]

Structural features: Close-packed O layers in h<sub>2</sub>c<sub>2</sub>(hc<sub>2</sub>)<sub>3</sub> stacking; Lu in octahedral, (Fe,Mn) in trigonal bipyramidal voids. Double and single layers of vertex-linked (Fe,Mn)O<sub>5</sub> trigonal bipyramids in the ratio 1:3 (also common edges for double layers).

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

Fe<sub>4.01</sub>Lu<sub>4</sub>Mn<sub>0.99</sub>O<sub>13</sub>

$a = 0.3453$ ,  $c = 5.188$  nm,  $c/a = 15.025$ ,  $V = 0.5357$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0199		tetrahedron Fe <sub>4</sub>
Lu2	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.082		octahedron O <sub>6</sub>
O3	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1366		non-coplanar triangle Fe <sub>3</sub>
Lu4	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1941		octahedron O <sub>6</sub>
M5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5235		trigonal bipyramid O <sub>5</sub>
O6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5624		tetrahedron FeLu <sub>3</sub>
O7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.7132		tetrahedron FeLu <sub>3</sub>
O8	4e	3m.	0	0	0.1019		tetrahedron FeLu <sub>3</sub>
M9	4e	3m.	0	0	0.1377		trigonal bipyramid O <sub>5</sub>
O10	4e	3m.	0	0	0.1738		tetrahedron FeLu <sub>3</sub>
M11	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		trigonal bipyramid O <sub>5</sub>
O12	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle Fe <sub>3</sub>

M5 = 0.70Fe + 0.30Mn; M9 = 0.87Fe + 0.13Mn; M11 = 0.87Fe + 0.13Mn

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

Remarks:  $\text{Lu}_4(\text{Mn}^{2+})(\text{Fe}^{3+})_4\text{O}_{13}$  from Mössbauer spectroscopy.

References: [1] Malaman B., Aqachmar E.H., Gérardin R., Evrard O. (1992), Mater. Res. Bull. 27, 855-865.

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hP44

$\text{Na}_3\text{Ce}_2[\text{CO}_3]_4\text{F}$	hP44	(194) $P6_3/mmc - k^2f^3ecb$
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**$\text{Na}_3\text{Ce}_2(\text{CO}_3)_4\text{F}$**  [1], lukechangite-(Ce)

Structural features:  $\text{CO}_3$  trigonal units arranged in approximately planar layers where C forms a triangle mesh (ABBAACCA stacking).  $\text{Ce}(\text{O}_9\text{F})$  polyhedra (an  $\text{O}_{12}$  antioctahedron with one triangle replaced by a single F) share vertices to form infinite slabs; C in trigonal, Na in trigonal prismatic voids in the slabs and between the slabs.

Grice J.D., Chao G.Y. (1997) [1]

$\text{C}_4\text{Ce}_2\text{FNa}_3\text{O}_{12}$

$a = 0.50612$ ,  $c = 2.282$  nm,  $c/a = 4.509$ ,  $V = 0.5062$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1448	0.2896	0.0625		single atom C
O2	12k	.m.	0.187	0.374	0.6759		single atom C
Ce3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.14553		10-vertex polyhedron $\text{FO}_9$
Na4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5223		9-vertex polyhedron $\text{O}_9$
C5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6761		coplanar triangle $\text{O}_3$
C6	4e	3m.	0	0	0.0642		non-coplanar triangle $\text{O}_3$
F7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear $\text{Ce}_2$
Na8	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism $\text{O}_6$

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

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

Remarks: Natural specimen from Mont Saint-Hilaire, Quebec. Composition  $\{\text{Na}_{2.99}\text{Ca}_{0.01}\text{Sr}_{0.01}\}\{\text{Ce}_{1.11}\text{La}_{0.62}\text{Nd}_{0.22}\text{Pr}_{0.07}\}(\text{CO}_3)_4\text{F}_{1.17}$  from electron microprobe analysis.

References: [1] Grice J.D., Chao G.Y. (1997), Am. Mineral. 82, 1255-1260.

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hP44

$\text{Rb}_2\text{Tb}_3\text{AlF}_{16}$	hP44	(194) $P6_3/mmc - k^2h^2fba$
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**$\text{Rb}_2\text{Tb}_3\text{AlF}_{16}$**  [2]

Structural features: Distorted  $\text{TbF}_6\text{F}_3$  tricapped trigonal prisms and  $\text{AlF}_6$  octahedra share vertices to form a 3D-framework.

Josse M. et al. (2004) [1]

$\text{AlF}_{16}\text{Rb}_2\text{Tb}_3$

$a = 0.7556$ ,  $c = 1.2397$  nm,  $c/a = 1.641$ ,  $V = 0.6130$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12k	.m.	0.1146	0.2292	0.5813		single atom Al
F2	12k	.m.	0.5503	0.1006	0.1531		non-colinear $\text{Tb}_2$
F3	6h	mm2	0.18	0.36	$\frac{1}{4}$		non-coplanar triangle $\text{Tb}_2\text{F}$
Tb4	6h	mm2	0.8291	0.6582	$\frac{1}{4}$		tricapped trigonal prism $\text{F}_9$



Rb5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0619	icosahedron F <sub>12</sub>
F6	2b	-6m2	0	0	$\frac{1}{4}$	coplanar triangle Tb <sub>3</sub>
Al7	2a	-3m.	0	0	0	octahedron F <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.027, T = 293 K

Remarks: The same data are reported in [2] (origin shifted by 0 0  $\frac{1}{2}$ ). In table 3a of [1] the z-coordinates of former Tb and F1 are misprinted as  $\frac{1}{4}$  instead of  $\frac{3}{4}$  (from comparison with [2]; checked on interatomic distances). In table 2a of [2] the x-coordinate of site F2 is misprinted as 0.1146 instead of -0.1146 (agreement with Wyckoff position 12k; checked on interatomic distances).

References: [1] Josse M., Dubois M., El Ghoszi M., Avignat D. (2004), J. Alloys Compd. 374, 213-218. [2] Josse M., Dubois M., El Ghoszi M., Avignat D. (2003), Solid State Sci. 5, 1141-1148.

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hP44

Ba <sub>5</sub> Nb <sub>2</sub> O <sub>9</sub> [O <sub>2</sub> ]	hP44	(194) P6 <sub>3</sub> /mmc – k <sup>2</sup> hf <sup>2</sup> ed
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**Ba<sub>5</sub>Nb<sub>2</sub>O<sub>9</sub>(O<sub>2</sub>)** [1]; Ba<sub>5</sub>Ru<sub>2</sub>O<sub>10</sub> [1]

Structural features: Double perovskite-type slabs (three close-packed BaO<sub>3</sub> layers, Nb in octahedral voids) alternate with triangle-mesh Ba<sub>2</sub>(O<sub>2</sub>) layers along [001] (O<sub>2</sub> dumbbells perpendicular to [001], 3-fold orientational disorder). Units of two face-linked NbO<sub>6</sub> octahedra (Nb<sub>2</sub> dumbbells).

Grasset F. et al. (1999) [1]

Ba<sub>5</sub>Nb<sub>2</sub>O<sub>11</sub>

$a = 0.6045$ ,  $c = 1.8316$  nm,  $c/a = 3.030$ ,  $V = 0.5796$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.0772	0.1544	0.0023	0.333	
O2	12k	.m.	0.5105	0.021	0.6214		single atom Nb
O3	6h	mm2	0.1905	0.381	$\frac{1}{4}$		non-collinear Nb <sub>2</sub>
Nb4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1699		octahedron O <sub>6</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5208		octahedron O <sub>6</sub>
Ba6	4e	3m.	0	0	0.1399		
Ba7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>

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

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.033

Remarks: Short interatomic distances for partly occupied site(s). Slightly different coordinates were obtained for site O1 in Ba<sub>5</sub>Ru<sub>2</sub>O<sub>10</sub>, which does not contain O<sub>2</sub> pairs (0.054 0.108 0.009, occ. =  $\frac{1}{6}$ ). Splitting of site Ba5 is reported for Ba<sub>5</sub>Ru<sub>2</sub>O<sub>9</sub>(O<sub>2</sub>) in [2]. In table 6 of [1] the Wyckoff position of former Ba(1) is misprinted as 4a instead of 4e.

References: [1] Grasset F., Zakhour M., Darriet J. (1999), J. Alloys Compd. 287, 25-31. [2] Grasset F., Dussarrat C., Darriet J. (1997), J. Mater. Chem. 7, 1911-1915.

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hP44

Ba <sub>0.8</sub> Sr <sub>0.6</sub> Ca <sub>1.6</sub> La <sub>2</sub> Mn <sub>2</sub> O <sub>10</sub>	hP44	(194) P6 <sub>3</sub> /mmc – kihf <sup>2</sup> ed
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**Ba<sub>0.8</sub>Sr<sub>0.6</sub>Ca<sub>1.6</sub>La<sub>2</sub>Mn<sub>2</sub>O<sub>10</sub>** [1]; K<sub>1.56</sub>Ba<sub>3.44</sub>Ir<sub>2</sub>O<sub>10</sub> [2]

Structural features: Double perovskite-type slabs (close-packed (Ba,Sr)O<sub>3</sub> and (La,Sr)O<sub>3</sub> layers, Mn in octahedral voids) alternate with triangle-mesh (Ca,La,Sr)<sub>2</sub>O layers along [001]. Units of two face-linked MnO<sub>6</sub> octahedra (Mn<sub>2</sub> dumbbells).

Bie L. et al. (2002) [1]

Ba<sub>0.80</sub>Ca<sub>1.60</sub>La<sub>2</sub>Mn<sub>2</sub>O<sub>10</sub>Sr<sub>0.60</sub>

$a = 0.56359$ ,  $c = 1.62843$  nm,  $c/a = 2.889$ ,  $V = 0.4479$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.5066	0.0132	0.6077	0.167	single atom Mn
O2	12 <i>i</i>	.2.	0.123	0	0		
O3	6 <i>h</i>	<i>mm</i> 2	0.1788	0.3576	<sup>1</sup> / <sub>4</sub>		non-collinear Mn <sub>2</sub>
Mn4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1706		octahedron O <sub>6</sub>
M5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5119		trigonal prism O <sub>6</sub>
M6	4 <i>e</i>	3 <i>m</i> .	0	0	0.1325		
M7	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		anticuboctahedron O <sub>12</sub>

M5 = 0.80Ca + 0.10La + 0.10Sr; M6 = 0.90La + 0.10Sr; M7 = 0.80Ba + 0.20Sr

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.087

Remarks: Short interatomic distances for partly occupied site(s). In footnote 7 of [1] the Wyckoff position of former Ba1 is misprinted as 2*d* instead of 2*c*.

References: [1] Bie L., Lin J., Wang Y., Loong C.K. (2002), Inorg. Chem. Commun. 5, 966-970. [2] Kim S.J., Smith M.D., Darriet J., Zur Loye H.C. (2004), J. Solid State Chem. 177, 1493-1500.

194  
hP44

Fe<sub>3</sub>Ge<sub>2.4</sub>Sb<sub>0.6</sub>

hP44

(194) *P*6<sub>3</sub>/*mmc* – kjgf<sup>2</sup>ea

**Fe<sub>3</sub>Ge<sub>2.4</sub>Sb<sub>0.6</sub>** [1]

Structural features: Fe<sub>9</sub>(Ge,□)<sub>3</sub> layers (a Fe Kagomé mesh, part of the hexagons are centered by Ge atoms, disorder) and Ge<sub>6</sub>(Sb<sub>2</sub>,□)<sub>3</sub> layers (a Ge hexagon mesh, part of the hexagons are centered by Sb<sub>2</sub> dumbbells perpendicular to the layer, disorder) alternate along [001].

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

Fe<sub>3</sub>Ge<sub>2.36</sub>Sb<sub>0.54</sub>

$a = 0.87958$ ,  $c = 0.8004$  nm,  $c/a = 0.910$ ,  $V = 0.5363$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12 <i>k</i>	. <i>m</i> .	0.16563	0.3312	0.00506		trigonal prism Fe <sub>6</sub>
Ge2	12 <i>j</i>	<i>m</i> ..	0.33972	0.01113	<sup>1</sup> / <sub>4</sub>		
Fe3	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		
Sb4	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0723	0.594	
Ge5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5032	0.29	
Sb6	4 <i>e</i>	3 <i>m</i> .	0	0	0.075	0.222	
Ge7	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.49	

Experimental: single crystal, diffractometer, X-rays, R = 0.041, T = 295 K

Remarks: Homogeneity range FeGe<sub>1-x</sub>Sb<sub>x</sub>, 0 < x < 0.4. Short interatomic distances for partly occupied site(s).

References: [1] Mills A.M., Mar A. (2000), J. Alloys Compd. 298, 82-92.

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hP44

Mg<sub>17.58</sub>Ce<sub>1.71</sub>

hP44

(194) *P*6<sub>3</sub>/*mmc* – kjgfedcb

**CeMg<sub>10.3</sub>** [1]; Ho<sub>2</sub>Fe<sub>17</sub> [2]

Structural features: Kagomé-mesh Mg<sub>9</sub> layers and CeCe<sub>2-x</sub>(Mg<sub>2</sub>)<sub>x</sub>Mg<sub>6</sub> layers (a Mg hexagon mesh, the hexagons of which are centered by a Ce atom or a Mg<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder).

Johnson Q., Smith G.S. (1967) [1]

Ce<sub>1.71</sub>Mg<sub>17.58</sub>

$a = 1.033$ ,  $c = 1.025$  nm,  $c/a = 0.992$ ,  $V = 0.9472$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	12 <i>k</i>	<i>m.</i>	0.1667	0.3334	0.0205		11-vertex polyhedron Mg <sub>11</sub>
Mg2	12 <i>j</i>	<i>m.</i>	0.3593	0.0321	$\frac{1}{4}$		
Mg3	6 <i>g</i>	<i>.2/m.</i>	$\frac{1}{2}$	0	0		
Mg4	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6004	0.985	pseudo Frank-Kasper Mg <sub>20</sub>
Mg5	4 <i>e</i>	3 <i>m.</i>	0	0	0.1118	0.305	
Ce6	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.015	
Ce7	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Ce8	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$	0.695	

Experimental: single crystal, diffractometer, X-rays,  $R = 0.053$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). In the title of [1] the chemical formula is misprinted as CeMg<sub>1.03</sub> instead of CeMg<sub>10.3</sub>.

References: [1] Johnson Q., Smith G.S. (1967), Acta Crystallogr. 23, 327-329. [2] Christensen A.N., Hazell R.G. (1980), Acta Chem. Scand. A 34, 455-459.

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hP44

Tb<sub>2</sub>Mn<sub>17</sub>C<sub>2.5</sub>

hP44

(194)  $P6_3/mmc$  – kjhgfc

**Tb<sub>2</sub>Mn<sub>17</sub>C<sub>x</sub>** [1]

Structural features: Filled-up derivative of Th<sub>2</sub>Ni<sub>17</sub> with C in octahedral (Tb<sub>2</sub>Mn<sub>4</sub>) voids. See Fig. III.43.

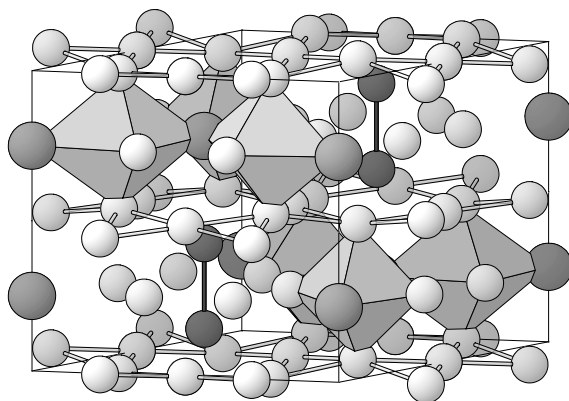


Fig. III.43. **Tb<sub>2</sub>Mn<sub>17</sub>C<sub>3-x</sub>**

Arrangement of C(Tb<sub>2</sub>Mn<sub>4</sub>) octahedra (Tb atoms large, Mn atoms small) and additional Mn atoms (Mn<sub>2</sub> dumbbells dark).

Block G., Jeitschko W. (1987) [1]

C<sub>2.43</sub>Mn<sub>17</sub>Tb<sub>2</sub>

$a = 0.8738$ ,  $c = 0.8511$  nm,  $c/a = 0.974$ ,  $V = 0.5628$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	12k	.m.	0.1687	0.3374	0.0239		single atom C
Mn2	12j	m..	0.3829	0.055	$\frac{1}{4}$		single atom C
C3	6h	mm2	0.165	0.33	$\frac{1}{4}$	0.81	octahedron Mn <sub>4</sub> Tb <sub>2</sub>
Mn4	6g	.2/m.	$\frac{1}{2}$	0	0		16-vertex polyhedron Mn <sub>10</sub> Tb <sub>2</sub> C <sub>4</sub>
Mn5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6077		14-vertex Frank-Kasper Mn <sub>13</sub> Tb
Tb6	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle C <sub>3</sub>
Tb7	2b	-6m2	0	0	$\frac{1}{4}$		coplanar triangle C <sub>3</sub>

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

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

Remarks: A refinement on data collected at 16 K is reported in [2] (partial disorder Tb/Mn<sub>2</sub>).

References: [1] Block G., Jeitschko W. (1987), J. Solid State Chem. 70, 271-280. [2] Hu Z., Luo H., Yelon W.B., De Groot C.H., De Boer F.R., Buschow K.H.J. (1997), J. Alloys Compd. 248, 121-124.

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hP46

Ba <sub>5</sub> Er <sub>2</sub> ZrAl <sub>2</sub> O <sub>13</sub>	hP46	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> f <sup>3</sup> edca
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### Ba<sub>5</sub>Er<sub>2</sub>Al<sub>2</sub>ZrO<sub>13</sub> [1]

Structural features: Four close-packed BaO<sub>3</sub> layers in c stacking alternate with hexagon-mesh BaO layers along [001]; Er and Zr in octahedral, Al in tetrahedral voids. ErO<sub>6</sub> and ZrO<sub>6</sub> octahedra share vertices to form triple perovskite-type slabs, which are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Shpanchenko R.V. et al. (1995) [1]

Al<sub>2</sub>Ba<sub>5</sub>Er<sub>2</sub>O<sub>13</sub>Zr

$a = 0.59476$ ,  $c = 2.46604$  nm,  $c/a = 4.146$ ,  $V = 0.7555$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.157	0.314	0.0502		non-colinear ZrEr
O2	12k	.m.	0.508	0.016	0.1589		non-colinear AlEr
Er3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1033		octahedron O <sub>6</sub>
Ba4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5431		cuboctahedron O <sub>12</sub>
Al5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6823		tetrahedron O <sub>4</sub>
Ba6	4e	3m.	0	0	0.1404		9-vertex polyhedron O <sub>9</sub>
O7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Ba8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O <sub>6</sub>
Zr9	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.033

References: [1] Shpanchenko R.V., Abakumov A.M., Antipov E.V., Nistor L., Van Tendeloo G., Amelinckx S. (1995), J. Solid State Chem. 118, 180-192.

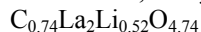
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hP46

Li <sub>0.52</sub> La <sub>2</sub> [CO <sub>3</sub> ] <sub>0.74</sub> O <sub>2.26</sub>	hP46	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> h <sup>2</sup> f <sup>2</sup> d
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### Li<sub>2x</sub>La<sub>2</sub>O<sub>2+x</sub>(CO<sub>3</sub>)<sub>1-x</sub> [1]

Structural features: Ordered  $\text{La}_2\text{O}_2$  slabs (edge-linked  $\text{OLa}_4$  tetrahedra) and disordered layers containing Li atoms and  $\text{CO}_3$  trigonal units (parallel to  $[001]$ ), in part replaced by simple O anions.

Attfield J.P., Ferey G. (1989) [1]



$a = 0.4058$ ,  $c = 1.62219$  nm,  $c/a = 3.998$ ,  $V = 0.2313$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.034	0.0681	0.6755	0.266	
O2	12k	.m.	0.131	0.262	0.633	0.067	
C3	6h	mm2	0.047	0.094	$\frac{1}{4}$	0.247	
O4	6h	mm2	0.228	0.456	$\frac{1}{4}$	0.247	coplanar triangle $\text{CO}_2$
La5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0943		non-coplanar hexagon $\text{O}_6$
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5569		non-coplanar triangle $\text{O}_3$
Li7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.52	coplanar hexagon $\text{O}_6$

Experimental: powder, diffractometer, neutrons, time-of-flight,  $wR_p = 0.040$ ,  $T = 293$  K

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

References: [1] Attfield J.P., Ferey G. (1989), J. Solid State Chem. 82, 132-138.

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hP46

$\text{Y}_2(\text{Ga}_{0.45}\text{Ge}_{0.55})_{3.36}$	hP46	(194) $P6_3/mmc - k^2h^2fec$
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**$\text{Y}_8(\text{Ge,Ga})_{15-x}$**  [1]

Structural features: 3D-framework of fused  $\text{Y}_6$  trigonal prisms centered by (Ge,Ga); every eighth prism in alternating interlayers remains vacant and the surrounding (Ge,Ga) atoms are displaced from the prism centers (additional partly disordered vacancies).

Venturini G., Vernière A. (2000) [1]



$a = 0.8097$ ,  $c = 1.6464$  nm,  $c/a = 2.033$ ,  $V = 0.9348$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	12k	.m.	0.156	0.312	0.005	0.74	tricapped trigonal prism $\text{Ge}_3\text{Y}_6$
Y2	12k	.m.	0.5013	0.0026	0.6224		19-vertex polyhedron $\text{Ge}_{11}\text{Y}_8$
M3	6h	mm2	0.156	0.312	$\frac{1}{4}$		tricapped trigonal prism $\text{Ge}_3\text{Y}_6$
M4	6h	mm2	0.798	0.596	$\frac{1}{4}$		10-vertex polyhedron $\text{Ge}_4\text{Y}_6$
M5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.508		tricapped trigonal prism $\text{Ge}_3\text{Y}_6$
Y6	4e	3m.	0	0	0.129		pseudo Frank-Kasper $\text{Ge}_{12}\text{Y}_8$
M7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism $\text{Ge}_3\text{Y}_6$

$\text{M1} = 0.55\text{Ge} + 0.45\text{Ga}$ ;  $\text{M3} = 0.55\text{Ge} + 0.45\text{Ga}$ ;  $\text{M4} = 0.55\text{Ge} + 0.45\text{Ga}$ ;  $\text{M5} = 0.55\text{Ge} + 0.45\text{Ga}$ ;  $\text{M7} = 0.55\text{Ge} + 0.45\text{Ga}$

Experimental: powder, diffractometer, X-rays,  $R = 0.092$

Remarks: Homogeneity range  $\text{Y}_{36}\text{Ge}_{64-x}\text{Ga}_x$ ,  $11 < x < 29$ . We assigned an approximate value to the Ge/Ga ratio of sites M based on the nominal composition of the sample ( $\text{Y}_{38}\text{Ga}_{28}\text{Ge}_{34}$ ).

References: [1] Venturini G., Vernière A. (2000), J. Alloys Compd. 298, 213-219.

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hP46

$\text{Cs}_3\text{Sb}_3[\text{Ge}_2\text{O}_7]\text{O}_6$	hP46	(194) $P6_3/mmc - k^2hgfd$
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**Cs<sub>3</sub>Sb<sub>3</sub>(Ge<sub>2</sub>O<sub>7</sub>)O<sub>6</sub> [1]**

Structural features: Infinite slabs of vertex-linked SbO<sub>6</sub> octahedra are interconnected via common vertices with units of two vertex-linked GeO<sub>4</sub> tetrahedra to form a 3D-framework.

Pagnoux C. et al. (1993) [1]

Cs<sub>2.99</sub>Ge<sub>2</sub>O<sub>13</sub>Sb<sub>3</sub>

$a = 0.73309$ ,  $c = 1.6775$  nm,  $c/a = 2.288$ ,  $V = 0.7807$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.2028	0.4056	0.02		non-colinear Sb <sub>2</sub>
O2	12k	.m.	0.5346	0.0692	0.1168		non-colinear GeSb
Cs3	6h	mm2	0.265	0.53	$\frac{1}{4}$	0.33	
Sb4	6g	.2/m.	$\frac{1}{2}$	0	0		octahedron O <sub>6</sub>
Ge5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6495		tetrahedron O <sub>4</sub>
Cs6	4e	3m.	0	0	0.1125		non-coplanar triangle O <sub>3</sub>
O7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Ge <sub>2</sub>

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

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

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

References: [1] Pagnoux C., Verbaere A., Piffard Y., Tournoux M. (1993), Eur. J. Solid State Inorg. Chem. 30, 111-123.

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hP46

SrMg <sub>5.2</sub>	hP46	(194) $P6_3/mmc - kh^2gfe^2ba$
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**SrMg<sub>5.2</sub> [1]**

Structural features: Puckered triangle-mesh Mg<sub>11</sub>(Mg,□) layers and Sr<sub>3</sub>Mg<sub>3</sub>(Mg,□) layers (Sr<sub>3</sub> trigonal clusters) alternate along [001]; disordered atom arrangement along 0 0  $z$ .

Erassme J. et al. (1988) [1]

Mg<sub>5.25</sub>Sr

$a = 1.0463$ ,  $c = 1.0834$  nm,  $c/a = 1.035$ ,  $V = 1.0272$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	12k	.m.	0.1601	0.3202	0.5898		
Sr2	6h	mm2	0.1955	0.3910	$\frac{1}{4}$		
Mg3	6h	mm2	0.5682	0.1364	$\frac{1}{4}$		icosahedron Mg <sub>10</sub> Sr <sub>2</sub>
Mg4	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Mg <sub>8</sub> Sr <sub>4</sub>
Mg5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5065		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Mg6	4e	3m.	0	0	0.079	0.26	
Mg7	4e	3m.	0	0	0.158	0.21	
Mg8	2b	-6m2	0	0	$\frac{1}{4}$	0.386	
Mg9	2a	-3m.	0	0	0	0.410	

Experimental: single crystal, diffractometer, X-rays, R = 0.023, T = 293 K

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

References: [1] Erassme J., Brauers T., Lueken H. (1988), J. Less-Common Met. 137, 155-161.

$\text{Mn}_5(\text{Ga}_{0.1}\text{Ge}_{0.9})_3$	<i>hP48</i>	(194) $P6_3/mmc - ih^6$
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**Mn<sub>5</sub>(Ga,Ge)<sub>3</sub> [1]**

Structural features: Infinite columns of face-linked Mn<sub>6</sub> octahedra and infinite linear -Mn- chains parallel to [001]. Distorted variant of Mn<sub>5</sub>Si<sub>3</sub>.

Noga A.S. et al. (1991) [1]

$\text{Ga}_{0.30}\text{Ge}_{2.70}\text{Mn}_{4.87}$

$a = 1.2492$ ,  $c = 0.50437$  nm,  $c/a = 0.404$ ,  $V = 0.6816$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Mn1	12i	.2.	0.331	0	0		14-vertex polyhedron Mn <sub>8</sub> Ge <sub>6</sub>
Mn2	6h	mm2	0.075	0.15	1/4		15-vertex polyhedron Ge <sub>5</sub> Mn <sub>10</sub>
M3	6h	mm2	0.199	0.398	1/4		pseudo Frank-Kasper Mn <sub>9</sub> Ge <sub>2</sub>
Mn4	6h	mm2	0.416	0.832	1/4	0.87	15-vertex polyhedron Ge <sub>5</sub> Mn <sub>10</sub>
M5	6h	mm2	0.53	0.06	1/4		pseudo Frank-Kasper Mn <sub>9</sub> Ge <sub>2</sub>
Mn6	6h	mm2	0.748	0.496	1/4		15-vertex polyhedron Ge <sub>5</sub> Mn <sub>10</sub>
M7	6h	mm2	0.873	0.746	1/4		pseudo Frank-Kasper Mn <sub>9</sub> Ge <sub>2</sub>

M3 = 0.9Ge + 0.1Ga; M5 = 0.9Ge + 0.1Ga; M7 = 0.9Ge + 0.1Ga

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

Experimental: single crystal, diffractometer, X-rays, R = 0.030

Remarks: Homogeneity range Mn<sub>5</sub>Ga<sub>x</sub>Ge<sub>3-x</sub>, 0.3 < x < 1.2. A slightly different atom distribution is proposed in [2] (Mn<sub>5</sub>Ge<sub>3</sub>Ga<sub>2</sub>). In table I of [1] the *z*-coordinate of former Ge(1) is misprinted as 1/4 instead of 3/4 (from fig. 1), and the *x*-coordinate of former Mn(3) as 0.169 instead of 0.584 (see [2]; checked on interatomic distances) and the occupation of sites M as Ce<sub>0.9</sub>Ga<sub>0.1</sub> instead of Ge<sub>0.9</sub>Ga<sub>0.1</sub>. In [2] the *x*-coordinate of X3 is misprinted as identical to the *x*-coordinate of Mn1 instead of a value close to 1/4.

References: [1] Noga A.S., Sichevich O.M., Zavodnik V.E., Fundamenskii V.S., Grin Y.N. (1991), Sov. Phys. Crystallogr. 36, 490-492 (Kristallografiya 36, 876-879). [2] Noga A.S., Zavodnik V.E., Grin' Y.N. (1989), Vses. Konf. Kristallokhim. Internet. Soeden., 5th, L'vov 1989, Coll. Abstr. p. 48.

$\text{Sm}_5\text{Co}_{19}$	<i>hP48</i>	(194) $P6_3/mmc - k^2f^3edcba$
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**Sm<sub>5</sub>Co<sub>19</sub> [1]**

Structural features: Intergrowth of Laves- and CaCu<sub>5</sub>-type slabs (common Kagomé-mesh layers) in the ratio 1:3, consecutive Laves-type slabs in h stacking.

Khan Y. (1974) [1]

Co<sub>19</sub>Sm<sub>5</sub>

$a = 0.50312$ ,  $c = 3.2265$  nm,  $c/a = 6.413$ ,  $V = 0.7073$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	12k	.m.	0.16667	0.33333	0.0625		icosahedron Co <sub>7</sub> Sm <sub>5</sub>
Co2	12k	.m.	0.16667	0.33333	0.1875		cuboctahedron Co <sub>8</sub> Sm <sub>4</sub>
Co3	4f	3m.	1/3	2/3	0.125		anticuboctahedron Co <sub>9</sub> Sm <sub>3</sub>
Sm4	4f	3m.	1/3	2/3	0.52185		16-vertex Frank-Kasper Co <sub>12</sub> Sm <sub>4</sub>
Sm5	4f	3m.	1/3	2/3	0.625		pseudo Frank-Kasper Co <sub>18</sub> Sm <sub>2</sub>
Co6	4e	3m.	0	0	0.125		anticuboctahedron Co <sub>9</sub> Sm <sub>3</sub>
Sm7	2d	-6m2	1/3	2/3	3/4		sixcapped hexagonal prism Co <sub>18</sub>

Co8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	anticuboctahedron Co <sub>9</sub> Sm <sub>3</sub>
Co9	2b	-6m2	0	0	$\frac{1}{4}$	anticuboctahedron Co <sub>9</sub> Sm <sub>3</sub>
Co10	2a	-3m.	0	0	0	icosahedron Co <sub>6</sub> Sm <sub>6</sub>

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

Experimental: powder, film, X-rays

Remarks: We derived idealized coordinates from formulae in table 1 of [1] ( $m = 3$ ,  $p = 1$ ,  $q = 0$ ,  $\alpha = 2$ ,  $\beta = 1$ ,  $\gamma = 2$ ).

References: [1] Khan Y. (1974), Phys. Status Solidi A 23, 425-434.

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hP48

Ca <sub>5</sub> Ni <sub>15</sub> B <sub>4</sub>	hP48	(194) $P6_3/mmc - k^2f^3edcba$
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#### Ca<sub>5</sub>Ni<sub>15</sub>B<sub>4</sub> [1]

Structural features: BNi<sub>6</sub> trigonal prisms share edges to form infinite slabs; no B-B contact. Intergrowth of binary Laves-, binary and ternary CaCu<sub>5</sub>-type (CeCo<sub>3</sub>B<sub>2</sub>) slabs (common Kagomé-mesh layers) in the ratio 1:1:2, consecutive Laves-type slabs in h stacking. Ordering variant of Sm<sub>5</sub>Co<sub>19</sub>.

Jung W., Weltzer M. (1991) [1]

B<sub>4</sub>Ca<sub>5</sub>Ni<sub>15</sub>

$a = 0.5115$ ,  $c = 2.7946$  nm,  $c/a = 5.464$ ,  $V = 0.6332$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	12k	.m.	0.1642	0.3284	0.07812		pseudo Frank-Kasper B <sub>2</sub> Ni <sub>6</sub> Ca <sub>5</sub>
Ni2	12k	.m.	0.1675	0.335	0.17784		pseudo Frank-Kasper B <sub>2</sub> Ni <sub>7</sub> Ca <sub>4</sub>
B3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1263		trigonal prism Ni <sub>6</sub>
Ca4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5188		16-vertex Frank-Kasper Ni <sub>12</sub> Ca <sub>4</sub>
Ca5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6314		pseudo Frank-Kasper Ni <sub>12</sub> B <sub>6</sub> Ca <sub>2</sub>
B6	4e	3m.	0	0	0.1288		trigonal prism Ni <sub>6</sub>
Ca7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper Ni <sub>18</sub> Ca <sub>2</sub>
Ni8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Ni <sub>9</sub> Ca <sub>3</sub>
Ni9	2b	-6m2	0	0	$\frac{1}{4}$		cuboctahedron Ni <sub>9</sub> Ca <sub>3</sub>
Ni10	2a	-3m.	0	0	0		icosahedron Ni <sub>6</sub> Ca <sub>6</sub>

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

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

References: [1] Jung W., Weltzer M. (1991), Z. Kristallogr. 196, 169-178.

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hP48

Ba <sub>5</sub> Fe <sub>5</sub> O <sub>14</sub>	hP48	(194) $P6_3/mmc - k^2f^3edcba$
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#### BaFeO<sub>2.65</sub> [1], perovskite 10H

Structural features: Four close-packed BaO<sub>3</sub> layers in h stacking alternate with triangle-mesh BaO<sub>2</sub> layers along [001]; Fe in octahedral and tetrahedral voids. Units of three face-linked FeO<sub>6</sub> octahedra (linear Fe<sub>3</sub> chains) share vertices with units of two vertex-linked FeO<sub>4</sub> tetrahedra to form a 3D-framework; additional O in compressed Ba<sub>5</sub> trigonal bipyramids.

Gomez M.I. et al. (2001) [1]

Ba<sub>5</sub>Fe<sub>5</sub>O<sub>13.27</sub>

$a = 0.57794$ ,  $c = 2.46087$  nm,  $c/a = 4.258$ ,  $V = 0.7118$  nm<sup>3</sup>,  $Z = 2$



site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1475	0.2949	0.54559	0.878	non-colinear Fe <sub>2</sub>
O2	12k	.m.	0.1649	0.3298	0.14925		non-colinear Fe <sub>2</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.03936		anticuboctahedron O <sub>12</sub>
Fe4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.17816		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.62778		10-vertex polyhedron O <sub>10</sub>
Fe6	4e	3m.	0	0	0.10771		octahedron O <sub>6</sub>
O7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		8-vertex polyhedron Ba <sub>5</sub> O <sub>3</sub>
O8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Fe <sub>2</sub>
Ba9	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>
Fe10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays, synchrotron, R<sub>B</sub> = 0.067

References: [1] Gomez M.I., Lucotti G., De Moran J.A., Aymonino P.J., Pagola S., Stephens P., Carbonio R.E. (2001), J. Solid State Chem. 160, 17-24.

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Ba <sub>5</sub> Co <sub>5</sub> ClO <sub>13</sub>	hP48	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> f <sup>3</sup> edcba
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### Ba<sub>5</sub>Co<sub>5</sub>O<sub>13</sub>Cl [1]

Structural features: Four close-packed BaO<sub>3</sub> layers in h stacking alternate with triangle-mesh BaOCl layers along [001]; Co in octahedral and tetrahedral voids. Units of three face-linked CoO<sub>6</sub> octahedra (linear Co<sub>3</sub> chains) share vertices with units of two vertex-linked CoO<sub>4</sub> tetrahedra to form a 3D-framework; Cl in compressed Ba<sub>5</sub> trigonal bipyramids. Ordering variant of Ba<sub>5</sub>Fe<sub>5</sub>O<sub>14</sub>.

Yamaura K. et al. (2001) [1]

Ba<sub>5</sub>ClCo<sub>5</sub>O<sub>13</sub>

$a = 0.5698$ ,  $c = 2.4469$  nm,  $c/a = 4.294$ ,  $V = 0.6880$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.146	0.292	0.5508		non-colinear Co <sub>2</sub>
O2	12k	.m.	0.161	0.322	0.1496		non-colinear Co <sub>2</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.04003		9-vertex polyhedron O <sub>9</sub>
Co4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.17671		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.62896		10-vertex polyhedron O <sub>9</sub> Cl
Co6	4e	3m.	0	0	0.10286		octahedron O <sub>6</sub>
Cl7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Ba <sub>2</sub>
O8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Co <sub>2</sub>
Ba9	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>
Co10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: twinned crystal, diffractometer, X-rays, R = 0.022

Remarks: An independent refinement is reported in [2].

References: [1] Yamaura K., Young D.P., Siegrist T., Besnard C., Svensson C., Liu Y., Cava R.J. (2001), J. Solid State Chem. 158, 175-179. [2] Tancrét N., Roussel P., Abraham F. (2004), J. Solid State Chem. 177, 1023-1031.

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hP48

$\text{Ba}_5\text{Fe}_4\text{PtClO}_{12.5}$	<i>hP48</i>	(194) $P6_3/mmc - k^2f^3$ edcba
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**Ba<sub>10</sub>Fe<sub>8</sub>Pt<sub>2</sub>O<sub>25</sub>Cl<sub>2</sub> [1]**

Structural features: Four close-packed BaO<sub>3</sub> layers in h stacking alternate with triangle-mesh BaOCl layers along [001]; Fe in octahedral and tetrahedral, Pt in octahedral voids. Units of one PtO<sub>6</sub> and two FeO<sub>6</sub> octahedra sharing faces (linear Fe-Pt-Fe chains) share vertices with units of two vertex-linked FeO<sub>4</sub> tetrahedra to form a 3D-framework; Cl in Ba<sub>5</sub> compressed trigonal bipyramids. Ordering variant of Ba<sub>5</sub>Fe<sub>5</sub>O<sub>14</sub>.

Leib W., Müller Buschbaum H. (1987) [1]

 $\text{Ba}_5\text{ClFe}_4\text{O}_{12.50}\text{Pt}$  $a = 0.58034$ ,  $c = 2.4997$  nm,  $c/a = 4.307$ ,  $V = 0.7291$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.153	0.306	0.549		non-colinear PtFe
O2	12k	.m.	0.165	0.33	0.149		non-colinear Fe <sub>2</sub>
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.04		anticuboctahedron O <sub>12</sub>
Fe4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1785		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6277		10-vertex polyhedron O <sub>9</sub> Cl
Fe6	4e	3m.	0	0	0.109		octahedron O <sub>6</sub>
Cl7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Ba <sub>2</sub>
O8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.5	colinear Fe <sub>2</sub>
Ba9	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>
Pt10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

References: [1] Leib W., Müller Buschbaum H. (1987), Z. Anorg. Allg. Chem. 551, 7-12.

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hP48

$\text{Ba}_5\text{IrAl}_2\text{In}_2\text{ClO}_{13}$	<i>hP48</i>	(194) $P6_3/mmc - k^2f^3$ edcba
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**Ba<sub>5</sub>IrIn<sub>2</sub>Al<sub>2</sub>O<sub>13</sub>Cl [1]**

Structural features: Four close-packed BaO<sub>3</sub> layers in h stacking alternate with triangle-mesh BaOCl layers along [001]; Ir and In in octahedral, Al in tetrahedral voids. Units of one IrO<sub>6</sub> and two InO<sub>6</sub> octahedra sharing faces (linear In-Ir-In chains) share vertices with units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework; Cl in Ba<sub>5</sub> compressed trigonal bipyramids. Ordering variant of Ba<sub>5</sub>Fe<sub>5</sub>O<sub>14</sub>.

Neubacher M., Müller Buschbaum H. (1992) [1]

 $\text{Al}_2\text{Ba}_5\text{ClIn}_2\text{IrO}_{13}$  $a = 0.586$ ,  $c = 2.5101$  nm,  $c/a = 4.283$ ,  $V = 0.7465$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.155	0.31	0.549		non-colinear IrIn
O2	12k	.m.	0.172	0.344	0.1564		non-colinear AlIn
Ba3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0399		9-vertex polyhedron O <sub>9</sub>
Al4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1836		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.63		10-vertex polyhedron O <sub>9</sub> Cl
In6	4e	3m.	0	0	0.1124		octahedron O <sub>6</sub>

Cl7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	colinear Ba <sub>2</sub>
O8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	colinear Al <sub>2</sub>
Ba9	2b	-6m2	0	0	$\frac{1}{4}$	trigonal prism O <sub>6</sub>
Ir10	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

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

References: [1] Neubacher M., Müller Buschbaum H. (1992), J. Alloys Compd. 183, 18-23.

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hP48

(Li <sub>0.5</sub> W <sub>0.5</sub> ) <sub>2</sub> Ba <sub>5</sub> W <sub>2</sub> O <sub>15</sub>	hP48	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> hf <sup>3</sup> ed
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### Ba<sub>5</sub>W<sub>3</sub>LiO<sub>15</sub> [1]

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>4</sub> stacking; W and (Li,W) in octahedral voids leaving every fifth interlayer vacant. Infinite layers of vertex-linked WO<sub>6</sub> octahedra share vertices with units of two face-linked (Li,W)O<sub>6</sub> octahedra to form quadruple perovskite-type slabs.

Jendrek E.F. Jr. et al. (1975) [1]

Ba<sub>5</sub>LiO<sub>15</sub>W<sub>3</sub>

$a = 0.57614$ ,  $c = 2.3719$  nm,  $c/a = 4.117$ ,  $V = 0.6818$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.174	0.348	0.5538		single atom W
O2	12k	.m.	0.5061	0.0122	0.1479		non-colinear WLi
O3	6h	mm2	0.174	0.3479	$\frac{1}{4}$		non-colinear Li <sub>2</sub>
Ba4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0489		cuboctahedron O <sub>12</sub>
M5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2004		7-vertex polyhedron O <sub>6</sub> Li
W6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5969		octahedron O <sub>6</sub>
Ba7	4e	3m.	0	0	0.1529		cuboctahedron O <sub>12</sub>
Ba8	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>

M5 = 0.5Li + 0.5W

Experimental: single crystal, diffractometer, X-rays, wR = 0.060

Remarks: The authors state that the true composition may be Ba<sub>5</sub>W<sub>3.2</sub>Li<sub>0.8</sub>O<sub>15</sub> or Ba<sub>5</sub>W<sub>3</sub>LiO<sub>14.5</sub>. A similar model in space group (186) *P6<sub>3</sub>mc* with an ordered arrangement of W and Li was tested and rejected.

References: [1] Jendrek E.F. Jr., Potoff A.D., Katz L. (1975), J. Solid State Chem. 14, 165-171.

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hP48

Mg <sub>15.65</sub> Eu <sub>3</sub>	hP48	(194) <i>P6<sub>3</sub>/mmc</i> – kh <sup>2</sup> gfe <sup>3</sup> a
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### (Eu<sub>3</sub>Mg<sub>14</sub>)Mg<sub>1.65</sub> [1]

Structural features: Puckered triangle-mesh Mg<sub>11</sub>(Mg,□) layers and Eu<sub>3</sub>Mg<sub>3</sub>(Mg,□) layers (Eu<sub>3</sub> trigonal clusters) alternate along [001]; disordered atom arrangement along 0 0 z.

Mühlpfordt W. (1997) [1]

Eu<sub>3</sub>Mg<sub>15.65</sub>

$a = 1.043$ ,  $c = 1.078$  nm,  $c/a = 1.034$ ,  $V = 1.0156$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	12k	.m.	0.1599	0.3198	0.5892		

Eu2	6h	mm2	0.19501	0.39002	$\frac{1}{4}$	
Mg3	6h	mm2	0.5676	0.1352	$\frac{1}{4}$	icosahedron Mg <sub>10</sub> Eu <sub>2</sub>
Mg4	6g	.2/m.	$\frac{1}{2}$	0	0	icosahedron Mg <sub>8</sub> Eu <sub>4</sub>
Mg5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5026	icosahedron Mg <sub>9</sub> Eu <sub>3</sub>
Mg6	4e	3m.	0	0	0.064	0.15
Mg7	4e	3m.	0	0	0.123	0.12
Mg8	4e	3m.	0	0	0.22	0.39
Mg9	2a	-3m.	0	0	0	0.33

Experimental: single crystal, diffractometer, X-rays, R = 0.016, T = 295 K

Remarks: Homogeneity range (Eu<sub>3</sub>Mg<sub>14</sub>)Mg<sub>x</sub>, 1 < x < 1.7. Short interatomic distances for partly occupied site(s).

References: [1] Mühlpfordt W. (1997), Z. Anorg. Allg. Chem. 623, 985-989.

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hP48

Mg(Ag <sub>0.03</sub> Zn <sub>0.97</sub> ) <sub>2</sub>	hP48	(194) <i>P6<sub>3</sub>/mmc</i> – khgt <sup>4</sup> e <sup>2</sup>
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**Mg(Zn,Ag)<sub>2</sub> 8H** [1], Laves phase 8H

Structural features: Mg[Mg<sub>4</sub>(Zn,Ag)<sub>12</sub>] Friauf polyhedra share the hexagonal faces of the truncated tetrahedra to form a 3D-framework. (Zn,Ag)<sub>4</sub> tetrahedra share faces and vertices to form a 3D-framework. Kagomé-mesh (Zn,Ag)<sub>3</sub> layers and puckered triangle-mesh Mg<sub>2</sub>(Zn,Ag) layers alternate along [001]. Laves-type slabs in h<sub>3</sub>c stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Komura Y., Tokunaga K. (1980) [1]

Ag<sub>0.06</sub>MgZn<sub>1.94</sub>

a = 0.521, c = 3.44 nm, c/a = 6.603, V = 0.8087 nm<sup>3</sup>, Z = 16

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.16451	0.32902	0.12494		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M2	6h	mm2	0.50221	0.00442	$\frac{1}{4}$		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M3	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.06235		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.18738		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.57808		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67139		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg8	4e	3m.	0	0	0.04598		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg9	4e	3m.	0	0	0.20389		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>

M1 = 0.97Zn + 0.03Ag; M2 = 0.97Zn + 0.03Ag; M3 = 0.97Zn + 0.03Ag; M4 = 0.97Zn + 0.03Ag; M5 = 0.97Zn + 0.03Ag

Experimental: single crystal, diffractometer, X-rays, wR = 0.074

Remarks: We assigned an approximate value to the Zn/Ag ratio of sites M based on the nominal composition.

References: [1] Komura Y., Tokunaga K. (1980), Acta Crystallogr. B 36, 1548-1554.

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hP48

Ce(Mn <sub>0.75</sub> Al <sub>0.25</sub> ) <sub>2</sub> H <sub>0.09</sub>	hP48	(194) <i>P6<sub>3</sub>/mmc</i> – lkhfa
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**CeMn<sub>1.5</sub>Al<sub>0.5</sub>H<sub>0.09</sub>** [1]

Structural features: Filled-up derivative of  $\text{MgZn}_2$  with H in tetrahedral ( $\text{Ce}_2(\text{Mn},\text{Al})_2$ ) and trigonal ( $\text{Ce}(\text{Mn},\text{Al})_2$ ) voids.

Gross K.J. et al. (2000) [1]

$\text{Al}_{0.50}\text{CeD}_{0.08}\text{Mn}_{1.50}$

$a = 0.54448$ ,  $c = 0.88915$  nm,  $c/a = 1.633$ ,  $V = 0.2283$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	24l	1	0.19	0.4	0.016	0.006	
D2	12k	.m.	0.51	0.02	0.63	0.016	non-colinear D <sub>2</sub>
M3	6h	mm2	0.1644	0.3288	$\frac{1}{4}$		non-coplanar square D <sub>4</sub>
Ce4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5618		
M5	2a	-3m.	0	0	0		

$\text{M3} = 0.777\text{Mn} + 0.223\text{Al}$ ;  $\text{M5} = 0.669\text{Mn} + 0.331\text{Al}$

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

Experimental: powder, diffractometer, neutrons,  $R_p = 0.046$

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

References: [1] Gross K.J., Chartouni D., Fauth F. (2000), J. Alloys Compd. 306, 203-218.

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hP50

BaMnO <sub>3</sub>	hP50	(194) $P6_3/mmc - k^2hf^3eba$
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**BaMnO<sub>3</sub> 10H** [1], perovskite 10H

Structural features: Close-packed BaO<sub>3</sub> layers in h<sub>2</sub>chc stacking; Mn in octahedral voids. Units of three and two face-linked MnO<sub>6</sub> octahedra (linear Mn<sub>3</sub> chains and Mn<sub>2</sub> dumbbells) share vertices to form a 3D-framework.

Negas T., Roth R.S. (1971) [1]

BaMnO<sub>3</sub>

$a = 0.568$ ,  $c = 2.3373$  nm,  $c/a = 4.115$ ,  $V = 0.6530$  nm<sup>3</sup>,  $Z = 10$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.16667	0.33333	0.15		colinear Mn <sub>2</sub>
O2	12k	.m.	0.16667	0.33333	0.55		non-colinear Mn <sub>2</sub>
O3	6h	mm2	0.5	0.0	$\frac{1}{4}$		non-colinear Mn <sub>2</sub>
Ba4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05		anticuboctahedron O <sub>12</sub>
Mn5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2		7-vertex polyhedron O <sub>6</sub> Mn
Ba6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.65		cuboctahedron O <sub>12</sub>
Mn7	4e	3m.	0	0	0.1		7-vertex polyhedron O <sub>6</sub> Mn
Ba8	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Mn9	2a	-3m.	0	0	0		8-vertex polyhedron O <sub>6</sub> Mn <sub>2</sub>

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

Experimental: powder, diffractometer, X-rays

Remarks: Idealized chemical formula. Phase stable at  $1748 < T < 1823$  K in air, homogeneity range BaMnO<sub>3-x</sub>,  $0.175 < x < 0.20$ .

References: [1] Negas T., Roth R.S. (1971), J. Solid State Chem. 3, 323-339.

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hP50

$\text{Ba}_5\text{Fe}_4\text{NiO}_{13.5}$	<i>hP50</i>	(194) $P6_3/mmc - k^2hf^3eba$
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**Ba<sub>5</sub>Fe<sub>4</sub>NiO<sub>13.5</sub>** [1], perovskite 10H

Structural features: Close-packed BaO<sub>3</sub> layers in h<sub>2</sub>chc stacking; Fe and Ni in octahedral voids. Units of three and two face-linked TO<sub>6</sub> octahedra (linear Fe-Ni-Fe chains and Fe<sub>2</sub> dumbbells) share vertices to form a 3D-framework. Ordering variant of BaMnO<sub>3</sub> 10H.

Takizawa H., Steinfink H. (1996) [1]

 $\text{Ba}_5\text{Fe}_4\text{NiO}_{13.50}$  $a = 0.57713$ ,  $c = 2.45812$  nm,  $c/a = 4.259$ ,  $V = 0.7091$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.157	0.314	0.047	0.9	non-colinear NiFe
O2	12 <i>k</i>	. <i>m</i> .	0.1703	0.3406	0.6502	0.9	non-colinear Fe <sub>2</sub>
O3	6 <i>h</i>	<i>mm</i> 2	0.522	0.044	$\frac{1}{4}$	0.9	non-colinear Fe <sub>2</sub>
Ba4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.127		9-vertex polyhedron O <sub>9</sub>
Ba5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.538		anticuboctahedron O <sub>12</sub>
Fe6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6814		octahedron O <sub>6</sub>
Fe7	4 <i>e</i>	3 <i>m</i> .	0	0	0.1091		octahedron O <sub>6</sub>
Ba8	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Ni9	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, X-rays, R = 0.042

Remarks: Different models for an ordered arrangement of O vacancies were tested and rejected.

References: [1] Takizawa H., Steinfink H. (1996), J. Solid State Chem. 121, 133-137.

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hP50

$\text{Ba}_5\text{Zr}(\text{Al}_{0.5}\text{In}_{0.5})_4\text{O}_{13}$	<i>hP50</i>	(194) $P6_3/mmc - k^2hf^3eca$
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**Ba<sub>5</sub>ZrIn<sub>2</sub>Al<sub>2</sub>O<sub>13</sub>** [1]

Structural features: Four close-packed BaO<sub>3</sub> layers in c stacking alternate with hexagon-mesh BaO layers (split O site) along [001]; Zr and (In,Al) in octahedral, (Al,In) in tetrahedral voids. ZrO<sub>6</sub> and (In,Al)O<sub>6</sub> octahedra share vertices to form triple perovskite-type slabs, which are interconnected via units of two vertex-linked (Al,In)O<sub>4</sub> tetrahedra to form a 3D-framework. Variant of Ba<sub>5</sub>Er<sub>2</sub>ZrAl<sub>2</sub>O<sub>13</sub> with site splitting.

Shpanchenko R.V. et al. (1994) [1]

 $\text{Al}_2\text{Ba}_5\text{In}_2\text{O}_{13}\text{Zr}$  $a = 0.58707$ ,  $c = 2.4445$  nm,  $c/a = 4.164$ ,  $V = 0.7296$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.0484		non-colinear ZrIn
O2	12 <i>k</i>	. <i>m</i> .	0.503	0.006	0.1536		non-colinear AlIn
O3	6 <i>h</i>	<i>mm</i> 2	0.705	0.41	$\frac{1}{4}$	0.333	
M4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1032		octahedron O <sub>6</sub>
Ba5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5446		cuboctahedron O <sub>12</sub>
M6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.685		
Ba7	4 <i>e</i>	3 <i>m</i> .	0	0	0.1435		9-vertex polyhedron O <sub>9</sub>
Ba8	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O <sub>6</sub>

Zr9      2a   -3*m*.      0      0      0      octahedron O<sub>6</sub>

M4 = 0.85In + 0.15Al; M6 = 0.85Al + 0.15In

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

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

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

References: [1] Shpanchenko R.V., Abakumov A.M., Antipov E.V., Kovba L.M. (1994), J. Alloys Compd. 206, 185-188.

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hP50

Li(Li<sub>0.5</sub>W<sub>0.5</sub>)<sub>2</sub>Ba<sub>5</sub>W<sub>2</sub>O<sub>15</sub>

hP50

(194) *P*6<sub>3</sub>/*mmc* – k<sup>2</sup>hf<sup>3</sup>eda

**Ba<sub>5</sub>W<sub>3</sub>Li<sub>2</sub>O<sub>15</sub>** [1], perovskite 10H

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>4</sub> stacking; Li, (W,Li) and W in octahedral voids (minor substitution ignored). Triple layers of vertex-linked LiO<sub>6</sub> and WO<sub>6</sub> octahedra share vertices with units of two face-linked (W,Li)O<sub>6</sub> octahedra to form a 3D-framework.

Jacobson A.J. et al. (1974) [1]

Ba<sub>5</sub>Li<sub>1.99</sub>O<sub>15</sub>W<sub>3.01</sub>

*a* = 0.57559, *c* = 2.3719 nm, *c/a* = 4.121, *V* = 0.6805 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1754	0.3508	0.5545		non-colinear WLi
O2	12 <i>k</i>	. <i>m</i> .	0.5056	0.0112	0.1482		non-colinear W <sub>2</sub>
O3	6 <i>h</i>	<i>mm</i> 2	0.1774	0.3548	$\frac{1}{4}$		non-colinear W <sub>2</sub>
Ba4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0498		cuboctahedron O <sub>12</sub>
M5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.2037		7-vertex polyhedron O <sub>6</sub> W
M6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5957		octahedron O <sub>6</sub>
Ba7	4 <i>e</i>	3 <i>m</i> .	0	0	0.1552		cuboctahedron O <sub>12</sub>
Ba8	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>
M9	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M5 = 0.555W + 0.445Li; M6 = 0.94W + 0.06Li; M9 = 0.98Li + 0.02W

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.065

References: [1] Jacobson A.J., Collins B.M., Fender B.E.F. (1974), Acta Crystallogr. B 30, 816-819.

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hP50

Cs<sub>5</sub>Cd(Cd<sub>0.12</sub>Ni<sub>0.88</sub>)<sub>2</sub>Ni<sub>2</sub>F<sub>15</sub>

hP50

(194) *P*6<sub>3</sub>/*mmc* – k<sup>2</sup>hf<sup>3</sup>eda

**Cs<sub>4</sub>Ni<sub>3</sub>CdF<sub>12</sub> ht** [1], perovskite 10H; Cs<sub>5</sub>CaNi<sub>4</sub>F<sub>15</sub> [2]

Structural features: Close-packed CsF<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Cd, Ni and (Ni,Cd) in octahedral voids. Units of four face-linked NiF<sub>6</sub> and (Ni,Cd)F<sub>6</sub> octahedra (linear M-Ni-Ni-M chains) share vertices with CdF<sub>6</sub> octahedra to form a 3D-framework.

Dance J.M. et al. (1984) [1]

Cd<sub>1.25</sub>Cs<sub>5</sub>F<sub>15</sub>Ni<sub>3.75</sub>

*a* = 0.6238, *c* = 2.5362 nm, *c/a* = 4.066, *V* = 0.8547 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>k</i>	. <i>m</i> .	0.1728	0.3456	0.0497		non-colinear NiCd

F2	12k	.m.	0.5256	0.0512	0.6469	non-colinear Ni <sub>2</sub>
F3	6h	mm2	0.1931	0.3862	<sup>1</sup> / <sub>4</sub>	non-colinear Ni <sub>2</sub>
M4	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.08987	octahedron F <sub>6</sub>
Ni5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1973	octahedron F <sub>6</sub>
Cs6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5581	cuboctahedron F <sub>12</sub>
Cs7	4e	3m.	0	0	0.15556	anticuboctahedron F <sub>12</sub>
Cs8	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	anticuboctahedron F <sub>12</sub>
Cd9	2a	-3m.	0	0	0	octahedron F <sub>6</sub>

M4 = 0.875Ni + 0.125Cd

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Phase stable at T > 1123 K. A fully ordered structure is reported for Cs<sub>5</sub>CaNi<sub>4</sub>F<sub>15</sub> in [2].

References: [1] Dance J.M., Darriet J., Tressaud A., Hagenmuller P. (1984), Z. Anorg. Allg. Chem. 508, 93-99. [2] Tressaud A., Demortain G., Bouree Vigneron F., Darriet J. (1987), Rev. Chim. Miner. 24, 621-630.

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hP50

Sm[BrO <sub>3</sub> ] <sub>3</sub> [H <sub>2</sub> O] <sub>9</sub>	hP50	(194) P6 <sub>3</sub> /mmc – k <sup>2</sup> jh <sup>2</sup> d
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### Sm(BrO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O [1]

Structural features: :BrO<sub>3</sub> ψ-tetrahedra (two-fold orientational disorder) and Sm atoms in a Mg<sub>3</sub>Cd-type arrangement, embedded in a H<sub>2</sub>O matrix.

Sikka S.K. (1969) [1]

Br<sub>3</sub>H<sub>18</sub>O<sub>18</sub>Sm

a = 1.186, c = 0.676 nm, c/a = 0.570, V = 0.8235 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.0943	0.1886	0.0515	0.5	single atom Br
O2	12k	.m.	0.5788	0.1576	0.0023		single atom Sm
O3	12j	m..	0.068	0.361	<sup>1</sup> / <sub>4</sub>		single atom Br
Br4	6h	mm2	0.1313	0.2626	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O5	6h	mm2	0.7908	0.5816	<sup>1</sup> / <sub>4</sub>		single atom Sm
Sm6	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		tricapped trigonal prism O <sub>9</sub>
H7	24l	1	0.1292	0.5036	0.0636		
H8	12j	m..	0.3686	0.1188	<sup>1</sup> / <sub>4</sub>		

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, neutrons, R = 0.098

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the Wyckoff position of former O(W2) is misprinted as 12h instead of 6h.

References: [1] Sikka S.K. (1969), Acta Crystallogr. A 25, 621-626.

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hP50

Ba <sub>2</sub> [CN <sub>2</sub> ][CN] <sub>2</sub>	hP50	(194) P6 <sub>3</sub> /mmc – k <sup>3</sup> hgc
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Ba<sub>2</sub>(CN<sub>2</sub>)(CN)<sub>2</sub> [1]; Sr<sub>2</sub>(CN<sub>2</sub>)(CN)<sub>2</sub> [1]



Structural features: N=C=N linear units (perpendicular to [001]) and CN units (part parallel, part perpendicular to [001]) in partial substitutional disorder.

Berger U. et al. (1995) [1]

Ba<sub>2</sub>C<sub>3</sub>N<sub>4</sub>

$a = 1.0634$ ,  $c = 0.6989$  nm,  $c/a = 0.657$ ,  $V = 0.6844$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.1441	0.2882	0.1695		
M2	12 <i>k</i>	. <i>m</i> .	0.532	0.064	0.503	0.333	
N3	12 <i>k</i>	. <i>m</i> .	0.5649	0.1298	0.0394	0.667	
Ba4	6 <i>h</i>	<i>mm</i> 2	0.81063	0.62126	$\frac{1}{4}$		
C5	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0	0.667	
Ba6	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		

M1 = 0.5C + 0.5N; M2 = 0.5C + 0.5N

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.012$ ,  $T = 173$  K

Remarks: Short interatomic distances for partly occupied site(s). Ambiguous data: the authors state that the structure at 293 K was refined considering splitting of site N3, however, the  $y$ -coordinate is omitted and the value calculated from the interatomic distances corresponds within the standard uncertainty to Wyckoff position 12*k*. In table 2 of [1] the  $z$ -coordinate of former N(1) at 293 K is misprinted as 0.0348 instead of 0.0384 (checked on interatomic distances).

References: [1] Berger U., Milius W., Schnick W. (1995), *Z. Anorg. Allg. Chem.* 621, 2075-2082.

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*hP50*

Mg <sub>15.55</sub> Eu <sub>3</sub>	<i>hP50</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $kh^2gfe^3ba$
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(Eu<sub>3</sub>Mg<sub>14</sub>)Mg<sub>1.55</sub> [1]

Structural features: Puckered triangle-mesh Mg<sub>11</sub>(Mg,□) layers and Eu<sub>3</sub>Mg<sub>3</sub>(Mg,□) layers (Eu<sub>3</sub> trigonal clusters) alternate along [001]; disordered atom arrangement along 0 0  $z$ .

Mühlpfordt W. (1997) [1]

Eu<sub>3</sub>Mg<sub>15.55</sub>

$a = 1.043$ ,  $c = 1.078$  nm,  $c/a = 1.034$ ,  $V = 1.0156$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	12 <i>k</i>	. <i>m</i> .	0.1599	0.3198	0.5891		
Eu2	6 <i>h</i>	<i>mm</i> 2	0.19551	0.39102	$\frac{1}{4}$		
Mg3	6 <i>h</i>	<i>mm</i> 2	0.5677	0.1354	$\frac{1}{4}$		icosahedron Mg <sub>10</sub> Eu <sub>2</sub>
Mg4	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		icosahedron Mg <sub>8</sub> Eu <sub>4</sub>
Mg5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5021		icosahedron Mg <sub>9</sub> Eu <sub>3</sub>
Mg6	4 <i>e</i>	3 <i>m</i> .	0	0	0.062	0.2	
Mg7	4 <i>e</i>	3 <i>m</i> .	0	0	0.117	0.14	
Mg8	4 <i>e</i>	3 <i>m</i> .	0	0	0.199	0.18	
Mg9	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$	0.23	
Mg10	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.28	

Experimental: single crystal, diffractometer, X-rays,  $R = 0.021$ ,  $T = 295$  K

Remarks: Homogeneity range (Eu<sub>3</sub>Mg<sub>14</sub>)Mg <sub>$x$</sub> ,  $1 < x < 1.7$ . Short interatomic distances for partly occupied site(s).

References: [1] Mühlpfordt W. (1997), *Z. Anorg. Allg. Chem.* 623, 985-989.

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hP50

$\text{Cs}_4\text{Cu}[\text{MoO}_4]_3$	hP50	(194) $P6_3/mmc - \text{kj}^4\text{e}^2\text{b}$
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**Cs<sub>4</sub>Cu(MoO<sub>4</sub>)<sub>3</sub> [1]**

Structural features: MoO<sub>4</sub> tetrahedra and CuO<sub>5</sub> trigonal bipyramids share vertices to form infinite slabs; statistical occupation of two face-sharing tetrahedra in the central layer, accompanied by a slight rotation (split sites).

Solodovnikov S.F. et al. (1988) [1]

 $\text{Cs}_4\text{CuMo}_3\text{O}_{12}$  $a = 0.6286$ ,  $c = 2.3669$  nm,  $c/a = 3.765$ ,  $V = 0.8100$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1506	0.3012	0.5695		single atom Mo
O2	12j	m..	0.1051	0.3726	$\frac{1}{4}$	0.5	single atom O
Cs3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0312		10-vertex polyhedron O <sub>10</sub>
O4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1637	0.5	single atom Mo
Mo5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2327	0.5	
Cs6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6646		15-vertex polyhedron O <sub>15</sub>
Mo7	4e	3m.	0	0	0.0952		tetrahedron O <sub>4</sub>
O8	4e	3m.	0	0	0.1716		colinear MoCu
Cu9	2b	-6m2	0	0	$\frac{1}{4}$		colinear O <sub>2</sub>

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

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

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

References: [1] Solodovnikov S.F., Klevtsova R.F., Glinskaya L.A., Klevtsov P.V. (1988), Sov. Phys. Crystallogr. 33, 820-824 (Kristallografiya 33, 1380-1386).

194  
hP50

$\text{Y}_2\text{Fe}_{17}\text{N}_{1.7}$	hP50	(194) $P6_3/mmc - \text{kjhgfedcb}$
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**Y<sub>2</sub>Fe<sub>17</sub>N<sub>x</sub> [1]; Tb<sub>2</sub>Mn<sub>17</sub>C<sub>x</sub> [2]**

Structural features: Filled-up derivative of Th<sub>2</sub>Ni<sub>17</sub> with N in octahedral (Y<sub>2</sub>Fe<sub>4</sub>) voids; partial disorder Y/Fe<sub>2</sub> corresponding to CeMg<sub>10.3</sub>.

Yelon W.B., Hadjipanayis G.C. (1992) [1]

 $\text{Fe}_{16.98}\text{N}_{1.68}\text{Y}_{1.76}$  $a = 0.86622$ ,  $c = 0.84702$  nm,  $c/a = 0.978$ ,  $V = 0.5504$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12k	.m.	0.1682	0.3364	0.0112		single atom N
Fe2	12j	m..	0.3843	0.0435	$\frac{1}{4}$		single atom N
N3	6h	mm2	0.1708	0.3416	$\frac{1}{4}$	0.56	coplanar square Fe <sub>4</sub>
Fe4	6g	.2/m.	$\frac{1}{2}$	0	0		10-vertex polyhedron Fe <sub>10</sub>
Fe5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6101	0.71	
Fe6	4e	3m.	0	0	0.1184	0.28	
Y7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.35	
Y8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle N <sub>3</sub>
Y9	2b	-6m2	0	0	$\frac{1}{4}$	0.41	

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

Experimental: powder, diffractometer, neutrons

Remarks: Occupancies of the metal atom sites from a refinement on the same sample before nitrogen absorption. Short interatomic distances for partly occupied site(s); impossible short distances occur for published site occupancies.

References: [1] Yelon W.B., Hadjipanayis G.C. (1992), IEEE Trans. Magn. 28, 2316-2321. [2] Hu Z., Luo H., Yelon W.B., De Groot C.H., De Boer F.R., Buschow K.H.J. (1997), J. Alloys Compd. 248, 121-124.

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hP50

$(\text{Cu}_{0.5}\text{V}_{0.5})_2\text{ZrH}_4$	hP50	(194) $P6_3/mmc - 1h^2f^2ea$
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### ZrVCuH<sub>4</sub> [1]

Structural features: Filled-up derivative of  $\text{MgZn}_2$  with H in tetrahedral  $(\text{Zr}_2(\text{Cu,V})_2, \text{Zr}(\text{Cu,V})_3$  and  $(\text{Cu,V})_4$ ) voids.

Yartys' V.A. et al. (1983) [1]

$\text{CuD}_{3.98}\text{VZr}$

$a = 0.5468$ ,  $c = 0.894$  nm,  $c/a = 1.635$ ,  $V = 0.2315$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	24l	1	0.035	0.331	0.085	0.34	non-coplanar triangle D <sub>2</sub> Cu
M2	6h	mm2	0.148	0.296	$\frac{1}{4}$		non-colinear D <sub>2</sub>
D3	6h	mm2	0.528	0.056	$\frac{1}{4}$		non-colinear Cu <sub>2</sub>
D4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.15	0.17	8-vertex polyhedron D <sub>7</sub> Zr
Zr5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.55		single atom D
D6	4e	3m.	0	0	0.21	0.27	
M7	2a	-3m.	0	0	0		bicapped hexagonal prism D <sub>14</sub>

$\text{M2} = 0.5\text{Cu} + 0.5\text{V}$ ;  $\text{M7} = 0.5\text{Cu} + 0.5\text{V}$

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

Experimental: powder, diffractometer, neutrons,  $R = 0.164$

Remarks: The same data are also reported in [2]. In [3] the space group is misprinted as  $P6_3/mcm$  instead of  $P6_3/mmc$ .

References: [1] Yartys' V.A., Burnasheva V.V., Tsirkunova S.E., Kozlov E.N., Semenenko K.N. (1983), Latv. PSR Zinat. Akad. Vestis, Fiz. Teh. Zinat. Ser. 1983, 14-20. [2] Yartys' V.A., Burnasheva V.V., Semenenko K.N. (1984), Russ. J. Inorg. Chem. 29, 357-360 (Zh. Neorg. Khim. 29, 615-621). [3] (1988), Structure Reports 50A, 30.

194  
hP50

$\text{Ca}[\text{CO}_3]$	hP50	(194) $P6_3/mmc - 1j^2a$
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### CaCO<sub>3</sub> μ [1], vaterite

Structural features: Ca atoms and CO<sub>3</sub> trigonal units (parallel to [001], orientational disorder) in a NiAs-type arrangement.

Meyer H.J. (1969) [1]

$\text{CCaO}_{3.01}$

$a = 0.4127$ ,  $c = 0.8475$  nm,  $c/a = 2.054$ ,  $V = 0.1250$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.2917	0.6326	0.1096	0.167	
O2	12j	<i>m.</i>	0.0567	0.2401	$\frac{1}{4}$	0.167	
C3	12j	<i>m.</i>	0.2462	0.5522	$\frac{1}{4}$	0.167	
Ca4	2a	-3 <i>m.</i>	0	0	0		

Experimental: single crystal, Weissenberg and rotation photographs, X-rays,  $R = 0.115$

Remarks: Short interatomic distances for partly occupied site(s). Average structure; additional reflections could be indexed with a 6-fold supercell (new axes  $2a+b, -a+b, 2c$ ). The data in [1] refer to a non-conventional setting with this large cell, however, no deviation from the subcell symmetry is proposed. A similar model with part of Ca in Wyckoff position 12*k* is also reported. Preliminary data in [2].

References: [1] Meyer H.J. (1969), Z. Kristallogr. 128, 183-212. [2] Meyer H.J. (1965), Z. Kristallogr. 121, 220-242.

194  
hP52

Ho <sub>2.18</sub> Co <sub>15.56</sub>	hP52	(194) $P6_3/mmc - k^2jgfdcb$
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### Ho<sub>2</sub>Co<sub>17</sub> [1]

Structural features: Kagomé-mesh Co<sub>9</sub> layers (site splitting) and Ho<sub>2</sub>(Co<sub>2</sub>)Co<sub>6</sub> layers (a Co hexagon mesh, the hexagons of which are centered by a Ho atom or a Co<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder).

Christensen A.N., Hazell R.G. (1980) [1]

Co<sub>15.56</sub>Ho<sub>2.18</sub>

$a = 0.8322$ ,  $c = 0.8113$  nm,  $c/a = 0.975$ ,  $V = 0.4866$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Co1	12 <i>k</i>	<i>m.</i>	0.165	0.33	0.032	0.18	
Co2	12 <i>k</i>	<i>m.</i>	0.165	0.33	0.532	0.82	
Co3	12 <i>j</i>	<i>m.</i>	0.044	0.374	$\frac{1}{4}$	0.82	
Co4	6 <i>g</i>	.2/ <i>m.</i>	$\frac{1}{2}$	0	0		
Co5	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.101	0.82	
Ho6	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		
Ho7	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.18	
Ho8	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		

Experimental: single crystal, diffractometer, neutrons,  $R = 0.058$ ,  $T = 300$  K

Remarks: Refinement of the occupancy of site Ho8 showed no significant deviation from unity. Short interatomic distances for partly occupied site(s).

References: [1] Christensen A.N., Hazell R.G. (1980), Acta Chem. Scand. A 34, 455-459.

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hP52

Ba <sub>4.5</sub> Nb <sub>2</sub> S <sub>10.5</sub>	hP52	(194) $P6_3/mmc - k^3hfcd$
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### Ba<sub>9</sub>Nb<sub>4</sub>S<sub>21</sub> [1]

Structural features: Three close-packed BaS<sub>3</sub> layers in h stacking alternate with triangle-mesh Ba<sub>2-x</sub>(S<sub>2</sub>)<sub>1-y</sub> layers (split sites, S<sub>2</sub> dumbbells perpendicular to [001]) along [001]. Units of two face-sharing NbS<sub>6</sub> octahedra (Nb<sub>2</sub> dumbbells).

Saeki M., Onoda M. (1991) [1]

$\text{Ba}_{4.50}\text{Nb}_2\text{S}_{10.50}$

$a = 0.69743$ ,  $c = 2.1599$  nm,  $c/a = 3.097$ ,  $V = 0.9098$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
S1	12 <i>k</i>	. <i>m</i> .	0.078	0.156	0.002	0.25	single atom Nb
S2	12 <i>k</i>	. <i>m</i> .	0.506	0.012	0.62		
Ba3	12 <i>k</i>	. <i>m</i> .	0.633	0.266	0.007	0.25	
S4	6 <i>h</i>	<i>mm</i> 2	0.159	0.318	$\frac{1}{4}$		non-colinear Nb <sub>2</sub> octahedron S <sub>6</sub>
Nb5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1686		
Ba6	4 <i>e</i>	3 <i>m</i> .	0	0	0.1363		anticuboctahedron S <sub>12</sub>
Ba7	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		

Experimental: powder, diffractometer, X-rays,  $R_B = 0.091$

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

References: [1] Saeki M., Onoda M. (1991), Bull. Chem. Soc. Jpn. 64, 2923-2925.

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*hP*52

$\text{SiO}_2$	<i>hP</i> 52	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – <i>ljif</i>
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**SiO<sub>2</sub> tridymite ht** [1], tridymite high

Structural features: SiO<sub>4</sub> tetrahedra share vertices to form a 3D-framework with large channels (6-membered rings; O in partial rotational disorder around the axes defined by the Si atoms).

Kihara K. (1978) [1]

O<sub>2</sub>Si

$a = 0.5052$ ,  $c = 0.827$  nm,  $c/a = 1.637$ ,  $V = 0.1828$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24 <i>l</i>	1	0.474	0.037	0.04	0.167	
O2	12 <i>j</i>	<i>m</i> ..	0.258	0.587	$\frac{1}{4}$	0.167	
O3	12 <i>i</i>	.2.	0.408	0	0	0.167	
Si4	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0624		

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.051$ ,  $T = 733$  K

Remarks: Phase stable at  $T > 693$  K. Short interatomic distances for partly occupied site(s). A similar model without site splitting gave slightly less good reliability factors ( $R = 0.067$ ). Space group (182) *P*6<sub>3</sub>22 was tested and rejected.

References: [1] Kihara K. (1978), Z. Kristallogr. 148, 237-253.

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*hP*54

$\text{V}_4\text{Al}_{23}$	<i>hP</i> 54	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – <i>k</i> <sup>3</sup> <i>h</i> <sup>2</sup> <i>fa</i>
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**V<sub>4</sub>Al<sub>23</sub>** [2]

Structural features: VAl<sub>12</sub> icosahedra and V<sub>3</sub>Al<sub>20</sub> units (V<sub>3</sub> trigonal cluster, each V inside a truncated (Al<sub>10</sub>□<sub>2</sub>) icosahedron) share vertices to form a 3D-framework.

Ray A.E., Smith J.F. (1960) [1]

Al<sub>23</sub>V<sub>4</sub>

$a = 0.7692$ ,  $c = 1.704$  nm,  $c/a = 2.215$ ,  $V = 0.8731$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.1261	0.2522	0.1164		12-vertex polyhedron V <sub>2</sub> Al <sub>10</sub>
Al2	12k	.m.	0.2112	0.4224	0.5295		11-vertex polyhedron Al <sub>10</sub> V
Al3	12k	.m.	0.5417	0.0834	0.1663		12-vertex polyhedron V <sub>2</sub> Al <sub>10</sub>
V4	6h	mm2	0.2177	0.4354	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>10</sub> V <sub>2</sub>
Al5	6h	mm2	0.8748	0.7496	<sup>1</sup> / <sub>4</sub>		12-vertex polyhedron V <sub>2</sub> Al <sub>10</sub>
Al6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1162		icosahedron V <sub>3</sub> Al <sub>9</sub>
V7	2a	-3m.	0	0	0		icosahedron Al <sub>12</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Cell parameters from [2]. Electron density study.

References: [1] Ray A.E., Smith J.F. (1960), Acta Crystallogr. 13, 876-884. [2] Smith J.F., Ray A.E. (1957), Acta Crystallogr. 10, 169-172.

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hP54

Zr(Mn <sub>0.8</sub> Ni <sub>0.2</sub> ) <sub>2</sub> H <sub>2.85</sub>	hP54	(194) P6 <sub>3</sub> /mmc – lkh <sup>2</sup> fa
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**ZrMn<sub>1.6</sub>Ni<sub>0.4</sub>H<sub>2.85</sub>** [1]; Zr(Cr<sub>0.6</sub>Ni<sub>0.4</sub>)<sub>2</sub>H<sub>3.3</sub> [2]

Structural features: Filled-up derivative of MgZn<sub>2</sub> with H in tetrahedral (Zr<sub>2</sub>(Mn,Ni)<sub>2</sub>) voids.

Soubeyroux J.L. et al. (1993) [1]

D<sub>2.85</sub>Mn<sub>1.66</sub>Ni<sub>0.34</sub>Zr

a = 0.5371, c = 0.8729 nm, c/a = 1.625, V = 0.2181 nm<sup>3</sup>, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	24l	1	0.058	0.345	0.073	0.203	non-coplanar triangle D <sub>3</sub>
D2	12k	.m.	0.539	0.078	0.627	0.343	non-coplanar triangle D <sub>3</sub>
M3	6h	mm2	0.174	0.348	<sup>1</sup> / <sub>4</sub>		10-vertex polyhedron D <sub>10</sub>
D4	6h	mm2	0.55	0.1	<sup>1</sup> / <sub>4</sub>	0.4	non-colinear D <sub>2</sub>
Zr5	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.558		21-vertex polyhedron D <sub>21</sub>
M6	2a	-3m.	0	0	0		hexagonal prism D <sub>12</sub>

M3 = 0.812Mn + 0.188Ni; M6 = 0.88Mn + 0.12Ni

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.011, T = 30 K

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

References: [1] Soubeyroux J.L., Pontonnier L., Miraglia S., Isnard O., Fruchart D., Akiba E., Hayakawa H., Fujitani S., Yonezu I. (1993), Z. Phys. Chem. 179, 187-198. [2] Bououdina M., Soubeyroux J.L., Fruchart D., De Rango P. (1997), J. Alloys Compd. 257, 82-90.

194  
hP56

KCu <sub>7</sub> Cd[SeO <sub>3</sub> ] <sub>2</sub> Cl <sub>9</sub> O <sub>2</sub>	hP56	(194) P6 <sub>3</sub> /mmc – k <sup>3</sup> hf <sup>2</sup> cba
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**KCdCu<sub>7</sub>O<sub>2</sub>(SeO<sub>3</sub>)<sub>2</sub>Cl<sub>9</sub>** [1], burnsite

Structural features: Single CdCl<sub>6</sub> octahedra, :SeO<sub>3</sub> ψ-tetrahedra and units of two vertex-linked OCu<sub>4</sub> tetrahedra (parallel to [001]); K and additional Cl between the units.

Burns P.C. et al. (2002) [1]

 $\text{CdCl}_9\text{Cu}_7\text{KOs}_8\text{Se}_2$  $a = 0.87805$ ,  $c = 1.5521$  nm,  $c/a = 1.768$ ,  $V = 1.0363$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12k	.m.	0.13697	0.27394	0.10178		non-coplanar triangle Cu <sub>2</sub> Cd
Cu2	12k	.m.	0.54736	0.09472	0.59057		octahedron O <sub>3</sub> Cl <sub>3</sub>
O3	12k	.m.	0.5696	0.1392	0.0447		coplanar triangle SeCu <sub>2</sub>
Cl4	6h	mm2	0.4945	0.989	$\frac{1}{4}$		non-coplanar triangle Cu <sub>3</sub>
O5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1267		tetrahedron Cu <sub>4</sub>
Se6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5973		non-coplanar triangle O <sub>3</sub>
Cu7	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear O <sub>2</sub>
K8	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism Cl <sub>6</sub>
Cd9	2a	-3m.	0	0	0		octahedron Cl <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.019

Remarks: Natural specimen from the Tolbachik volcano, Kamchatka, Russia. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Burns P.C., Cooper M.A., Hawthorne F.C. (2002), Can. Mineral. 40, 1587-1595.

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hP56

$\text{Ba}_5\text{Ru}_2\text{O}_9[\text{O}_2]$	hP56	(194) $P6_3/mmc - k^3hf^2ec$
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**Ba<sub>5</sub>Ru<sub>2</sub>O<sub>9</sub>(O<sub>2</sub>)** [1]Structural features: Double perovskite-type slabs (three close-packed BaO<sub>3</sub> layers, Ru in octahedral voids) alternate with triangle-mesh Ba<sub>2</sub>(O<sub>2</sub>) layers along [001] (O<sub>2</sub> dumbbells perpendicular to [001], 3-fold rotational disorder; splitting of the Ba site). Units of two face-linked RuO<sub>6</sub> octahedra (Ru<sub>2</sub> dumbbells).

Grasset F. et al. (1997) [1]

 $\text{Ba}_{4.90}\text{O}_{10.80}\text{Ru}_2$  $a = 0.5947$ ,  $c = 1.8043$  nm,  $c/a = 3.034$ ,  $V = 0.5526$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.0677	0.1354	0.0037	0.3	
Ba2	12k	.m.	0.3611	0.7222	0.015	0.13	
O3	12k	.m.	0.5116	0.0232	0.1181		single atom Ru
O4	6h	mm2	0.8168	0.6336	$\frac{1}{4}$		non-coplanar Ru <sub>2</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0155	0.56	
Ru6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6738		octahedron O <sub>6</sub>
Ba7	4e	3m.	0	0	0.1392		
Ba8	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.027

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

References: [1] Grasset F., Dussarrat C., Darriet J. (1997), J. Mater. Chem. 7, 1911-1915.

194  
hP56

$\text{Ba}(\text{Tl}_{0.2}\text{Pb}_{0.8})_3$	hP56	(194) $P6_3/mmc - k^3hf^2ed$
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**Ba(Pb<sub>0.8</sub>Tl<sub>0.2</sub>)<sub>3</sub>** [1]

Structural features: Close-packed Ba(Pb,Tl)<sub>3</sub> layers (Ba forms a triangle mesh) in h<sub>3</sub>ch<sub>2</sub>c stacking.

Havinga E.E., Van Vucht J.H.N. (1970) [1]

BaPb<sub>2.40</sub>Tl<sub>0.60</sub>

$a = 0.7342$ ,  $c = 3.945$  nm,  $c/a = 5.373$ ,  $V = 1.8417$  nm<sup>3</sup>,  $Z = 14$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.152	0.304	0.53571		anticuboctahedron Pb <sub>8</sub> Ba <sub>4</sub>
M2	12 <i>k</i>	. <i>m</i> .	0.16667	0.33333	0.10714		cuboctahedron Pb <sub>8</sub> Ba <sub>4</sub>
M3	12 <i>k</i>	. <i>m</i> .	0.515	0.03	0.67857		anticuboctahedron Pb <sub>8</sub> Ba <sub>4</sub>
M4	6 <i>h</i>	<i>mm</i> 2	0.182	0.364	<sup>1</sup> / <sub>4</sub>		anticuboctahedron Pb <sub>8</sub> Ba <sub>4</sub>
Ba5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.034		anticuboctahedron Pb <sub>12</sub>
Ba6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.60714		cuboctahedron Pb <sub>12</sub>
Ba7	4 <i>e</i>	3 <i>m</i> .	0	0	0.181		anticuboctahedron Pb <sub>12</sub>
Ba8	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		anticuboctahedron Pb <sub>12</sub>

M1 = 0.8Pb + 0.2Tl; M2 = 0.8Pb + 0.2Tl; M3 = 0.8Pb + 0.2Tl; M4 = 0.8Pb + 0.2Tl

Experimental: powder, diffractometer, X-rays,  $R_B = 0.180$

Remarks: Idealized coordinates.

References: [1] Havinga E.E., Van Vucht J.H.N. (1970), Acta Crystallogr. B 26, 653-655.

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hP56

Y <sub>2</sub> Fe <sub>17</sub>	hP56	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kj <sup>2</sup> gfedcb
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**Y<sub>2</sub>Fe<sub>17</sub>** [1]

Structural features: Kagomé-mesh Fe<sub>9</sub> layers and Y<sub>2</sub>(Fe<sub>2</sub>)Fe<sub>6</sub> layers (a Fe hexagon mesh, the hexagons of which are centered by an Y atom or a Fe<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder). Variant of Th<sub>2</sub>Ni<sub>17</sub> with a partly disordered arrangement of Y atoms and Fe<sub>2</sub> dumbbells.

Moze O. et al. (1994) [1]

Fe<sub>17.06</sub>Y<sub>1.97</sub>

$a = 0.8462$ ,  $c = 0.829$  nm,  $c/a = 0.980$ ,  $V = 0.5141$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	12 <i>k</i>	. <i>m</i> .	0.169	0.338	0.013		
Fe2	12 <i>j</i>	<i>m</i> ..	0.047	0.374	<sup>1</sup> / <sub>4</sub>	0.71	
Fe3	12 <i>j</i>	<i>m</i> ..	0.297	0.001	<sup>1</sup> / <sub>4</sub>	0.29	
Fe4	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		
Fe5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.105	0.8	
Fe6	4 <i>e</i>	3 <i>m</i> .	0	0	0.097	0.23	
Y7	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		
Y8	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.2	
Y9	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.77	

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

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

References: [1] Moze O., Caciuffo R., Gillon B., Calestani G., Kayzel F.E., Franse J.J.M. (1994), Phys. Rev. B: Condens. Matter 50, 9293-9299.



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hP56

$\text{U}_2\text{Fe}_2(\text{Fe}_{0.75}\text{Si}_{0.25})_{15}$	<i>hP56</i>	(194) <i>P6<sub>3</sub>/mmc</i> – kj <sup>2</sup> gfedcb
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**U<sub>2</sub>Fe<sub>13.3</sub>Si<sub>3.7</sub> [1]**

Structural features: Kagomé-mesh (Fe,Si)<sub>9</sub> layers and U<sub>2</sub>(Fe<sub>2</sub>)(Fe,Si)<sub>6</sub> layers (a (Fe,Si) hexagon mesh, the hexagons of which are centered by a U atom or a Fe<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder). Ordering variant of Y<sub>2</sub>Fe<sub>17</sub>.

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

Fe<sub>13.29</sub>Si<sub>3.71</sub>U<sub>2</sub>

$a = 0.8352$ ,  $c = 0.8218$  nm,  $c/a = 0.984$ ,  $V = 0.4965$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	. <i>m</i> .	0.1603	0.3206	0.0174		
Fe2	12 <i>j</i>	<i>m</i> ..	0.008	0.304	<sup>1</sup> / <sub>4</sub>	0.167	
M3	12 <i>j</i>	<i>m</i> ..	0.3627	0.0377	<sup>1</sup> / <sub>4</sub>	0.833	
M4	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		
Fe5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.601	0.833	
Fe6	4 <i>e</i>	3 <i>m</i> .	0	0	0.101	0.167	
U7	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.167	
U8	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		
U9	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.833	

M1 = 0.83Fe + 0.17Si; M3 = 0.66Fe + 0.34Si; M4 = 0.67Fe + 0.33Si

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.066

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

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

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hP56

$\text{Er}_2\text{Fe}_{17}\text{N}_{4.5}$	<i>hP56</i>	(194) <i>P6<sub>3</sub>/mmc</i> – kjihgfc <b>b</b>
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**Er<sub>2</sub>Fe<sub>17</sub>N<sub>4.5</sub> [1]**

Structural features: Filled-up derivative of Th<sub>2</sub>Ni<sub>17</sub> with N in octahedral (Er<sub>2</sub>Fe<sub>4</sub>) and tetrahedral (Er<sub>2</sub>Fe<sub>2</sub>) voids.

Yan Q.W. et al. (1995) [1]

Er<sub>2</sub>Fe<sub>17</sub>N<sub>4.44</sub>

$a = 0.865$ ,  $c = 0.8529$  nm,  $c/a = 0.986$ ,  $V = 0.5527$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	12 <i>k</i>	. <i>m</i> .	0.1702	0.3404	0.0184		non-coplanar triangle N <sub>3</sub>
Fe2	12 <i>j</i>	<i>m</i> ..	0.37963	0.0463	<sup>1</sup> / <sub>4</sub>		single atom N
N3	12 <i>i</i>	.2.	0.1303	0	0	0.33	non-colinear N <sub>2</sub>
N4	6 <i>h</i>	<i>mm</i> 2	0.1657	0.3315	<sup>1</sup> / <sub>4</sub>	0.82	coplanar square Fe <sub>4</sub>
Fe5	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		10-vertex polyhedron Fe <sub>10</sub>
Fe6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6049		14-vertex Frank-Kasper Fe <sub>13</sub> Er
Er7	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle N <sub>3</sub>
Er8	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		

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

Experimental: powder, diffractometer, neutrons,  $R = 0.030$

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

References: [1] Yan Q.W., Zhang P.L., Wei Y.N., Sun K., Hu B.P., Wang Y.Z., Liu G.C., Gou C., Chen D.F. (1995), J. Alloys Compd. 222, 141-142.

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hP56

$\text{Na}_3\text{La}_2[\text{CO}_3]_4\text{F}$	hP56	(194) $P6_3/mmc - 1k^3\text{edb}$
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### $\text{Na}_3\text{La}_2(\text{CO}_3)_4\text{F}$ [1]

Structural features:  $\text{CO}_3$  trigonal units arranged in approximately planar layers where C forms a triangle mesh (ABBAACCA stacking, splitting of the O site).  $\text{La}(\text{O}_9\text{F})$  polyhedra (an  $\text{O}_{12}$  anticuboctahedron with one triangle replaced by a single F) share vertices to form infinite slabs; C in trigonal, Na in trigonal prismatic voids in the slabs and between the slabs.

Mercier N. et al. (1993) [1]

$\text{C}_4\text{FLa}_2\text{Na}_3\text{O}_{12}$

$a = 0.5083$ ,  $c = 2.3034$  nm,  $c/a = 4.532$ ,  $V = 0.5154$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.286	0.096	0.062	0.5	single atom C
O2	12k	.m.	0.1883	0.3766	0.1761		
Na3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0221		
C4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1768		non-coplanar triangle $\text{O}_3$
La5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6454		
C6	4e	3m.	0	0	0.0632		colinear $\text{La}_2$ trigonal prism $\text{O}_6$
F7	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		
Na8	2b	-6m2	0	0	$\frac{1}{4}$		

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

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

Remarks: Short interatomic distances for partly occupied site(s). Space group (190)  $P-62c$  was tested and rejected.

References: [1] Mercier N., Taulelle F., Leblanc M. (1993), Eur. J. Solid State Inorg. Chem. 30, 609-617.

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hP58

$\text{Ba}_6\text{Co}_6\text{O}_{15.6}$	hP58	(194) $P6_3/mmc - k^2hf^4e^2da$
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### $\text{BaCoO}_{2.6}$ 12H [1]

Structural features: Five close-packed  $\text{BaO}_3$  layers ( $\text{ch}_3\text{c}$  stacking) and triangle-mesh  $\text{BaO}_2$  layers alternate along [001]; Co in octahedral and tetrahedral voids. Units of four face-linked  $\text{CoO}_6$  octahedra (linear  $\text{Co}_4$  chains) are interconnected via  $\text{CoO}_4$  tetrahedra to form infinite slabs.

Jacobson A.J., Hutchison J.L. (1980) [1]

$\text{Ba}_6\text{Co}_6\text{O}_{15.92}$

$a = 0.5671$ ,  $c = 2.8545$  nm,  $c/a = 5.034$ ,  $V = 0.7950$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1428	0.2856	0.6663	0.92	non-colinear $\text{Co}_2$
O2	12k	.m.	0.1647	0.3294	0.0811	0.94	non-colinear $\text{Co}_2$

O3	6h	mm2	0.1513	0.3026	$\frac{1}{4}$	0.88	non-colinear Co <sub>2</sub>
Co4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0581		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1758		9-vertex polyhedron O <sub>9</sub>
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5042		single atom Co
Ba7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.595		10-vertex polyhedron O <sub>10</sub>
Co8	4e	3m.	0	0	0.1226		octahedron O <sub>6</sub>
Co9	4e	3m.	0	0	0.2072		octahedron O <sub>6</sub>
Ba10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>
Ba11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons, wR = 0.104, T = 4.2 K

References: [1] Jacobson A.J., Hutchison J.L. (1980), J. Solid State Chem. 35, 334-340.

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hP58

Ba <sub>6</sub> Nd <sub>2</sub> Ti <sub>4</sub> O <sub>17</sub>	hP58	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> hf <sup>5</sup> eba
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#### Ba<sub>6</sub>Nd<sub>2</sub>Ti<sub>4</sub>O<sub>17</sub> [1]

Structural features: Five close-packed BaO<sub>3</sub> layers (c<sub>2</sub>hc<sub>2</sub> stacking) and triangle-mesh BaO<sub>2</sub> layers alternate along [001]; Nd in octahedral, Ti in octahedral and tetrahedral voids. Units of two face-linked TiO<sub>6</sub> octahedra (Ti<sub>2</sub> dumbbells) share vertices with NdO<sub>6</sub> octahedra and TiO<sub>4</sub> tetrahedra to form infinite slabs.

Kuang X. et al. (2002) [1]

Ba<sub>6</sub>Nd<sub>2</sub>O<sub>17</sub>Ti<sub>4</sub>

$a = 0.59928$ ,  $c = 2.99289$  nm,  $c/a = 4.994$ ,  $V = 0.9309$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1705	0.341	0.0754		non-colinear TiNd
O2	12k	.m.	0.1782	0.3564	0.66999		non-colinear TiNd
O3	6h	mm2	0.522	0.044	$\frac{1}{4}$		non-colinear Ti <sub>2</sub>
Ti4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0527		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.18529		9-vertex polyhedron O <sub>9</sub>
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5039		single atom Ti
Ba7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.58775		10-vertex polyhedron O <sub>10</sub>
Ti8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7051		octahedron O <sub>6</sub>
Nd9	4e	3m.	0	0	0.12641		octahedron O <sub>6</sub>
Ba10	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Ba11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons, time-of-flight, R<sub>p</sub> = 0.064

Remarks: In table 1 of [1] the Wyckoff positions of former Nd and Ba(3) are misprinted as 4f and 4e, instead of 4e and 4f.

References: [1] Kuang X., Jing X., Loong C.K., Lachowski E.E., Skakle J.M.S., West A.R. (2002), Chem. Mater. 14, 4359-4363.

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hP58

Na <sub>2</sub> Ba <sub>6</sub> V <sub>2</sub> Ru <sub>2</sub> O <sub>17</sub>	hP58	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2</sup> hf <sup>5</sup> eba
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#### Ba<sub>6</sub>Ru<sub>2</sub>Na<sub>2</sub>V<sub>2</sub>O<sub>17</sub> [1]

Structural features: Five close-packed BaO<sub>3</sub> layers (c<sub>2</sub>hc<sub>2</sub> stacking) and triangle-mesh BaO<sub>2</sub> layers alternate along [001]; Ru and Na in octahedral, V in tetrahedral voids. Units of two face-linked RuO<sub>6</sub> octahedra (Ru<sub>2</sub> dumbbells) share vertices with NaO<sub>6</sub> octahedra and VO<sub>4</sub> tetrahedra to form infinite slabs. Ordering variant of Ba<sub>6</sub>Nd<sub>2</sub>Ti<sub>4</sub>O<sub>17</sub>.

Quarez E. et al. (2003) [1]

Ba<sub>6</sub>Na<sub>2</sub>O<sub>17</sub>Ru<sub>2</sub>V<sub>2</sub>

$a = 0.58506$ ,  $c = 2.96241$  nm,  $c/a = 5.063$ ,  $V = 0.8782$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.177	0.354	0.0732		single atom V
O2	12k	.m.	0.1773	0.355	0.6703		non-collinear RuNa
O3	6h	mm2	0.512	0.024	$\frac{1}{4}$		non-collinear Ru <sub>2</sub>
V4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05247		tetrahedron O <sub>4</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.17907		9-vertex polyhedron O <sub>9</sub>
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5054		single atom V
Ba7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.59261		10-vertex polyhedron O <sub>10</sub>
Ru8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.70468		octahedron O <sub>6</sub>
Na9	4e	3m.	0	0	0.1245		octahedron O <sub>6</sub>
Ba10	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Ba11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

References: [1] Quarez E., Abraham F., Mentré O. (2003), J. Solid State Chem. 176, 137-150.

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hP58

NaAl <sub>11</sub> O <sub>17</sub>	hP58	(194) $P6_3/mmc - k^3f^3edca$
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NaAl<sub>11</sub>O<sub>17</sub> [2], diaoyudaoite,  $\beta$  alumina-Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and NaO layers (Na at BR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework. See Fig. III.44.

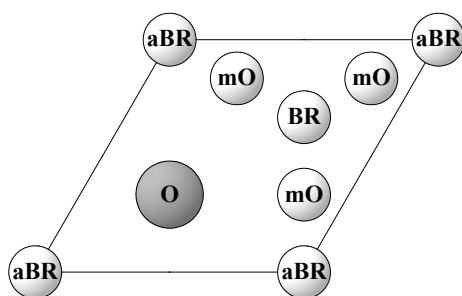


Fig. III.44. NaAl<sub>11</sub>O<sub>17</sub>

Framework O site and commonly occupied interstitial sites at  $z = \frac{1}{4}$  in  $\beta$ -aluminas (BR = Beevers-Ross, aBR = antiBeevers-Ross, mO = mid-oxygen).

Yamaguchi G., Suzuki K. (1968) [1]

Al<sub>11</sub>NaO<sub>17</sub>

$a = 0.5593$ ,  $c = 2.261$  nm,  $c/a = 4.043$ ,  $V = 0.6125$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.167	0.334	0.05		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.167	0.334	0.606		octahedron O <sub>6</sub>

O3	12k	.m.	0.5	0.0	0.144	non-coplanar triangle Al <sub>3</sub>
Al4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.022	tetrahedron O <sub>4</sub>
Al5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.178	tetrahedron O <sub>4</sub>
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.55	tetrahedron Al <sub>4</sub>
O7	4e	3m.	0	0	0.144	non-coplanar triangle Al <sub>3</sub>
Na8	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	trigonal prism O <sub>6</sub>
O9	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	colinear Al <sub>2</sub>
Al10	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

Experimental: powder, diffractometer, X-rays,  $R_B = 0.300$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Supersedes a structure proposal for so-called  $\frac{1}{2}\text{Na}_2\text{O} \cdot 11\frac{1}{2}\text{Al}_2\text{O}_3$  in [3]. In the table of [1] the *x*- and *y*-coordinates of former O(3) are misprinted as 0.1667 0.3333 instead of 0.3333 0.6667 (agreement with expected interatomic distances).

References: [1] Yamaguchi G., Suzuki K. (1968), Bull. Chem. Soc. Jpn. 41, 93-99. [2] Beevers C.A., Ross M.A.S. (1937), Z. Kristallogr. 97, 59-66. [3] Bragg W.L., Gottfried C., West J. (1931), Z. Kristallogr. 77, 255-274.

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hP58

(Ba<sub>0.91</sub>Eu<sub>0.09</sub>)(Mg<sub>0.5</sub>Al<sub>0.5</sub>)<sub>2</sub>Al<sub>9</sub>O<sub>17</sub>

hP58

(194)  $P6_3/mmc - k^3f^3edca$

#### Ba<sub>1-x</sub>Eu<sub>x</sub>MgAl<sub>10</sub>O<sub>17</sub> [2]

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral, (Mg,Al) in tetrahedral voids) and (Ba,Eu)O layers alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Mg,Al)O<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Kim K.B. et al. (2003) [1]

Al<sub>9.95</sub>Ba<sub>0.98</sub>Eu<sub>0.02</sub>Mg<sub>1.05</sub>O<sub>17</sub>

$a = 0.5626$ ,  $c = 2.266$  nm,  $c/a = 4.028$ ,  $V = 0.6211$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	.m.	0.1535	0.3071	0.0514		tetrahedron MgAl <sub>3</sub>
Al2	12k	.m.	0.1651	0.3302	0.6054		octahedron O <sub>6</sub>
O3	12k	.m.	0.5045	0.009	0.1481		non-coplanar triangle Al <sub>3</sub>
M4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0229		tetrahedron O <sub>4</sub>
Al5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1745		tetrahedron O <sub>4</sub>
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5585		tetrahedron MgAl <sub>3</sub>
O7	4e	3m.	0	0	0.1446		non-coplanar triangle Al <sub>3</sub>
M8	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		trigonal prism O <sub>6</sub>
O9	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Al <sub>2</sub>
Al10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M4 = 0.526Mg + 0.474Al; M8 = 0.980Ba + 0.020Eu

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.081$

Remarks: Refinement on combined X-ray and neutron diffraction data considering also parameters of EuMgAl<sub>11</sub>O<sub>19</sub>. Cell parameters omitted in [1], we took approximate values from [3]. When relevant, we changed the last digit of partial occupancies to respect constraints on total occupancy.

References: [1] Kim K.B., Koo K.W., Cho T.Y., Chun H.G. (2003), Mater. Chem. Phys. 80, 682-689. [2] Kim K.B., Kim Y.I., Chun H.G., Cho T.Y., Jung J.S., Kang J.G. (2002), Chem. Mater. 14, 5045-5052. [3] Kim Y.I., Kim K.B., Jung M.J., Hong J.S. (2002), J. Lumin. 99, 91-100.

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hP58

$\text{Ti}(\text{V}_{0.4}\text{Mn}_{0.6})_{1.9}\text{H}_{2.4}$	<i>hP58</i>	(194) $P6_3/mmc - \text{Ikh}^2\text{f}^2\text{a}$
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**Ti(V<sub>0.40</sub>Mn<sub>0.60</sub>)<sub>1.87</sub>H<sub>2.36</sub> [1]**

Structural features: Filled-up derivative of MgZn<sub>2</sub> with H in tetrahedral (Ti<sub>2</sub>(Mn,V)<sub>2</sub> and Ti(Mn,V)<sub>3</sub>) voids.

Mayer H.W. et al. (1982) [1]

$\text{D}_{2.47}\text{Mn}_{1.12}\text{TiV}_{0.75}$

$a = 0.5229$ ,  $c = 0.8581$  nm,  $c/a = 1.641$ ,  $V = 0.2032$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	24l	1	0.319	0.02	0.086	0.212	single atom D
D2	12k	.m.	0.538	0.076	0.603	0.199	non-coplanar triangle D <sub>3</sub>
M3	6h	mm2	0.171	0.342	1/4	0.935	non-coplanar square D <sub>4</sub>
D4	6h	mm2	0.555	0.11	1/4	0.238	non-coplanar D <sub>2</sub>
D5	4f	3m.	1/3	2/3	0.126	0.239	non-coplanar triangle D <sub>3</sub>
Ti6	4f	3m.	1/3	2/3	0.573		7-vertex polyhedron D <sub>7</sub>
M7	2a	-3m.	0	0	0	0.935	hexagonal prism D <sub>12</sub>

M3 = 0.60Mn + 0.40V; M7 = 0.60Mn + 0.40V

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

Experimental: powder, diffractometer, neutrons, R = 0.132

Remarks: We assigned an approximate value to the Mn/V ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s). In [1] the Wyckoff position of the second mixed site Me is misprinted as 6b instead of 6h.

References: [1] Mayer H.W., Alasafi K.M., Bernauer O. (1982), J. Less-Common Met. 88, L7-L10.

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hP60

$\text{Mg}(\text{Ag}_{0.10}\text{Zn}_{0.90})_2$	<i>hP60</i>	(194) $P6_3/mmc - \text{k}^2\text{hf}^5\text{e}^2\text{a}$
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**Mg(Zn,Ag)<sub>2</sub> 10H [2], Laves phase 10H**

Structural features: (Zn,Ag)<sub>4</sub> tetrahedra share faces and vertices to form a 3D-framework. Laves-type slabs in hchh stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Komura Y., Tokunaga K. (1980) [1]

$\text{Ag}_{0.20}\text{MgZn}_{1.80}$

$a = 0.522$ ,  $c = 4.3$  nm,  $c/a = 8.238$ ,  $V = 1.0147$  nm<sup>3</sup>,  $Z = 20$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12k	.m.	0.16661	0.33322	0.14998		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M2	12k	.m.	0.1694	0.3388	0.55002		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M3	6h	mm2	0.50237	0.00474	1/4		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg4	4f	3m.	1/3	2/3	0.01306		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg5	4f	3m.	1/3	2/3	0.08712		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
M6	4f	3m.	1/3	2/3	0.19987		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg7	4f	3m.	1/3	2/3	0.61282		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg8	4f	3m.	1/3	2/3	0.68696		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
M9	4e	3m.	0	0	0.10003		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg10	4e	3m.	0	0	0.2122		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>

M11      2a   -3m.      0      0      0      icosahedron Zn<sub>6</sub>Mg<sub>6</sub>

M1 = 0.90Zn + 0.10Ag; M2 = 0.90Zn + 0.10Ag; M3 = 0.90Zn + 0.10Ag; M6 = 0.90Zn + 0.10Ag; M9 = 0.90Zn + 0.10Ag; M11 = 0.90Zn + 0.10Ag

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

Experimental: single crystal, diffractometer, X-rays, R = 0.079

Remarks: We assigned an approximate value to the Zn/Ag ratio of sites M based on the nominal composition.

References: [1] Komura Y., Tokunaga K. (1980), Acta Crystallogr. B 36, 1548-1554. [2] Komura Y., Kishida E., Inoue M. (1967), J. Phys. Soc. Jpn. 23, 398-404.

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hP60

Na <sub>1.5</sub> Al <sub>10.83</sub> O <sub>17</sub>	hP60	(194) P6 <sub>3</sub> /mmc – k <sup>3</sup> f <sup>3</sup> edcba
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**Na<sub>1.50</sub>Al<sub>10.83</sub>O<sub>17</sub>** [1], β alumina-Na; KFe<sub>11</sub>O<sub>17</sub> [2]

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and NaO layers (Na at BR and aBR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Yamaguchi G., Suzuki K. (1968) [1]

Al<sub>11</sub>Na<sub>1.50</sub>O<sub>17</sub>

a = 0.5592, c = 2.2711 nm, c/a = 4.061, V = 0.6150 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.167	0.334	0.05		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.167	0.334	0.605		octahedron O <sub>6</sub>
O3	12k	.m.	0.5	0.0	0.144		non-coplanar triangle Al <sub>3</sub>
Al4	4f	3m.	1/3	2/3	0.03		tetrahedron O <sub>4</sub>
Al5	4f	3m.	1/3	2/3	0.17		tetrahedron O <sub>4</sub>
O6	4f	3m.	1/3	2/3	0.55		tetrahedron Al <sub>4</sub>
O7	4e	3m.	0	0	0.144		non-coplanar triangle Al <sub>3</sub>
Na8	2d	-6m2	1/3	2/3	3/4	0.75	icosahedron O <sub>9</sub> Na <sub>3</sub>
O9	2c	-6m2	1/3	2/3	1/4		colinear Al <sub>2</sub>
Na10	2b	-6m2	0	0	1/4	0.75	colinear O <sub>2</sub>
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.260

Remarks: Composition Na<sub>2</sub>O·7.02Al<sub>2</sub>O<sub>3</sub> from chemical analysis. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions.

References: [1] Yamaguchi G., Suzuki K. (1968), Bull. Chem. Soc. Jpn. 41, 93-99. [2] Ito S., Kurosawa H., Akashi K., Michiue Y., Watanabe M. (1996), Solid State Ionics 86/88, 745-750.

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hP60

U <sub>3</sub> Ni <sub>2</sub> F <sub>16</sub> [H <sub>2</sub> O] <sub>9</sub>	hP60	(194) P6 <sub>3</sub> /mmc – k <sup>3</sup> h <sup>2</sup> fecb
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**Ni<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>U<sub>3</sub>F<sub>16</sub>·3H<sub>2</sub>O** [1]

Structural features: Infinite layers of edge-linked UF<sub>6</sub>F monocapped square antiprisms (UF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms) sharing vertices with single Ni[F<sub>3</sub>(OH<sub>2</sub>)<sub>3</sub>] octahedra; additional H<sub>2</sub>O between the slabs.

Bean A.C. et al. (2003) [1]



$a = 0.79863$ ,  $c = 1.6566$  nm,  $c/a = 2.074$ ,  $V = 0.9150$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
(OH <sub>2</sub> )1	12 <i>k</i>	. <i>m</i> .	0.2072	0.4145	0.5148		single atom Ni
F2	12 <i>k</i>	. <i>m</i> .	0.22	0.4401	0.6763		non-coplanar triangle U <sub>2</sub> F
F3	12 <i>k</i>	. <i>m</i> .	0.5482	0.0964	0.6224		non-coplanar NiU
F4	6 <i>h</i>	<i>mm</i> 2	0.1611	0.3223	$\frac{1}{4}$		coplanar square (OH <sub>2</sub> )U <sub>2</sub> F
U5	6 <i>h</i>	<i>mm</i> 2	0.50149	0.00298	$\frac{1}{4}$		tricapped trigonal prism F <sub>9</sub>
Ni6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.05152		octahedron F <sub>3</sub> (OH <sub>2</sub> ) <sub>3</sub>
(OH <sub>2</sub> )7	4 <i>e</i>	3 <i>m</i> .	0	0	0.1115		single atom (OH <sub>2</sub> )
F8	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		icosahedron U <sub>3</sub> F <sub>9</sub>
(OH <sub>2</sub> )9	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal bipyramid F <sub>3</sub> (OH <sub>2</sub> ) <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.024$ ,  $T = 193$  K

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

References: [1] Bean A.C., Sullens T.A., Runde W., Albrecht Schmitt T.E. (2003), Inorg. Chem. 42, 2628-2633.

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hP60

Al <sub>11</sub> O <sub>16</sub> [OH]	hP60	(194) $P6_3/mmc - k^3hf^3ea$
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**HA<sub>11</sub>O<sub>17</sub>** [2],  $\beta$  alumina-H

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and OH layers (split O site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked Al(O<sub>3</sub>OH) tetrahedra to form a 3D-framework.

Newsam J.M. et al. (1985) [1]



$a = 0.56037$ ,  $c = 2.26169$  nm,  $c/a = 4.036$ ,  $V = 0.6151$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1575	0.315	0.0494		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.1643	0.3286	0.6065		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5007	0.0014	0.1457		non-coplanar triangle Al <sub>3</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.37	0.74	$\frac{1}{4}$	0.333	
Al5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0237		tetrahedron O <sub>4</sub>
Al6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1708		
O7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5564		tetrahedron Al <sub>4</sub>
O8	4 <i>e</i>	3 <i>m</i> .	0	0	0.1396		non-coplanar triangle Al <sub>3</sub>
Al9	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>
D10	6 <i>h</i>	<i>mm</i> 2	0.464	0.928	$\frac{1}{4}$	0.333	

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.096$ ,  $T = 298$  K

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



References: [1] Newsam J.M., Cheetham A.K., Tofield B.C. (1985), J. Solid State Chem. 60, 214-229. [2] Tofield B.C., Jacobson A.J., England W.A., Clarke P.J., Thomas M.W. (1979), J. Solid State Chem. 30, 1-22.

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hP60

$K_2[SO_4]$	<i>hP60</i>	(194) $P6_3/mmc - I^2f^3$
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### $K_2SO_4 \alpha$ [1]

Structural features: K atoms and  $SO_4$  tetrahedra (partial orientational disorder) in a  $Ni_2In$ -type (ht- $Co_2Ge$ ) arrangement (K and S displaced from the ideal positions).

Van Den Berg A.J., Tuinstra F. (1978) [1]

$K_2O_4S$

$a = 0.59$ ,  $c = 0.811$  nm,  $c/a = 1.375$ ,  $V = 0.2445$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
K1	24I	1	0.039	0.002	0.019	0.083	
O2	24I	1	0.185	0.411	0.195	0.25	
O3	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.076	0.5	
S4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.248	0.5	
K5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.703	0.5	

Experimental: powder, film, X-rays,  $wR = 0.034$ ,  $T = 903$  K

Remarks: Phase stable at  $T > 853$  K. Short interatomic distances for partly occupied site(s). Space groups (159)  $P31c$ , (163)  $P-31c$ , (186)  $P6_3mc$  and (188)  $P-6c2$  were tested and rejected.

References: [1] Van Den Berg A.J., Tuinstra F. (1978), Acta Crystallogr. B 34, 3177-3181.

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hP60

$ZrMn_2H_3$	<i>hP60</i>	(194) $P6_3/mmc - Ikh^3fa$
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### $ZrMn_2H_3$ [2]

Structural features: Filled-up derivative of  $MgZn_2$  with H in tetrahedral ( $Zr_2Mn_2$ ) voids. See Fig. III.45.

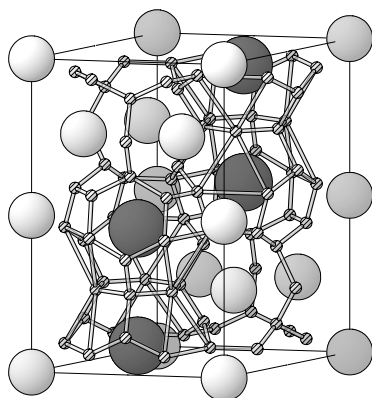


Fig. III.45.  $ZrMn_2H_3$

Arrangement of Zr (large) and Mn (medium) atoms; solid lines connect partly occupied H sites (small).

Pontonnier L. et al. (1992) [1]

$D_{3.05}Mn_2Zr$

$a = 0.54055$ ,  $c = 0.87964$  nm,  $c/a = 1.627$ ,  $V = 0.2226$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	24l	1	0.0398	0.3249	0.0647	0.211	non-coplanar triangle D <sub>3</sub>
D2	12k	.m.	0.5406	0.0812	0.6261	0.372	non-coplanar triangle D <sub>3</sub>
Mn3	6h	mm2	0.1634	0.3268	<sup>1</sup> / <sub>4</sub>		cuboctahedron D <sub>12</sub>
D4	6h	mm2	0.534	0.068	<sup>1</sup> / <sub>4</sub>	0.369	tetrahedron D <sub>4</sub>
D5	6h	mm2	0.7979	0.5958	<sup>1</sup> / <sub>4</sub>	0.079	non-colinear D <sub>2</sub>
Zr6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5629		24-vertex polyhedron D <sub>24</sub>
Mn7	2a	-3m.	0	0	0		hexagonal prism D <sub>12</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.057

References: [1] Pontonnier L., Miraglia S., Fruchart D., Soubeyrou J.L., Baudry A., Boyer P. (1992), J. Alloys Compd. 186, 241-248. [2] Didisheim J.J., Yvon K., Shaltiel D., Fischer P. (1979), Solid State Commun. 31, 47-50.

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hP62

Lu <sub>1.87</sub> Fe <sub>17.26</sub> H <sub>3</sub>	hP62	(194) P <sub>63</sub> /mmc – kj <sup>2</sup> hgfedcb
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### Lu<sub>2</sub>Fe<sub>17</sub>H<sub>3</sub> [1]

Structural features: Filled-up derivative of Th<sub>2</sub>Ni<sub>17</sub> with H in octahedral (Lu<sub>2</sub>Fe<sub>4</sub>) voids; partial disorder Lu/Fe<sub>2</sub> and splitting of the Fe site forming the hexagon mesh.

Tereshina I.S. et al. (2001) [1]

Fe<sub>17.26</sub>H<sub>3</sub>Lu<sub>1.86</sub>

*a* = 0.8509, *c* = 0.8308 nm, *c/a* = 0.976, *V* = 0.5209 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12k	.m.	0.1669	0.3339	0.0159		single atom H
Fe2	12j	m..	0.3004	0.0066	<sup>1</sup> / <sub>4</sub>	0.13	
Fe3	12j	m..	0.3777	0.047	<sup>1</sup> / <sub>4</sub>	0.87	
H4	6h	mm2	0.177	0.354	<sup>1</sup> / <sub>4</sub>		non-colinear Fe <sub>2</sub>
Fe5	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		
Fe6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6053	0.94	
Fe7	4e	3m.	0	0	0.1061	0.19	
Lu8	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.06	
Lu9	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle H <sub>3</sub>
Lu10	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>	0.8	

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.042, T = 293 K

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

References: [1] Tereshina I.S., Nikitin S.A., Stepien Damm J., Gulay L.D., Pankratov N.Y., Salamova A.A., Verbetsky V.N., Suski W. (2001), J. Alloys Compd. 329, 31-36.

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hP62

Ho <sub>2</sub> Fe <sub>17</sub> H <sub>3.6</sub>	hP62	(194) P <sub>63</sub> /mmc – kjihg fedcb
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### Ho<sub>2</sub>Fe<sub>17</sub>H<sub>3.6</sub> [1]

Structural features: Filled-up derivative of  $\text{Th}_2\text{Ni}_{17}$  with H in octahedral ( $\text{Ho}_2\text{Fe}_4$ ) and tetrahedral ( $\text{Fe}_4$ ) voids; partial disorder Ho/Fe<sub>2</sub>.

Isnard O. et al. (1990) [1]

$\text{D}_{3.39}\text{Fe}_{16.79}\text{Ho}_{1.91}$

$a = 0.85363$ ,  $c = 0.83519$  nm,  $c/a = 0.978$ ,  $V = 0.5271$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Fe1	12 <i>k</i>	. <i>m</i> .	0.1667	0.3334	0.0139		non-collinear D <sub>2</sub>
Fe2	12 <i>j</i>	. <i>m</i> ..	0.3704	0.0456	$\frac{1}{4}$	0.936	single atom D
D3	12 <i>i</i>	.2.	0.137	0	0	0.1	non-collinear D <sub>2</sub>
D4	6 <i>h</i>	<i>mm</i> 2	0.156	0.312	$\frac{1}{4}$	0.93	coplanar square Fe <sub>4</sub>
Fe5	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		10-vertex polyhedron Fe <sub>10</sub>
Fe6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.612	0.841	
Fe7	4 <i>e</i>	3 <i>m</i> .	0	0	0.088	0.244	
Ho8	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.158	
Ho9	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		23-vertex polyhedron D <sub>3</sub> Fe <sub>20</sub>
Ho10	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$	0.756	

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

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.166$ ,  $T = 280$  K

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

References: [1] Isnard O., Miraglia S., Soubeyroux J.L., Fruchart D., Stergiou A. (1990), J. Less-Common Met. 162, 273-284.

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*hP62*

Ca[CO <sub>3</sub> ]	<i>hP62</i>	(194) <i>P6<sub>3</sub>/mmc</i> – <i>Ij</i> <sup>2</sup> <i>ia</i>
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**CaCO<sub>3</sub> μ** [1], vaterite

Structural features: Ca atoms (in part displaced from the ideal positions) and CO<sub>3</sub> trigonal units (parallel to [001], orientational disorder) in a NiAs-type arrangement.

Meyer H.J. (1969) [1]

$\text{CCaO}_{3.01}$

$a = 0.4127$ ,  $c = 0.8475$  nm,  $c/a = 2.054$ ,  $V = 0.1250$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24 <i>l</i>	1	0.2838	0.6294	0.11	0.167	
O2	12 <i>j</i>	. <i>m</i> ..	0.0575	0.2408	$\frac{1}{4}$	0.167	
C3	12 <i>j</i>	. <i>m</i> ..	0.2496	0.5578	$\frac{1}{4}$	0.167	
Ca4	12 <i>i</i>	.2.	0.0405	0	0	0.111	
Ca5	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.333	

Experimental: single crystal, Weissenberg and rotation photographs, X-rays,  $R = 0.113$

Remarks: Short interatomic distances for partly occupied site(s). Average structure; additional reflections could be indexed with a 6-fold supercell (new axes 2a+b, -a+b, 2c). The data in [1] refer to a non-conventional setting with this large cell, however, no deviation from the subcell symmetry is proposed. A similar model with Ca exclusively in Wyckoff position 2*a* is also reported. Preliminary data in [2].

References: [1] Meyer H.J. (1969), Z. Kristallogr. 128, 183-212. [2] Meyer H.J. (1965), Z. Kristallogr. 121, 220-242.

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hP64

$\text{Na}_{0.5}\text{Al}_{11.5}\text{O}_{17.5}$	<i>hP64</i>	(194) $P6_3/mmc - k^3f^4edcba$
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**Na<sub>0.5</sub>Al<sub>11.5</sub>O<sub>17.5</sub>** [1],  $\beta$  alumina-Na, Strukturbericht notation D5<sub>6</sub>

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, partial disorder for the latter) and Na<sub>x</sub>O<sub>1+y</sub> layers (partial disorder) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra (partial disorder) to form a 3D-framework.

Bragg W.L. et al. (1931) [1]

 $\text{Al}_{11.50}\text{Na}_{0.50}\text{O}_{17.50}$  $a = 0.556$ ,  $c = 2.255$  nm,  $c/a = 4.056$ ,  $V = 0.6037$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.16667	0.33333	0.106		octahedron O <sub>6</sub>
O2	12k	.m.	0.16667	0.33333	0.55		tetrahedron Al <sub>4</sub>
O3	12k	.m.	0.5	0.0	0.144		tetrahedron Al <sub>4</sub>
O4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05		tetrahedron Al <sub>4</sub>
Al5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.178	0.75	tetrahedron O <sub>4</sub>
Al6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.522		tetrahedron O <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.678	0.75	tetrahedron O <sub>4</sub>
O8	4e	3m.	0	0	0.144		non-coplanar triangle Al <sub>3</sub>
O9	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.75	colinear Al <sub>2</sub>
O10	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.75	colinear Al <sub>2</sub>
Na11	2b	-6m2	0	0	$\frac{1}{4}$	0.5	colinear O <sub>2</sub>
Al12	2a	-3m.	0	0	0	0.5	octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays

Remarks: The structure was redetermined in [2] (ideal composition NaAl<sub>11</sub>O<sub>17</sub>).

References: [1] Bragg W.L., Gottfried C., West J. (1931), Z. Kristallogr. 77, 255-274. [2] Beevers C.A., Ross M.A.S. (1937), Z. Kristallogr. 97, 59-66.

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hP64

$\text{Fe}_{12}\text{PbO}_{19}$	<i>hP64</i>	(194) $P6_3/mmc - k^3hf^3edba$
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**PbFe<sub>12</sub>O<sub>19</sub>** [1], magnetoplumbite, ferrite M-type; Nd<sub>2</sub>Fe<sub>15</sub>Al<sub>9</sub>O<sub>38</sub> [3]

Structural features: Close-packed O<sub>4</sub> and PbO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Fe in octahedral, tetrahedral and trigonal bipyramidal voids. Intergrowth of spinel-type slabs (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells), FeO<sub>5</sub> trigonal bipyramids and Pb atoms.

Adelsköld V. (1938) [1]

 $\text{Fe}_{12}\text{O}_{19}\text{Pb}$  $a = 0.5877$ ,  $c = 2.302$  nm,  $c/a = 3.917$ ,  $V = 0.6886$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.167	0.334	0.05		tetrahedron Fe <sub>4</sub>
Fe2	12k	.m.	0.167	0.334	0.608		octahedron O <sub>6</sub>
O3	12k	.m.	0.5	0.0	0.15		non-coplanar triangle Fe <sub>3</sub>
O4	6h	mm2	0.186	0.372	$\frac{1}{4}$		coplanar triangle Fe <sub>3</sub>

Fe5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.028	tetrahedron O <sub>4</sub>
Fe6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.189	octahedron O <sub>6</sub>
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.55	tetrahedron Fe <sub>4</sub>
O8	4e	3m.	0	0	0.15	tetrahedron Fe <sub>4</sub>
Pb9	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	anticuboctahedron O <sub>12</sub>
Fe10	2b	-6m2	0	0	$\frac{1}{4}$	trigonal bipyramid O <sub>5</sub>
Fe11	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

Remarks: Natural specimen. In [1] the *z*-coordinate of former Fe(5) is misprinted as 39° instead of -39° (see [2]). Partial ordering of Fe and Al is reported for Nd<sub>2</sub>Fe<sub>15</sub>Al<sub>9</sub>O<sub>38</sub> in [3] (no Al in Wyckoff position 4f). Similar partial ordering of Fe and In is reported for BaIn<sub>3.4</sub>Fe<sub>8.6</sub>O<sub>19</sub> in [4], where, however, O was not located.

References: [1] Adelsköld V. (1938), Ark. Kemi Mineral. Geol. 12A(29), 1-9. [2] Braun P.B. (1957), Philips Res. Rep. 12, 491-548. [3] Lehmann U., Müller Buschbaum H. (1982), Z. Anorg. Allg. Chem. 486, 45-48. [4] Aleshko Ozhevskii O.P., Lyubimtsev V.A., Namtalishvili M.I., Yamzin I.I. (1972), Sov. Phys. Crystallogr. 16, 711-712 (Kristallografiya 16, 823-824).

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hP64

K <sub>1.44</sub> (Mg <sub>0.22</sub> Ga <sub>0.78</sub> ) <sub>2</sub> Ga <sub>9</sub> O <sub>17</sub>	hP64	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> hf <sup>3</sup> edca
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**K<sub>1.47</sub>Mg<sub>0.44</sub>Ga<sub>10.56</sub>O<sub>17.015</sub>** [1], β alumina(Ga,Mg)-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Ga in octahedral and outer tetrahedral, (Ga,Mg) in inner tetrahedral voids) and K<sub>x</sub>O layers (K at BR and near mO positions) alternate along [001]. Infinite slabs of edge-linked GaO<sub>6</sub> octahedra sharing vertices with single (Ga,Mg)O<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked GaO<sub>4</sub> tetrahedra to form a 3D-framework.

Ikawa H. et al. (1985) [1]

Ga<sub>10.66</sub>K<sub>1.50</sub>Mg<sub>0.34</sub>O<sub>17</sub>

*a* = 0.5857, *c* = 2.333 nm, *c/a* = 3.983, *V* = 0.6931 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	.m.	0.157	0.314	0.5513		tetrahedron Ga <sub>4</sub>
Ga2	12k	.m.	0.1674	0.3348	0.10611		octahedron O <sub>6</sub>
O3	12k	.m.	0.5055	0.011	0.6483		non-coplanar triangle Ga <sub>3</sub>
K4	6h	mm2	0.1187	0.2374	$\frac{1}{4}$	0.273	
O5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0566		tetrahedron Ga <sub>4</sub>
M6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52471		tetrahedron O <sub>4</sub>
Ga7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67418		tetrahedron O <sub>4</sub>
O8	4e	3m.	0	0	0.143		non-coplanar triangle Ga <sub>3</sub>
O9	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Ga <sub>2</sub>
K10	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.68	
Ga11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M6 = 0.83Ga + 0.17Mg

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

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

Remarks: Part of Mg not located; the authors state that Mg probably also partly substitutes for Ga on octahedral sites. Short interatomic distances for partly occupied site(s).

References: [1] Ikawa H., Tsurumi T., Ishimori M., Urabe K., Udagawa S. (1985), J. Solid State Chem. 60, 51-61.

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hP64

CsU <sub>6</sub> F <sub>25</sub>	hP64	(194) $P6_3/mmc - k^3ihfed$
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CsU<sub>6</sub>F<sub>25</sub> [1]; KU<sub>6</sub>F<sub>25</sub> [2]; KTh<sub>6</sub>F<sub>25</sub> [2]; PbZr<sub>6</sub>O<sub>22</sub>F<sub>22</sub> [3]Structural features: UF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework.

Brunton G. (1971) [1]

CsF<sub>25</sub>U<sub>6</sub> $a = 0.82424$ ,  $c = 1.6412$  nm,  $c/a = 1.991$ ,  $V = 0.9656$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12k	.m.	0.121	0.242	0.649		single atom F
U2	12k	.m.	0.1737	0.3474	0.11146		tricapped trigonal prism F <sub>9</sub>
F3	12k	.m.	0.515	0.03	0.644		non-collinear U <sub>2</sub>
F4	12i	.2.	0.322	0	0		non-collinear U <sub>2</sub>
F5	6h	mm2	0.184	0.368	$\frac{1}{4}$		non-collinear U <sub>2</sub>
F6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.068		non-coplanar triangle U <sub>3</sub>
F7	4e	3m.	0	0	0.076		non-coplanar triangle F <sub>3</sub>
Cs8	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		hexagonal prism F <sub>12</sub>

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

Remarks: Only cell parameters are reported for KU<sub>6</sub>F<sub>25</sub> and KTh<sub>6</sub>F<sub>25</sub> in [2]. In table 1 of [1] the Wyckoff position of former F(1) is misprinted as 12j instead of 6h. Additional reflections observed for PbZr<sub>6</sub>O<sub>22</sub>F<sub>22</sub> in [3] could be indexed with a 3-fold supercell, space group (193)  $P6_3/mcm$ ; refinement of the average structure showed substitution by O exclusively on site F4 and partial occupation of site F5.

References: [1] Brunton G. (1971), Acta Crystallogr. B 27, 245-247. [2] Zachariasen W.H. (1948), J. Am. Chem. Soc. 70, 2147-2151. [3] Laval J.P., Frit B. (1983), Rev. Chim. Miner. 20, 368-384.

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hP66

AgAl <sub>11</sub> O <sub>17</sub>	hP66	(194) $P6_3/mmc - k^3h^2f^3ea$
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AgAl<sub>11</sub>O<sub>17</sub> [1],  $\beta$  alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and AgO layers (split sites, Ag near BR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Newsam J.M., Tofield B.C. (1981) [1]

Ag<sub>1.02</sub>Al<sub>11</sub>O<sub>17</sub> $a = 0.55871$ ,  $c = 2.25131$  nm,  $c/a = 4.029$ ,  $V = 0.6086$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1576	0.3152	0.05009		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1665	0.333	0.6066		octahedron O <sub>6</sub>
O3	12k	.m.	0.5029	0.0058	0.14603		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.2972	0.5944	$\frac{1}{4}$	0.333	
Ag5	6h	mm2	0.7763	0.5526	$\frac{1}{4}$	0.34	non-collinear Ag <sub>2</sub>
Al6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0251		tetrahedron O <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1754		
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5548		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.1415		non-coplanar triangle Al <sub>3</sub>

Al10    2a   -3m.    0    0    0    octahedron O<sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $R_B = 0.051$ ,  $T = 4.2$  K

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

References: [1] Newsam J.M., Tofield B.C. (1981), J. Phys. C: Solid State Phys. 14, 1545-1554.

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hP66

[H<sub>3</sub>O]Al<sub>11</sub>O<sub>17</sub>    hP66    (194)  $P6_3/mmc - k^3h^2f^3ea$

**HAl<sub>11</sub>O<sub>17</sub>·H<sub>2</sub>O** [2],  $\beta$  alumina-H<sub>3</sub>O

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (H<sub>3</sub>O)O layers (split sites, H<sub>3</sub>O near BR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Colomban P. et al. (1978) [1]

Al<sub>11</sub>H<sub>3</sub>O<sub>18</sub>

$a = 0.5614$ ,  $c = 2.262$  nm,  $c/a = 4.029$ ,  $V = 0.6174$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1578	0.3156	0.0499		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1677	0.3354	0.6066		octahedron O <sub>6</sub>
O3	12k	.m.	0.5027	0.0054	0.1453		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.3191	0.6382	$\frac{1}{4}$	0.333	
(OH <sub>3</sub> )5	6h	mm2	0.7039	0.4078	$\frac{1}{4}$	0.333	
Al6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0248		tetrahedron O <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1757		
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5551		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.141		non-coplanar triangle Al <sub>3</sub>
Al10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.059$

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] Colomban P., Boilot J.P., Kahn A., Lucazeau G. (1978), Nouv. J. Chim. 2, 21-32. [2] Kato K., Saalfeld H. (1977), Acta Crystallogr. B 33, 1596-1598.

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hP66

Sr(Mg<sub>0.5</sub>Al<sub>0.5</sub>)<sub>2</sub>Al<sub>9</sub>O<sub>17</sub>    hP66    (194)  $P6_3/mmc - k^3h^2f^3ea$

**SrMgAl<sub>10</sub>O<sub>17</sub>** [1],  $\beta$  alumina(Al,Mg)-Sr

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral, (Al,Mg) in tetrahedral voids) and SrO layers (split O site, Sr near BR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Iyi N., Göbbels M. (1996) [1]

Al<sub>10</sub>MgO<sub>17</sub>Sr<sub>0.92</sub>

$a = 0.562$ ,  $c = 2.24$  nm,  $c/a = 3.986$ ,  $V = 0.6127$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1537	0.3074	0.05222		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1659	0.3318	0.60688		octahedron O <sub>6</sub>
O3	12k	.m.	0.5055	0.011	0.15003		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.3085	0.617	<sup>1</sup> / <sub>4</sub>	0.333	
Sr5	6h	mm2	0.6891	0.3782	<sup>1</sup> / <sub>4</sub>	0.306	
M6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.02412		tetrahedron O <sub>4</sub>
Al7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.17491		
O8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5596		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.1456		non-coplanar triangle Al <sub>3</sub>
Al10	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M6 = 0.5Al + 0.5Mg

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

Remarks: The authors state that Mg substitutes for Al preferentially on site M6. We assigned an approximate value to the Al/Mg ratio of site M6 based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 3 of [1] the Wyckoff position of former Al(1) is misprinted as 12h instead of 12k.

References: [1] Iyi N., Göbbels M. (1996), J. Solid State Chem. 122, 46-52.

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hP66

Cs <sub>4</sub> Nb <sub>5</sub> Si <sub>3</sub> O <sub>20.5</sub>	hP66	(194) $P6_3/mmc - k^3h^2gf^2e$
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**Cs<sub>8</sub>Nb<sub>10</sub>O<sub>23</sub>(Si<sub>3</sub>O<sub>9</sub>)<sub>2</sub>** [1]

Structural features: Infinite slabs of vertex-linked NbO<sub>6</sub> octahedra are interconnected via common vertices with units of three vertex-linked SiO<sub>4</sub> tetrahedra to form a 3D-framework.

Crosnier M.P. et al. (1991) [1]

Cs<sub>4</sub>Nb<sub>5</sub>O<sub>20.50</sub>Si<sub>3</sub>

$a = 0.7342$ ,  $c = 2.2166$  nm,  $c/a = 3.019$ ,  $V = 1.0348$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.2057	0.4114	0.6898		non-colinear SiNb
O2	12k	.m.	0.209	0.418	0.0184	0.917	non-colinear Nb <sub>2</sub>
O3	12k	.m.	0.5457	0.0914	0.0863		non-colinear Nb <sub>2</sub>
O4	6h	mm2	0.117	0.234	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
Si5	6h	mm2	0.8623	0.7246	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
Nb6	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		octahedron O <sub>6</sub>
Cs7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.15558		non-coplanar triangle O <sub>3</sub>
Nb8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.63573		octahedron O <sub>6</sub>
Cs9	4e	3m.	0	0	0.09183		octahedron O <sub>6</sub>

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

References: [1] Crosnier M.P., Pagnoux C., Guyomard D., Verbaere A., Piffard Y., Tournoux M. (1991), Eur. J. Solid State Inorg. Chem. 28, 971-981.

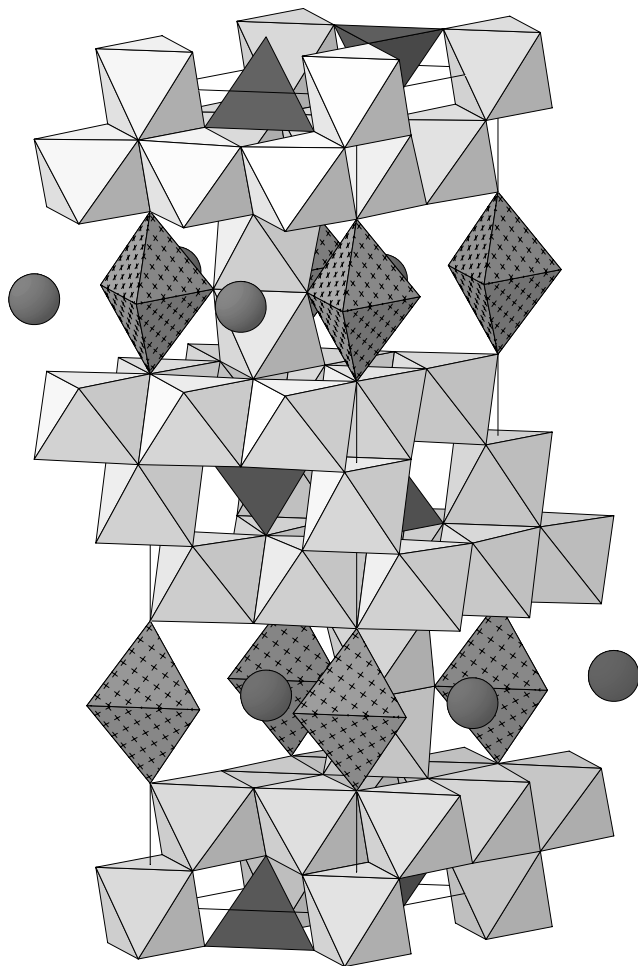
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hP66

BaFe <sub>12</sub> O <sub>19</sub>	hP66	(194) $P6_3/mmc - k^3hf^3e^2da$
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**BaFe<sub>12</sub>O<sub>19</sub>** [2], ferrite M-type, magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and BaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Fe in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells), FeO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Ba atoms. See Fig. III.46.

Fig. III.46. **BaFe<sub>12</sub>O<sub>19</sub>**

Arrangement of FeO<sub>4</sub> tetrahedra (dark), FeO<sub>5</sub> trigonal bipyramids (medium), FeO<sub>6</sub> octahedra (light) and Ba atoms.

Obradors X. et al. (1985) [1]

BaFe<sub>12</sub>O<sub>19</sub>

$a = 0.5892$ ,  $c = 2.3183$  nm,  $c/a = 3.935$ ,  $V = 0.6970$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.15647	0.31294	0.05192		tetrahedron Fe <sub>4</sub>
Fe2	12 <i>k</i>	. <i>m</i> .	0.16867	0.33735	0.60825		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5026	0.0052	0.14957		non-coplanar triangle Fe <sub>3</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.18213	0.36426	<sup>1</sup> / <sub>4</sub>		coplanar triangle Fe <sub>3</sub>
Fe5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.02713		tetrahedron O <sub>4</sub>
Fe6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1903		octahedron O <sub>6</sub>
O7	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.55454		tetrahedron Fe <sub>4</sub>
O8	4 <i>e</i>	3 <i>m</i> .	0	0	0.15094		tetrahedron Fe <sub>4</sub>
Fe9	4 <i>e</i>	3 <i>m</i> .	0	0	0.24267	0.5	trigonal bipyramid O <sub>5</sub>

Ba10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	anticuboctahedron O <sub>12</sub>
Fe11	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). Refinements on data collected at 4.2 and 743 K are reported in [3].

References: [1] Obradors X., Collomb A., Pernet M., Samaras D., Joubert J.C. (1985), J. Solid State Chem. 56, 171-181. [2] Townes W.D., Fang J.H., Perrotta A.J. (1967), Z. Kristallogr. 125, 437-449. [3] Collomb A., Wolfers P., Obradors X. (1986), J. Magn. Magn. Mater. 62, 57-67.

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hP66

SrCr <sub>9</sub> Ga <sub>3</sub> O <sub>19</sub>	hP66	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>3</sup> e <sup>2</sup> da
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**SrCr<sub>9</sub>Ga<sub>3</sub>O<sub>19</sub>** [2], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and SrO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Cr in octahedral, Ga in tetrahedral voids. Intergrowth of spinel-type (edge-linked CrO<sub>6</sub> octahedra sharing vertices with single GaO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked CrO<sub>6</sub> octahedra (Cr<sub>2</sub> dumbbells), GaO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Sr atoms.

Graetsch H., Gebert W. (1996) [1]

Cr<sub>9</sub>Ga<sub>3</sub>O<sub>19</sub>Sr

*a* = 0.5796, *c* = 2.26579 nm, *c/a* = 3.909, *V* = 0.6592 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1558	0.3116	0.0521		tetrahedron GaCr <sub>3</sub>
Cr2	12 <i>k</i>	. <i>m</i> .	0.1682	0.3364	0.6079		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5061	0.0122	0.1509		non-coplanar triangle Cr <sub>3</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.1846	0.3692	$\frac{1}{4}$		coplanar square Ga <sub>2</sub> Cr <sub>2</sub>
Ga5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0279		tetrahedron O <sub>4</sub>
Cr6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1919		octahedron O <sub>6</sub>
O7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5552		tetrahedron GaCr <sub>3</sub>
O8	4 <i>e</i>	3 <i>m</i> .	0	0	0.1517		tetrahedron Cr <sub>3</sub> Ga
Ga9	4 <i>e</i>	3 <i>m</i> .	0	0	0.2443	0.5	
Sr10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		anticuboctahedron O <sub>12</sub>
Cr11	2a	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.038

Remarks: Homogeneity range SrCr<sub>x</sub>Ga<sub>12-x</sub>O<sub>19</sub>, 0 < *x* < 9. Short interatomic distances for partly occupied site(s).

References: [1] Graetsch H., Gebert W. (1996), Z. Kristallogr. 211, 25-30. [2] Obradors X., Labarta A., Isalgue A., Tejada J., Rodriguez J., Pernet M. (1988), Solid State Commun. 65, 189-192.

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hP66

Al <sub>11</sub> O <sub>16</sub> [OH]	hP66	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> j <sup>3</sup> e <sup>3</sup> ea
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**Al<sub>11</sub>O<sub>17</sub>** [1], β alumina-H

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and OH layers (split O site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked Al(O<sub>3</sub>OH) tetrahedra to form a 3D-framework.

Tofield B.C. et al. (1979) [1]

$\text{Al}_{11}\text{D}_{0.87}\text{O}_{17}$

$a = 0.56062$ ,  $c = 2.26191$  nm,  $c/a = 4.035$ ,  $V = 0.6157$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.15518	0.31036	0.04966		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.16701	0.33402	0.60718		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.50199	0.00395	0.14549		non-coplanar triangle Al <sub>3</sub>
O4	12 <i>j</i>	. <i>m</i> ..	0.2481	0.6006	$\frac{1}{4}$	0.167	
Al5	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.02376		tetrahedron O <sub>4</sub>
Al6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.17295		
O7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.55588		tetrahedron Al <sub>4</sub>
O8	4 <i>e</i>	3 <i>m</i> .	0	0	0.14099		non-coplanar triangle Al <sub>3</sub>
Al9	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>
D10	12 <i>j</i>	. <i>m</i> ..	0.0471	0.4798	$\frac{1}{4}$	0.145	

Experimental: powder, diffractometer, neutrons,  $R_B = 0.034$ ,  $T = 4.5$  K

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

References: [1] Tofield B.C., Jacobson A.J., England W.A., Clarke P.J., Thomas M.W. (1979), J. Solid State Chem. 30, 1-22.

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hP66

$\text{Zr}(\text{Nb}_{0.5}\text{V}_{0.5})_2\text{H}_{5.4}$	<i>hP66</i>	(194) $P6_3/mmc - 1k^2h^2fa$
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**ZrNbVH<sub>5.4</sub>** [1]

Structural features: Filled-up derivative of  $\text{MgZn}_2$  with H in tetrahedral  $(\text{Zr}_2(\text{Nb},\text{V})_2$  and  $\text{Zr}(\text{Nb},\text{V})_3$ ) voids.

Yartys' V.A. et al. (1983) [1]

$\text{D}_{5.40}\text{NbVZr}$

$a = 0.569$ ,  $c = 0.9288$  nm,  $c/a = 1.632$ ,  $V = 0.2604$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	24 <i>l</i>	1	0.365	0.082	0.068	0.25	non-colinear D <sub>2</sub>
D2	12 <i>k</i>	. <i>m</i> .	0.13	0.26	0.13	0.05	non-colinear D <sub>2</sub>
D3	12 <i>k</i>	. <i>m</i> .	0.539	0.078	0.117	0.79	non-colinear D <sub>2</sub>
D4	6 <i>h</i>	<i>mm</i> 2	0.244	0.488	$\frac{1}{4}$	0.92	tetrahedron D <sub>4</sub>
M5	6 <i>h</i>	<i>mm</i> 2	0.858	0.716	$\frac{1}{4}$		square prism (cube) D <sub>8</sub>
Zr6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.065		pseudo Frank-Kasper D <sub>18</sub>
M7	2 <i>a</i>	-3 <i>m</i> .	0	0	0		18-vertex polyhedron D <sub>18</sub>

$M5 = 0.5\text{Nb} + 0.5\text{V}$ ;  $M7 = 0.5\text{Nb} + 0.5\text{V}$

Experimental: powder, diffractometer, neutrons,  $R = 0.117$

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. The same data are also reported in [2]. In table 1 of [1] the occupancies of former D(3) and D(4) expressed in percent are misprinted as 35 and 15 % instead of 25 and 5 %, respectively (from the occupancies expressed in number of atoms per cell). In [3] the space group is misprinted as  $P6_3/mcm$  instead of  $P6_3/mmc$ .

References: [1] Yartys' V.A., Burnasheva V.V., Tsirkunova S.E., Kozlov E.N., Semenenko K.N. (1983), Latv. PSR Zinat. Akad. Vestis, Fiz. Teh. Zinat. Ser. 1983, 14-20. [2] Yartys' V.A., Burnasheva V.V., Semenenko K.N. (1984), Russ. J. Inorg. Chem. 29, 357-360 (Zh. Neorg. Khim. 29, 615-621). [3] (1988), Structure Reports 50A, 34.

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hP68

$\text{Ba}_7\text{Sc}_6\text{Al}_2\text{O}_{19}$	<i>hP68</i>	(194) $P6_3/mmc - k^3f^6e^2cb$
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### **Ba<sub>7</sub>Sc<sub>6</sub>Al<sub>2</sub>O<sub>19</sub> [1]**

Structural features: Slabs of six close-packed BaO<sub>3</sub> layers in ABCCAB stacking alternate with BaO layers along [001]; Sc in octahedral and trigonal prismatic (displaced from the prism center), Al in tetrahedral voids. Double perovskite-type slabs of vertex-linked ScO<sub>6</sub> octahedra share faces with ScO<sub>6</sub> trigonal prisms on one side and vertices with units of two vertex-linked AlO<sub>4</sub> tetrahedra on the other side to form a 3D-framework.

Shpanchenko R.V. et al. (1991) [1]

$\text{Al}_2\text{Ba}_7\text{O}_{19}\text{Sc}_6$

$a = 0.58056$ ,  $c = 3.5248$  nm,  $c/a = 6.071$ ,  $V = 1.0289$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.154	0.308	0.614		non-colinear Sc <sub>2</sub>
O2	12k	.m.	0.182	0.364	0.1856		single atom Al
O3	12k	.m.	0.509	0.018	0.0405		coplanar triangle Sc <sub>3</sub>
Sc4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0091		trigonal prism O <sub>6</sub>
Ba5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1079		cuboctahedron O <sub>12</sub>
Al6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2017		tetrahedron O <sub>4</sub>
Sc7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5748		octahedron O <sub>6</sub>
Ba8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6739		9-vertex polyhedron O <sub>9</sub>
Ba9	4e	3m.	0	0	0.0528		9-vertex polyhedron O <sub>9</sub>
Sc10	4e	3m.	0	0	0.1476		octahedron O <sub>6</sub>
O11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Al <sub>2</sub>
Ba12	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays, R = 0.071

References: [1] Shpanchenko R.V., Antipov E.V., Paromova M.V., Kovba L.M. (1991), Russ. J. Inorg. Chem. 36, 797-799 (Zh. Neorg. Khim. 36, 1402-1407).

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hP68

$\text{MgLaAl}_{11}\text{O}_{19}$	<i>hP68</i>	(194) $P6_3/mmc - k^3h^2f^3eba$
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### **LaMgAl<sub>11</sub>O<sub>19</sub> [1], magnetoplumbite family**

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; (Al,Mg) in octahedral, trigonal bipyramidal and tetrahedral voids. Intergrowth of spinel-type (edge-linked (Al,Mg)O<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked (Al,Mg)O<sub>6</sub> octahedra, (Al,Mg)O<sub>5</sub> trigonal bipyramids and La atoms (split site).

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

$\text{Al}_{11}\text{LaMgO}_{19}$

$a = 0.5589$ ,  $c = 2.202$  nm,  $c/a = 3.94$ ,  $V = 0.5957$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.152	0.304	0.053		tetrahedron Al <sub>4</sub>
M2	12k	.m.	0.1676	0.3352	0.6082		octahedron O <sub>6</sub>
O3	12k	.m.	0.505	0.01	0.1508		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.182	0.364	1/4		coplanar triangle Al <sub>3</sub>
La5	6h	mm2	0.678	0.356	1/4	0.333	
M6	4f	3m.	1/3	2/3	0.0273		tetrahedron O <sub>4</sub>
M7	4f	3m.	1/3	2/3	0.1895		octahedron O <sub>6</sub>
O8	4f	3m.	1/3	2/3	0.5576		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.1499		tetrahedron Al <sub>4</sub>
M10	2b	-6m2	0	0	1/4		trigonal bipyramid O <sub>5</sub>
M11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M2 = 0.917Al + 0.083Mg; M6 = 0.917Al + 0.083Mg; M7 = 0.917Al + 0.083Mg; M10 = 0.917Al + 0.083Mg; M11 = 0.917Al + 0.083Mg

Experimental: single crystal, diffractometer, X-rays, R = 0.039

Remarks: No attempt was made to distinguish Al and Mg. We assigned an approximate value to the Al/Mg ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Kahn A., Lejus A.M., Madsac M., Thery J., Vivien D., Bernier J.C. (1981), J. Appl. Phys. 52, 6864-6869.

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hP68

AgAl <sub>11</sub> O <sub>17</sub>	hP68	(194) $P6_3/mmc - k^3h^2f^3eba$
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**AgAl<sub>11</sub>O<sub>17</sub>** [1],  $\beta$  alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and AgO layers (split sites, Ag near BR and at aBR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Newsam J.M. et al. (1990) [1]

AgAl<sub>11</sub>O<sub>17</sub>

$a = 0.55913$ ,  $c = 2.25293$  nm,  $c/a = 4.029$ ,  $V = 0.6100$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1569	0.3138	0.05		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1665	0.333	0.6067		octahedron O <sub>6</sub>
O3	12k	.m.	0.5021	0.0042	0.1459		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.306	0.612	1/4	0.333	
Ag5	6h	mm2	0.762	0.524	1/4	0.247	
Al6	4f	3m.	1/3	2/3	0.0254		tetrahedron O <sub>4</sub>
Al7	4f	3m.	1/3	2/3	0.1753		
O8	4f	3m.	1/3	2/3	0.5551		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.1421		non-coplanar triangle Al <sub>3</sub>
Ag10	2b	-6m2	0	0	1/4	0.26	trigonal bipyramid Ag <sub>3</sub> O <sub>2</sub>
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.042, T = 298 K

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

References: [1] Newsam J.M., Cheetham A.K., Tofield B.C. (1990), J. Phys.: Condens. Matter 2, 2335-2344.

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hP68

$\text{Na}_{1.3}\text{Al}_{10.9}\text{O}_{17}$	<i>hP68</i>	(194) $P6_3/mmc - k^3h^2f^3eda$
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**$\text{Na}_{1.3}\text{Al}_{10.9}\text{O}_{17}$**  [1],  $\beta$  alumina-Na;  $\text{K}_{1.55}\text{Fe}_{10.92}\text{O}_{17}$  [2], ferrite M-type

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and NaO layers (Na near BR and mO positions) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Peters C.R. et al. (1971) [1]

$\text{Al}_{11}\text{Na}_{1.27}\text{O}_{17}$

$a = 0.5594$ ,  $c = 2.253$  nm,  $c/a = 4.028$ ,  $V = 0.6106$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.15711	0.31421	0.55011		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.16775	0.3355	0.1063		octahedron O <sub>6</sub>
O3	12k	.m.	0.50318	0.00636	0.64678		non-coplanar triangle Al <sub>3</sub>
Na4	6h	mm2	0.1269	0.2538	$\frac{1}{4}$	0.174	
Na5	6h	mm2	0.2938	0.5876	$\frac{1}{4}$	0.25	
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05552		tetrahedron Al <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52477		tetrahedron O <sub>4</sub>
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67555		tetrahedron O <sub>4</sub>
O9	4e	3m.	0	0	0.14253		non-coplanar triangle Al <sub>3</sub>
O10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

Remarks: The authors of [1] give as probable cell content  $\text{Na}_{2.58}\text{Al}_{21.81}\text{O}_{34}$ . Refinement of the occupancies of the Al and O sites showed no significant deviation from unity. Short interatomic distances for partly occupied site(s).

References: [1] Peters C.R., Bettmann M., Moore J.W., Glick M.D. (1971), Acta Crystallogr. B 27, 1826-1834. [2] Boilot J.P., Colomban P., Collin G., Comes R. (1980), Solid State Ionics 1, 69-76.

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hP68

$\text{K}_{1.62}(\text{Mg}_{0.31}\text{Al}_{0.69})_2\text{Al}_9\text{O}_{17}$	<i>hP68</i>	(194) $P6_3/mmc - k^3h^2f^3eda$
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**$\text{K}_{1+x}\text{Mg}_x\text{Al}_{11-x}\text{O}_{17}$**  [1],  $\beta$  alumina(Al,Mg)-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and outer tetrahedral, (Al,Mg) in inner tetrahedral voids) and  $\text{K}_{1+x}\text{O}$  layers (K near BR and mO positions) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single (Al,Mg) $\text{O}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Collin G. et al. (1980) [1]

$\text{Al}_{10.38}\text{K}_{1.62}\text{Mg}_{0.62}\text{O}_{17}$

$a = 0.5608$ ,  $c = 2.256$  nm,  $c/a = 4.023$ ,  $V = 0.6144$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1543	0.3086	0.5508		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.167	0.334	0.1056		octahedron O <sub>6</sub>
O3	12k	.m.	0.5023	0.0046	0.6463		non-coplanar triangle Al <sub>3</sub>
K4	6h	mm2	0.1156	0.2312	1/4	0.313	
K5	6h	mm2	0.3284	0.6568	1/4	0.228	
O6	4f	3m.	1/3	2/3	0.057		tetrahedron Al <sub>4</sub>
M7	4f	3m.	1/3	2/3	0.5249		tetrahedron O <sub>4</sub>
Al8	4f	3m.	1/3	2/3	0.6742		tetrahedron O <sub>4</sub>
O9	4e	3m.	0	0	0.1434		non-coplanar triangle Al <sub>3</sub>
O10	2d	-6m2	1/3	2/3	3/4		colinear Al <sub>2</sub>
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M7 = 0.69Al + 0.31Mg

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

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

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

References: [1] Collin G., Comes R., Boilot J.P., Colomban P. (1980), Solid State Ionics 1, 59-68.

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hP68

Ba <sub>0.98</sub> Eu <sub>0.02</sub> (Mg <sub>0.5</sub> Al <sub>0.5</sub> ) <sub>2</sub> Al <sub>9</sub> O <sub>17</sub>	hP68	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>2</sup> f <sup>3</sup> eda
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**BaMgAl<sub>10</sub>O<sub>17</sub>:Eu<sup>2+</sup>** [1], β alumina(Al,Mg)-Ba,Eu

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Ba,Eu)<sub>x</sub>O layers (split O site, Ba at and Eu near BR positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Chernaya N.G. et al. (1989) [1]

Al<sub>11</sub>Ba<sub>0.91</sub>Eu<sub>0.02</sub>O<sub>17</sub>

*a* = 0.5645, *c* = 2.26958 nm, *c/a* = 4.021, *V* = 0.6263 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1542	0.3084	0.0511		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1662	0.3324	0.6055		octahedron O <sub>6</sub>
O3	12k	.m.	0.5041	0.0082	0.1479		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.315	0.63	1/4	0.333	
Eu5	6h	mm2	0.7039	0.4078	1/4	0.008	
Al6	4f	3m.	1/3	2/3	0.024		tetrahedron O <sub>4</sub>
Al7	4f	3m.	1/3	2/3	0.1745		
O8	4f	3m.	1/3	2/3	0.5583		tetrahedron Al <sub>4</sub>
O9	4e	3m.	0	0	0.1439		non-coplanar triangle Al <sub>3</sub>
Ba10	2d	-6m2	1/3	2/3	3/4	0.909	
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.027

Remarks: Mg not located. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). In [1] the Wyckoff positions of former Eu and O(5) are misprinted as 2d and 2c instead of 6h (site splitting).

References: [1] Chernaya N.G., Efremov V.A., Trunov V.K., Pisarenko V.F. (1989), 12th Eur. Crystallogr. Meet., Moscow 1989, Coll. Abstr. vol. 2, p. 48.

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hP68

MgEuAl <sub>11</sub> O <sub>19</sub>	hP68	(194) $P6_3/mmc - k^3hf^4edba$
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**EuMgAl<sub>11</sub>O<sub>19</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and EuO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and trigonal bipyramidal, (Mg,Al) in tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Mg,Al)O<sub>4</sub> tetrahedra, distinct positions for Mg and Al) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>5</sub> trigonal bipyramids and Eu atoms.

Kim K.B. et al. (2003) [1]

Al<sub>11</sub>EuMgO<sub>19</sub>

$a = 0.557$ ,  $c = 2.2$  nm,  $c/a = 3.95$ ,  $V = 0.5911$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1497	0.2994	0.0615		
Al2	12k	.m.	0.1894	0.3788	0.6095		single atom O
O3	12k	.m.	0.5088	0.0176	0.6591		single atom Al
O4	6h	mm2	0.143	0.2861	1/4		single atom Al
Mg5	4f	3m.	1/3	2/3	0.0166	0.5	
Al6	4f	3m.	1/3	2/3	0.0181	0.5	
Al7	4f	3m.	1/3	2/3	0.1853		non-coplanar triangle O <sub>3</sub>
O8	4f	3m.	1/3	2/3	0.5987		non-coplanar triangle Al <sub>3</sub>
O9	4e	3m.	0	0	0.1629		single atom Al
Eu10	2d	-6m2	1/3	2/3	3/4		anticuboctahedron O <sub>12</sub>
Al11	2b	-6m2	0	0	1/4		trigonal bipyramid O <sub>5</sub>
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.081

Remarks: Refinement on combined X-ray and neutron diffraction data, considering also parameters of Ba<sub>1-x</sub>Eu<sub>x</sub>MgAl<sub>10</sub>O<sub>17</sub>. Cell parameters omitted in [1], we took approximate values from the literature. Short interatomic distances for partly occupied site(s). Large differences between interatomic distances within the same coordination polyhedra. We assume that in table 1b of [1] the z-coordinate of former Al(2) is misprinted as 0.0811 instead of 0.0181 (better agreement with the description of the structure). Several site labels in table 2 (interatomic distances) do not correspond to those assigned in table 1.

References: [1] Kim K.B., Koo K.W., Cho T.Y., Chun H.G. (2003), Mater. Chem. Phys. 80, 682-689.

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hP68

NaNp <sub>3</sub> F <sub>13</sub>	hP68	(194) $P6_3/mmc - k^3ihf^2ed$
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**NaNp<sub>3</sub>F<sub>13</sub>** [1]

Structural features: NpF<sub>8</sub>F monocapped square antiprisms (NpF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms) share atoms to form a 3D-framework; additional F in hexagonal prismatic, Na in tetrahedral voids.

Cousson A. et al. (1983) [1]

F<sub>13</sub>NaNp<sub>3</sub>

$a = 0.8022$ ,  $c = 1.6513$  nm,  $c/a = 2.058$ ,  $V = 0.9203$  nm<sup>3</sup>,  $Z = 4$



site	Wyck.	sym.	x	y	z	occ.	atomic environment
Np1	12k	.m.	0.1619	0.3238	0.1129		tricapped trigonal prism F <sub>9</sub>
F2	12k	.m.	0.168	0.336	0.6479		non-colinear Np <sub>2</sub>
F3	12k	.m.	0.5385	0.077	0.6642		non-colinear Np <sub>2</sub>
F4	12i	.2.	0.3305	0	0		non-colinear Np <sub>2</sub>
F5	6h	mm2	0.135	0.27	<sup>1</sup> / <sub>4</sub>		non-colinear Np <sub>2</sub>
F6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0571		single atom Na
Na7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5896		trigonal bipyramid F <sub>5</sub>
F8	4e	3m.	0	0	0.0862		non-coplanar triangle Np <sub>3</sub>
F9	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		colinear Na <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.066

References: [1] Cousson A., Abazli H., Pages M., Gasperin M. (1983), Acta Crystallogr. C 39, 318-320.

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hP68

Er <sub>1.85</sub> Fe <sub>17.30</sub> N <sub>2.58</sub>	hP68	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kj <sup>2</sup> h <sup>2</sup> gfedcb
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### Er<sub>1.85</sub>Fe<sub>17.30</sub>N<sub>2.58</sub> [1]

Structural features: Filled-up derivative of Th<sub>2</sub>Ni<sub>7</sub> with N in octahedral (Er<sub>2</sub>Fe<sub>4</sub>) voids; partial disorder Er/Fe<sub>2</sub> and complex splitting of the site forming the hexagon mesh.

Voronin V.I. et al. (1998) [1]

Er<sub>1.85</sub>Fe<sub>17.30</sub>N<sub>2.58</sub>

*a* = 0.86193, *c* = 0.84896 nm, *c/a* = 0.985, *V* = 0.5462 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12k	.m.	0.1674	0.3347	0.0196		single atom N
Fe2	12j	m..	0.297	0.012	<sup>1</sup> / <sub>4</sub>	0.2	
Fe3	12j	m..	0.387	0.055	<sup>1</sup> / <sub>4</sub>	0.8	
N4	6h	mm2	0.162	0.324	<sup>1</sup> / <sub>4</sub>	0.82	non-colinear Fe <sub>2</sub>
N5	6h	mm2	0.828	0.656	<sup>1</sup> / <sub>4</sub>	0.04	
Fe6	6g	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		
Fe7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6091	0.89	
Fe8	4e	3m.	0	0	0.111	0.26	
Er9	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.08	
Er10	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		coplanar triangle N <sub>3</sub>
Er11	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>	0.77	

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.026

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

References: [1] Voronin V.I., Zinin A.V., Kudrevatykh N.V., Pirogov A.N. (1998), J. Alloys Compd. 266, 39-42.

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hP68

Yb <sub>1.85</sub> Fe <sub>17.30</sub>	hP68	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – kj <sup>3</sup> gfedcb
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**Yb<sub>1.85</sub>Fe<sub>17.30</sub>** [1]

Structural features: Kagomé-mesh Fe<sub>9</sub> layers and YbYb<sub>2-x</sub>(Fe<sub>2</sub>)<sub>x</sub>Fe<sub>6</sub> layers (a Fe hexagon mesh, the hexagons of which are centered by an Yb atom or a Fe<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder). Variant of Th<sub>2</sub>Ni<sub>17</sub> with a partly disordered arrangement of Yb atoms and Fe<sub>2</sub> dumbbells and complex splitting of the site forming the hexagon mesh.

Cerny R. et al. (2003) [1]

Fe<sub>17.31</sub>Yb<sub>1.85</sub>

$a = 0.8413$ ,  $c = 0.8297$  nm,  $c/a = 0.986$ ,  $V = 0.5086$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	12 <i>k</i>	. <i>m</i> .	0.1664	0.3328	0.0151		
Fe2	12 <i>j</i>	<i>m</i> ..	0.0	0.289	<sup>1</sup> / <sub>4</sub>	0.14	
Fe3	12 <i>j</i>	<i>m</i> ..	0.0	0.3333	<sup>1</sup> / <sub>4</sub>	0.046	
Fe4	12 <i>j</i>	<i>m</i> ..	0.3704	0.0415	<sup>1</sup> / <sub>4</sub>	0.814	
Fe5	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		
Fe6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6064	0.883	
Fe7	4 <i>e</i>	3 <i>m</i> .	0	0	0.106	0.271	
Yb8	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.117	
Yb9	2 <i>c</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		
Yb10	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.729	

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.019$

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

References: [1] Cerny R., Pacheco V., Yanson T., Manyako M., Bodak O. (2003), Z. Kristallogr. 218, 802-810.

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hP70

La<sub>0.9</sub>(Co<sub>0.375</sub>Al<sub>0.625</sub>)<sub>2</sub>Al<sub>9.95</sub>O<sub>18.9</sub>

hP70

(194) *P6<sub>3</sub>/mmc* –  $k^3h^2f^3e^2a$

**La<sub>0.9</sub>Co<sub>0.75</sub>Al<sub>11.2</sub>O<sub>18.9</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral, (Al,Co) in tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Al,Co)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (split site).

Gasparin M. et al. (1984) [1]

Al<sub>11.13</sub>Co<sub>0.75</sub>La<sub>0.90</sub>O<sub>19</sub>

$a = 0.5577$ ,  $c = 2.2003$  nm,  $c/a = 3.945$ ,  $V = 0.5927$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.153	0.306	0.0536		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.1675	0.335	0.6079		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5034	0.0068	0.1505		non-coplanar triangle Al <sub>3</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.1853	0.3706	<sup>1</sup> / <sub>4</sub>		
La5	6 <i>h</i>	<i>mm</i> 2	0.677	0.354	<sup>1</sup> / <sub>4</sub>	0.3	
M6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0265		tetrahedron O <sub>4</sub>
Al7	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1894		octahedron O <sub>6</sub>
O8	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5571		tetrahedron Al <sub>4</sub>
O9	4 <i>e</i>	3 <i>m</i> .	0	0	0.15		tetrahedron Al <sub>4</sub>

Al10	4e	3m.	0	0	0.2382	0.44
Al11	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

M6 = 0.625Al + 0.375Co

Experimental: single crystal, diffractometer, X-rays, R = 0.060

Remarks: The authors state that Co substitutes for Al mainly on site M6 and in minor amounts on site Al11. We assigned an approximate value to the Co/Al ratio of site M6 based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Gasperin M., Saine M.C., Kahn A., Laville F., Lejus A.M. (1984), J. Solid State Chem. 54, 61-69.

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hP70

TlAl <sub>11</sub> O <sub>17</sub>	hP70	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>2</sup> f <sup>3</sup> edba
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TlAl<sub>11</sub>O<sub>17</sub> [1], β alumina-Tl

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and TlO layers (Tl near BR, at aBr and between aBr and mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Collin G. et al. (1977) [1]

Al<sub>11</sub>O<sub>17</sub>Tl<sub>1.24</sub>

*a* = 0.5596, *c* = 2.2912 nm, *c/a* = 4.094, *V* = 0.6214 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	.m.	0.1577	0.3154	0.5488		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	.m.	0.1676	0.3352	0.1042		octahedron O <sub>6</sub>
O3	12 <i>k</i>	.m.	0.5021	0.0042	0.6437		non-coplanar triangle Al <sub>3</sub>
Tl4	6 <i>h</i>	<i>mm</i> 2	0.0901	0.1802	<sup>1</sup> / <sub>4</sub>	0.085	
Tl5	6 <i>h</i>	<i>mm</i> 2	0.3193	0.6386	<sup>1</sup> / <sub>4</sub>	0.292	
O6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0548		tetrahedron Al <sub>4</sub>
Al7	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5246		tetrahedron O <sub>4</sub>
Al8	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6748		tetrahedron O <sub>4</sub>
O9	4 <i>e</i>	3 <i>m</i> .	0	0	0.1397		non-coplanar triangle Al <sub>3</sub>
O10	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		colinear Al <sub>2</sub>
Tl11	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.105	
Al12	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). In table II of [1] the Wyckoff position of former O(5) is misprinted as 6*h* instead of 2*c*.

References: [1] Collin G., Boilot J.P., Kahn A., Thery J., Comes R. (1977), J. Solid State Chem. 21, 283-292.

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hP70

(Mg <sub>0.5</sub> Al <sub>0.5</sub> ) <sub>2</sub> (La <sub>0.95</sub> Al <sub>0.05</sub> )Al <sub>11</sub> O <sub>19</sub>	hP70	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>2</sup> f <sup>3</sup> edba
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La<sub>1-x</sub>MgAl<sub>11+x</sub>O<sub>19</sub> [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and (La,Al)O<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and trigonal bipyramidal, (Al,Mg) in tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>5</sub> trigonal bipyramids and (La,Al) atoms (in part displaced from the ideal position).

Abrahams S.C. et al. (1987) [1]

Al<sub>11.05</sub>La<sub>0.95</sub>MgO<sub>19</sub>

$a = 0.55898$ ,  $c = 2.19738$  nm,  $c/a = 3.931$ ,  $V = 0.5946$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.15236	0.30471	0.05344		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.16752	0.33505	0.60795		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5048	0.00961	0.15093		non-coplanar triangle Al <sub>3</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.18127	0.36254	<sup>1</sup> / <sub>4</sub>		coplanar triangle Al <sub>3</sub>
M5	6 <i>h</i>	<i>mm</i> 2	0.7269	0.4538	<sup>1</sup> / <sub>4</sub>	0.017	
M6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0273		tetrahedron O <sub>4</sub>
Al7	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.18957		octahedron O <sub>6</sub>
O8	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.55791		tetrahedron Al <sub>4</sub>
O9	4 <i>e</i>	3 <i>m</i> .	0	0	0.15086		tetrahedron Al <sub>4</sub>
M10	2 <i>d</i>	-6 <i>m</i> 2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>	0.948	
Al11	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>		trigonal bipyramid O <sub>5</sub>
Al12	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M5 = 0.95La + 0.05Al; M6 = 0.5Al + 0.5Mg; M10 = 0.95La + 0.05Al

Experimental: single crystal, diffractometer, X-rays, R = 0.014, T = 295 K

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

References: [1] Abrahams S.C., Marsh P., Brandle C.D. (1987), J. Chem. Phys. 86, 4221-4227.

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hP70

BaCrO <sub>3</sub>	hP70	(194) <i>P6</i> <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> hf <sup>4</sup> e <sup>2</sup> da
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**BaCrO<sub>3</sub> 14H** [1], perovskite 14H

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub>hchc stacking; Cr in octahedral (O<sub>6</sub>) voids. Units of two face-linked CrO<sub>6</sub> octahedra (Cr<sub>2</sub> dumbbells) and single CrO<sub>6</sub> octahedra share vertices to form a 3D-framework.

Chamberland B.L., Katz L. (1982) [1]

BaCrO<sub>3</sub>

$a = 0.565$ ,  $c = 3.2467$  nm,  $c/a = 5.746$ ,  $V = 0.8976$  nm<sup>3</sup>,  $Z = 14$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1664	0.3328	0.6779		non-colinear Cr <sub>2</sub>
O2	12 <i>k</i>	. <i>m</i> .	0.1676	0.3352	0.5344		non-colinear Cr <sub>2</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5179	0.0358	0.1061		non-colinear Cr <sub>2</sub>
O4	6 <i>h</i>	<i>mm</i> 2	0.1511	0.3022	<sup>1</sup> / <sub>4</sub>		non-colinear Cr <sub>2</sub>
Ba5	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.03904		cuboctahedron O <sub>12</sub>
Ba6	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.17328		cuboctahedron O <sub>12</sub>
Cr7	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.56492		octahedron O <sub>6</sub>
Cr8	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.64506		octahedron O <sub>6</sub>
Ba9	4 <i>e</i>	3 <i>m</i> .	0	0	0.10499		anticuboctahedron O <sub>12</sub>
Cr10	4 <i>e</i>	3 <i>m</i> .	0	0	0.20886		octahedron O <sub>6</sub>

Ba11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	anticuboctahedron O <sub>12</sub>
Cr12	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. In table 1 of [1] the *y*-coordinate of former O(4) is misprinted as 0.3203 instead of 0.3023, the *x*-coordinate of former O(3) as 0.1644 instead of 0.1664 and the *z*-coordinate of the same site as 0.6799 instead of 0.6779 (agreement with Wyckoff positions 6*h* and 12*k*; checked on interatomic distances).

References: [1] Chamberland B.L., Katz L. (1982), Acta Crystallogr. B 38, 54-57.

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hP70

Na <sub>11</sub> Ba <sub>7</sub> Ca <sub>0.5</sub> N <sub>3</sub>	hP70	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>4</sup> hgfea
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### Na<sub>22</sub>Ba<sub>14</sub>CaN<sub>6</sub> [2]

Structural features: CaN<sub>6</sub>Ba<sub>14</sub> clusters (a central Ca atom surrounded by a N<sub>6</sub> octahedron, a Ba<sub>8</sub> cube and a large Ba<sub>6</sub> octahedron) in a matrix of Na atoms; disorder described as a superposition of rods in two different orientations.

Steinbrenner U., Simon A. (1997) [1]

Ba<sub>7</sub>Ca<sub>0.50</sub>N<sub>3</sub>Na<sub>11</sub>

*a* = 1.2666, *c* = 1.2635 nm, *c/a* = 0.998, *V* = 1.7554 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	12 <i>k</i>	. <i>m</i> .	0.096	0.192	0.1183	0.5	coplanar triangle Ba <sub>2</sub> Ca
Ba2	12 <i>k</i>	. <i>m</i> .	0.14085	0.2817	0.58732	0.5	
Na3	12 <i>k</i>	. <i>m</i> .	0.1599	0.3198	0.5651	0.5	
Ba4	12 <i>k</i>	. <i>m</i> .	0.18986	0.37972	0.23102	0.5	
Na5	6 <i>h</i>	<i>mm</i> 2	0.5677	0.1354	$\frac{1}{4}$		octahedron N <sub>6</sub>
Na6	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		
Na7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0073		
Ba8	4 <i>e</i>	3 <i>m</i> .	0	0	0.2382	0.5	
Ca9	2 <i>a</i>	-3 <i>m</i> .	0	0	0	0.5	

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.036, T = 293 K

Remarks: Short interatomic distances for partly occupied site(s). A slightly different model for disorder is proposed for data collected at 128 K. The same data are reported in [2].

References: [1] Steinbrenner U., Simon A. (1997), Z. Kristallogr. 212, 428-438. [2] Simon A., Steinbrenner U. (1996), J. Chem. Soc., Faraday Trans. 92, 2117-2123.

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hP72

MgLaGa <sub>11</sub> O <sub>19</sub>	hP72	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>2</sup> f <sup>3</sup> e <sup>2</sup> da
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### LaMgGa<sub>11</sub>O<sub>19</sub> [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Ga and (Ga,Mg) in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked GaO<sub>6</sub> and (Ga,Mg)O<sub>6</sub> octahedra sharing vertices with single (Ga,Mg)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked GaO<sub>6</sub> octahedra, GaO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (ideal and split site).

Lefebvre D. et al. (1985) [1]

$\text{Ga}_{10.95}\text{La}_{0.95}\text{MgO}_{19}$

$a = 0.5806$ ,  $c = 2.2727$  nm,  $c/a = 3.914$ ,  $V = 0.6635$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.152	0.304	0.053		tetrahedron Ga <sub>4</sub>
Ga2	12k	.m.	0.1644	0.3288	0.6084		octahedron O <sub>6</sub>
O3	12k	.m.	0.505	0.01	0.1508		non-coplanar triangle Ga <sub>3</sub>
O4	6h	mm2	0.182	0.364	$\frac{1}{4}$		
La5	6h	mm2	0.7234	0.4468	$\frac{1}{4}$	0.06	
M6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0265		tetrahedron O <sub>4</sub>
Ga7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1884		octahedron O <sub>6</sub>
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5576		tetrahedron Ga <sub>4</sub>
O9	4e	3m.	0	0	0.1499		tetrahedron Ga <sub>4</sub>
Ga10	4e	3m.	0	0	0.2414	0.475	
La11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.77	
M12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M6 = 0.625Ga + 0.375Mg; M12 = 0.75Ga + 0.25Mg

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

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

References: [1] Lefebvre D., Kahn A., Thery J. (1985), C. R. Acad. Sci., Ser. II 300, 263-268.

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hP72

TlAl <sub>11</sub> O <sub>17</sub>	hP72	(194) $P6_3/mmc - k^3h^2f^3edcba$
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**TlAl<sub>11</sub>O<sub>17</sub>** [1],  $\beta$  alumina-Tl; RbAl<sub>11</sub>O<sub>17</sub> [2],  $\beta$  alumina-Rb

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and TlO layers (partial disorder, Tl near and at BR and aBr positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Kodama T., Muto G. (1976) [1]

Al<sub>11</sub>O<sub>17</sub>Tl<sub>1.33</sub>

$a = 0.5598$ ,  $c = 2.293$  nm,  $c/a = 4.096$ ,  $V = 0.6223$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1581	0.3162	0.5489		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1677	0.3353	0.1042		octahedron O <sub>6</sub>
O3	12k	.m.	0.5015	0.003	0.6445		non-coplanar triangle Al <sub>3</sub>
Tl4	6h	mm2	0.0767	0.1535	$\frac{1}{4}$	0.122	
Tl5	6h	mm2	0.3312	0.6624	$\frac{1}{4}$	0.22	
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0547		tetrahedron Al <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5244		tetrahedron O <sub>4</sub>
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.675		tetrahedron O <sub>4</sub>
O9	4e	3m.	0	0	0.1401		non-coplanar triangle Al <sub>3</sub>
O10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Tl11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.27	
Tl12	2b	-6m2	0	0	$\frac{1}{4}$	0.036	
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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

References: [1] Kodama T., Muto G. (1976), J. Solid State Chem. 17, 61-70. [2] Kodama T., Muto G. (1976), J. Solid State Chem. 19, 35-44.

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hP72

$K_{1.27}Al_{10.91}O_{17}$	hP72	(194) $P6_3/mmc - k^3h^3f^3ea$
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$K_{1.25}Al_{10.915}O_{17}$  [1],  $\beta$  alumina-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and KO layers (partial disorder, K near BR and mO positions) alternate along [001]. Infinite slabs of edge-linked  $AlO_6$  octahedra sharing vertices with single  $AlO_4$  tetrahedra are interconnected via units of two vertex-linked  $AlO_4$  tetrahedra to form a 3D-framework.

Dernier P.D., Remeika J.P. (1976) [1]

$Al_{11}K_{1.32}O_{16.95}$

$a = 0.5591$ ,  $c = 2.2711$  nm,  $c/a = 4.062$ ,  $V = 0.6148$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.157	0.314	0.54944		tetrahedron $Al_4$
Al2	12k	.m.	0.16797	0.33594	0.10489		octahedron $O_6$
O3	12k	.m.	0.5029	0.0058	0.64602		non-coplanar triangle $Al_3$
K4	6h	mm2	0.1148	0.2296	$\frac{1}{4}$	0.203	
K5	6h	mm2	0.3117	0.6234	$\frac{1}{4}$	0.237	
O6	6h	mm2	0.6892	0.3784	$\frac{1}{4}$	0.318	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0551		tetrahedron $Al_4$
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52455		tetrahedron $O_4$
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67484		
O10	4e	3m.	0	0	0.1416		non-coplanar triangle $Al_3$
Al11	2a	-3m.	0	0	0		octahedron $O_6$

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

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

Remarks: The authors state that excess K found with respect to stoichiometric  $KAl_{11}O_{17}$  is probably compensated for by Al vacancies, however, the occupancies of the Al sites were fixed to unity for the refinement. Short interatomic distances for partly occupied site(s).

References: [1] Dernier P.D., Remeika J.P. (1976), J. Solid State Chem. 17, 245-253.

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hP72

$K_{1.25}Co_{0.1}Al_{10.85}O_{17}$	hP72	(194) $P6_3/mmc - k^3h^3f^3ea$
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$K_{1.25}Co_{0.1}Al_{10.85}O_{17}$  [1],  $\beta$  alumina(Al,Co)-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and outer tetrahedral, (Al,Co) in inner tetrahedral voids) and  $K_xO$  layers (split O site, K near BR and mO positions) alternate along [001]. Infinite slabs of edge-linked  $AlO_6$  octahedra sharing vertices with single  $AlO_4$  tetrahedra are interconnected via units of two vertex-linked  $AlO_4$  tetrahedra to form a 3D-framework.

Dernier P.D., Remeika J.P. (1976) [1]

$\text{Al}_{10.70}\text{Co}_{0.30}\text{K}_{1.34}\text{O}_{16.90}$

$a = 0.5601$ ,  $c = 2.2722$  nm,  $c/a = 4.057$ ,  $V = 0.6173$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1564	0.3128	0.5497		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.16777	0.33554	0.10505		octahedron O <sub>6</sub>
O3	12k	.m.	0.503	0.006	0.64591		non-coplanar triangle Al <sub>3</sub>
K4	6h	mm2	0.115	0.23	$\frac{1}{4}$	0.203	
K5	6h	mm2	0.3117	0.6234	$\frac{1}{4}$	0.243	
O6	6h	mm2	0.6872	0.3744	$\frac{1}{4}$	0.3	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0554		tetrahedron Al <sub>4</sub>
M8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52446		tetrahedron O <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67465		
O10	4e	3m.	0	0	0.1414		non-coplanar triangle Al <sub>3</sub>
Al11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M8 = 0.85Al + 0.15Co

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

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

Remarks: The authors state that excess K is probably compensated for by Al vacancies. Short interatomic distances for partly occupied site(s). In table I of [1] the y-coordinate of former O(5) is misprinted as 0.6526 instead of 0.6256 (agreement with Wyckoff position 6h).

References: [1] Dernier P.D., Remeika J.P. (1976), J. Solid State Chem. 17, 245-253.

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hP74

$\text{Na}_{0.77}\text{Nd}_{0.26}(\text{Al}_{0.66}\text{Ga}_{0.34})_{11}\text{O}_{17.27}$

hP74

(194)  $P6_3/mmc - k^3h^3f^3eba$

**Na<sub>0.77</sub>Nd<sub>0.26</sub>(Al,Ga)<sub>11</sub>O<sub>17.27</sub>** [1], β alumina(Al,Ga)-Na,Nd

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, (Al,Ga) in octahedral and outer tetrahedral, Ga in inner tetrahedral voids) and (Na,Nd,O)<sub>x</sub>O layers (split framework O site, Nd near BR, Na at aBR, (Na,O) near mO positions) alternate along [001]. Infinite slabs of edge-linked (Al,Ga)O<sub>6</sub> octahedra sharing vertices with single GaO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked (Al,Ga)O<sub>4</sub> tetrahedra to form a 3D-framework.

Kahn Harari A. et al. (1991) [1]

$\text{Al}_{7.28}\text{Ga}_{3.72}\text{Na}_{0.76}\text{Nd}_{0.26}\text{O}_{17.28}$

$a = 0.5644$ ,  $c = 2.261$  nm,  $c/a = 4.006$ ,  $V = 0.6237$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.153	0.306	0.5506		tetrahedron GaAl <sub>3</sub>
M2	12k	.m.	0.1675	0.335	0.1083		octahedron O <sub>6</sub>
O3	12k	.m.	0.5043	0.0086	0.6477		non-coplanar triangle Al <sub>3</sub>
M4	6h	mm2	0.1991	0.3982	$\frac{1}{4}$	0.28	
Nd5	6h	mm2	0.3108	0.6216	$\frac{1}{4}$	0.087	
O6	6h	mm2	0.621	0.242	$\frac{1}{4}$	0.333	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0573		tetrahedron GaAl <sub>3</sub>
Ga8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5246		tetrahedron O <sub>4</sub>
M9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6774		
O10	4e	3m.	0	0	0.1433		non-coplanar triangle Al <sub>3</sub>
Na11	2b	-6m2	0	0	$\frac{1}{4}$	0.2	trigonal bipyramid Na <sub>3</sub> O <sub>2</sub>



M12    2a   -3m.    0    0    0    octahedron O<sub>6</sub>

M2 = 0.83Al + 0.17Ga; M4 = 0.667Na + 0.333O; M9 = 0.7Al + 0.3Ga; M12 = 0.90Al + 0.10Ga

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

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: We set the *z*-coordinate of former (Na<sub>2</sub>O) equal to  $\frac{1}{4}$  since the refined value within the standard uncertainty corresponds to Wyckoff position 6*h*. Short interatomic distances for partly occupied site(s).

References: [1] Kahn Harari A., Aka G., Thery J. (1991), J. Solid State Chem. 91, 71-81.

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hP74

Na <sub>1.32</sub> (Al <sub>0.65</sub> Ga <sub>0.35</sub> ) <sub>11</sub> O <sub>17.16</sub>	hP74	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>3</sup> f <sup>3</sup> eca
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**Na<sub>1.32</sub>(Al,Ga)<sub>11</sub>O<sub>17.16</sub>** [1], β alumina(Al,Ga)-Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, (Al,Ga) in octahedral and outer tetrahedral, Ga in inner tetrahedral voids) and Na<sub>1+2x</sub>O<sub>1+x</sub> layers (split framework O site, Na at and near BR, (Na,O) near mO positions) alternate along [001]. Infinite slabs of edge-linked (Al,Ga)O<sub>6</sub> octahedra sharing vertices with GaO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked (Al,Ga)O<sub>4</sub> tetrahedra to form a 3D-framework.

Kahn Harari A. et al. (1991) [1]

Al<sub>7.16</sub>Ga<sub>3.84</sub>Na<sub>1.31</sub>O<sub>17.16</sub>

*a* = 0.5667, *c* = 2.2663 nm, *c/a* = 3.999, *V* = 0.6303 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1531	0.3062	0.5511		tetrahedron GaAl <sub>3</sub>
M2	12 <i>k</i>	. <i>m</i> .	0.1676	0.3352	0.1079		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5038	0.0076	0.6475		non-coplanar triangle Al <sub>3</sub>
M4	6 <i>h</i>	<i>mm</i> 2	0.0997	0.1994	$\frac{1}{4}$	0.21	
Na5	6 <i>h</i>	<i>mm</i> 2	0.2297	0.4594	$\frac{1}{4}$	0.04	
O6	6 <i>h</i>	<i>mm</i> 2	0.6977	0.3954	$\frac{1}{4}$	0.333	
O7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0573		tetrahedron GaAl <sub>3</sub>
M8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5248		tetrahedron O <sub>4</sub>
M9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6758		
O10	4 <i>e</i>	3 <i>m</i> .	0	0	0.1441		non-coplanar triangle Al <sub>3</sub>
Na11	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.72	
M12	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M2 = 0.81Al + 0.19Ga; M4 = 0.75Na + 0.25O; M8 = 0.97Ga + 0.03Al; M9 = 0.67Al + 0.33Ga; M12 = 0.90Al + 0.10Ga

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

Experimental: single crystal, diffractometer, X-rays, R = 0.029

Remarks: We assigned an approximate value to the Na/O ratio of former Na(mO) based on the nominal composition. The authors state that small (not defined) amounts of Al(Ga) were detected in Wyckoff position 12*k*: -0.1667 2x 0.1745 (0.1667 2x 0.1745 after standardization). Short interatomic distances for partly occupied site(s).

References: [1] Kahn Harari A., Aka G., Thery J. (1991), J. Solid State Chem. 91, 71-81.

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hP76

La(Mn <sub>0.5</sub> Al <sub>0.5</sub> ) <sub>2</sub> Al <sub>9</sub> O <sub>19</sub>	hP76	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>3</sup> h <sup>3</sup> f <sup>3</sup> e <sup>2</sup> a
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**LaMnAl<sub>11</sub>O<sub>19</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral, (Al,Mn) in tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Al,Mn)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (two split sites).

Gasperin M. et al. (1984) [1]

Al<sub>11</sub>La<sub>0.99</sub>MnO<sub>19</sub>

$a = 0.5574$ ,  $c = 2.2008$  nm,  $c/a = 3.948$ ,  $V = 0.5922$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1539	0.3078	0.0526		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1672	0.3344	0.6083		octahedron O <sub>6</sub>
O3	12k	.m.	0.5056	0.0112	0.1501		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.1811	0.3622	$\frac{1}{4}$		
La5	6h	mm2	0.6676	0.3352	$\frac{1}{4}$	0.28	
La6	6h	mm2	0.7373	0.4746	$\frac{1}{4}$	0.05	
M7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0275		tetrahedron O <sub>4</sub>
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1899		octahedron O <sub>6</sub>
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5568		tetrahedron Al <sub>4</sub>
O10	4e	3m.	0	0	0.1492		tetrahedron Al <sub>4</sub>
Al11	4e	3m.	0	0	0.2399	0.5	
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M7 = 0.50Al + 0.50Mn

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

Remarks: Short interatomic distances for partly occupied site(s). In table II of [1] the y-coordinate of former La(1) is misprinted as 0.3552 instead of 0.3352 (agreement with Wyckoff position 6h).

References: [1] Gasperin M., Saine M.C., Kahn A., Laville F., Lejus A.M. (1984), J. Solid State Chem. 54, 61-69.

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hP76

Na <sub>0.08</sub> Nd <sub>0.38</sub> Al <sub>11</sub> O <sub>17.10</sub>	hP76	(194) $P6_3/mmc - k^3h^3f^3edba$
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**Na<sub>0.08</sub>Nd<sub>0.38</sub>Al<sub>11</sub>O<sub>17.10</sub>** [1], β alumina-Nd

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Na,Al,O)<sub>x</sub>O layers (split framework O site, Nd at and near BR, (Na,Al) at aBR, additional O near mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Tietz F., Urland W. (1992) [1]

Al<sub>10.96</sub>Na<sub>0.06</sub>Nd<sub>0.37</sub>O<sub>17.26</sub>

$a = 0.55848$ ,  $c = 2.2406$  nm,  $c/a = 4.012$ ,  $V = 0.6052$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1573	0.3146	0.0502		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1678	0.3356	0.6077		octahedron O <sub>6</sub>
O3	12k	.m.	0.5032	0.0064	0.1477		non-coplanar triangle Al <sub>3</sub>
O4	6h	mm2	0.18	0.36	$\frac{1}{4}$	0.12	non-colinear O <sub>2</sub>
O5	6h	mm2	0.392	0.784	$\frac{1}{4}$	0.3	

Nd6	6h	mm2	0.769	0.538	$\frac{1}{4}$	0.017	
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0248		tetrahedron O <sub>4</sub>
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1776	0.96	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5562		tetrahedron Al <sub>4</sub>
O10	4e	3m.	0	0	0.1427		non-coplanar triangle Al <sub>3</sub>
Nd11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.32	
M12	2b	-6m2	0	0	$\frac{1}{4}$	0.104	coplanar triangle O <sub>3</sub>
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M12 = 0.615Na + 0.385Al

Experimental: single crystal, diffractometer, X-rays, wR = 0.045, T = 298 K

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

References: [1] Tietz F., Urland W. (1992), J. Solid State Chem. 100, 255-261.

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hP76

Fe <sub>12</sub> PbO <sub>19</sub>	hP76	(194) $P6_3/mmc - k^3jh^3e^2a$
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### **PbFe<sub>12</sub>O<sub>19</sub>** [1], magnetoplumbite

Structural features: Close-packed O<sub>4</sub> and PbO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Fe in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells), FeO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Pb atoms (lone-electron pair, split site).

Moore P.B. et al. (1989) [1]

Fe<sub>12</sub>O<sub>19</sub>Pb

$a = 0.5873$ ,  $c = 2.3007$  nm,  $c/a = 3.917$ ,  $V = 0.6872$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1565	0.313	0.0524		tetrahedron Fe <sub>4</sub>
Fe2	12k	.m.	0.1687	0.3374	0.60881		octahedron O <sub>6</sub>
O3	12k	.m.	0.5035	0.007	0.1499		non-coplanar triangle Fe <sub>3</sub>
Pb4	12j	m..	0.616	0.28	$\frac{1}{4}$	0.167	
O5	6h	mm2	0.1839	0.3678	$\frac{1}{4}$		
Fe6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.02733		tetrahedron O <sub>4</sub>
Fe7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.19019		octahedron O <sub>6</sub>
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5546		tetrahedron Fe <sub>4</sub>
O9	4e	3m.	0	0	0.1511		tetrahedron Fe <sub>4</sub>
Fe10	4e	3m.	0	0	0.2441	0.5	
Fe11	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Remarks: Short interatomic distances for partly occupied site(s). Supersedes a structure proposal with no site splitting in [2]. In [2] the z-coordinate of former Fe(5) is misprinted as 39° instead of -39° (see [3]).

References: [1] Moore P.B., Gupta P.K.S., Le Page Y. (1989), Am. Mineral. 74, 1186-1194. [2] Adelsköld V. (1938), Ark. Kemi Mineral. Geol. 12A(29), 1-9. [3] Braun P.B. (1957), Philips Res. Rep. 12, 491-548.

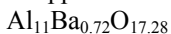
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hP76

Ba <sub>0.75</sub> Al <sub>11</sub> O <sub>17.25</sub>	hP76	(194) $P6_3/mmc - k^4hf^3edca$
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**Ba<sub>0.75</sub>Al<sub>11</sub>O<sub>17.25</sub>** [2],  $\beta$  alumina-Ba

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Ba<sub>1/2+x</sub>O<sub>1+x</sub> layers (Ba at BR, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Groppi G. et al. (1995) [1]



$a = 0.55876$ ,  $c = 2.2727$  nm,  $c/a = 4.067$ ,  $V = 0.6145$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.159	0.318	0.1745	0.094	trigonal bipyramid AlO <sub>4</sub>
O2	12k	.m.	0.1594	0.3189	0.55		tetrahedron Al <sub>4</sub>
Al3	12k	.m.	0.1672	0.3345	0.1044	0.906	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.5036	0.0072	0.6457		square pyramid Al <sub>5</sub>
O5	6h	mm2	0.125	0.25	<sup>1</sup> / <sub>4</sub>	0.094	non-colinear Al <sub>2</sub>
O6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0545		tetrahedron Al <sub>4</sub>
Al7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5239		tetrahedron O <sub>4</sub>
Al8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6753		tetrahedron O <sub>4</sub>
O9	4e	3m.	0	0	0.1426		trigonal prism Al <sub>6</sub>
O10	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		colinear Al <sub>2</sub>
Ba11	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.717	coplanar triangle O <sub>3</sub>
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, wR<sub>p</sub> = 0.169

Remarks: Short interatomic distances for partly occupied site(s). In table 1B of [1] the z-coordinate of former O1 is misprinted as 0.500 instead of 0.0500 (checked on interatomic distances).

References: [1] Groppi G., Assandri F., Bellotto M., Cristiani C., Forzatti P. (1995), J. Solid State Chem. 114, 326-336. [2] Van Berkel F.P.F., Zandbergen H.W., Verschoor G.C., Ijdo D.J.W. (1984), Acta Crystallogr. C 40, 1124-1127.

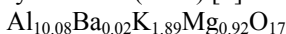
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hP78

$\text{K}_{1.88}\text{Ba}_{0.02}(\text{Mg}_{0.46}\text{Al}_{0.54})_2\text{Al}_9\text{O}_{17}$	<i>hP78</i>	(194) $P6_3/mmc - k^3h^3f^3edcba$
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**K<sub>1.88</sub>Ba<sub>0.02</sub>Mg<sub>0.92</sub>Al<sub>10.08</sub>O<sub>17</sub>** [1],  $\beta$  alumina(Al,Mg)-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and outer tetrahedral, (Al,Mg) in inner tetrahedral voids) and (K,Ba)<sub>x</sub>O layers (Ba near BR positions, K disordered within a hexagon mesh) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Iyi N. et al. (1986) [1]



$a = 0.56408$ ,  $c = 2.2645$  nm,  $c/a = 4.015$ ,  $V = 0.6240$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1533	0.3066	0.5515		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.167	0.334	0.10521		octahedron O <sub>6</sub>
O3	12k	.m.	0.5035	0.007	0.64714		non-coplanar triangle Al <sub>3</sub>
K4	6h	mm2	0.0888	0.1776	<sup>1</sup> / <sub>4</sub>	0.22	

K5	6h	mm2	0.179	0.358	$\frac{1}{4}$	0.12	
Ba6	6h	mm2	0.383	0.766	$\frac{1}{4}$	0.007	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05815		tetrahedron Al <sub>4</sub>
M8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52481		tetrahedron O <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67345		tetrahedron O <sub>4</sub>
O10	4e	3m.	0	0	0.14389		non-coplanar triangle Al <sub>3</sub>
O11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
K12	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.67	
K13	2b	-6m2	0	0	$\frac{1}{4}$	0.2	
Al14	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M8 = 0.54Al + 0.46Mg

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

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

Remarks: The authors state that Mg substitutes for Al mainly on site M8. We assigned an approximate value to the Mg/Al ratio of site M8 based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Iyi N., Inoue Z., Kimura S. (1986), J. Solid State Chem. 61, 236-244.

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hP78

Ag <sub>1.2</sub> Al <sub>11</sub> O <sub>17.1</sub>	hP78	(194) $P6_3/mmc - k^3h^4f^3ea$
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Ag<sub>1.20</sub>Al<sub>11</sub>O<sub>17.10</sub> [1], β alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and AgO layers (split framework O site, Ag near BR, aBR and mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Roth W.L. (1972) [1]

Ag<sub>1.27</sub>Al<sub>11</sub>O<sub>16.96</sub>

$a = 0.5595$ ,  $c = 2.2488$  nm,  $c/a = 4.019$ ,  $V = 0.6097$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1566	0.3132	0.5503		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1679	0.3358	0.1064		octahedron O <sub>6</sub>
O3	12k	.m.	0.5027	0.0054	0.647		non-coplanar triangle Al <sub>3</sub>
Ag4	6h	mm2	0.0247	0.0494	$\frac{1}{4}$	0.144	
Ag5	6h	mm2	0.1928	0.3856	$\frac{1}{4}$	0.056	
Ag6	6h	mm2	0.2903	0.5806	$\frac{1}{4}$	0.224	
O7	6h	mm2	0.6926	0.3852	$\frac{1}{4}$	0.319	
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0553		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5248		tetrahedron O <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6755		
O11	4e	3m.	0	0	0.1428		non-coplanar triangle Al <sub>3</sub>
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.065

Remarks: Part of O not located. Short interatomic distances for partly occupied site(s).

References: [1] Roth W.L. (1972), J. Solid State Chem. 4, 60-75.

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hP78

$\text{Na}_{0.5}\text{Li}_{0.74}\text{Al}_{11}\text{O}_{17.12}$	<i>hP78</i>	(194) $P6_3/mmc - k^4h^2f^3ea$
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**Na<sub>0.5</sub>Li<sub>0.74</sub>Al<sub>11</sub>O<sub>17.12</sub>** [1],  $\beta$  alumina-Li,Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Na,Li)O layers (split O site, Na near BR, Li above and below mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Tofield B.C., Farrington G.C. (1979) [1]

 $\text{Al}_{11}\text{Li}_{0.57}\text{Na}_{0.45}\text{O}_{17}$  $a = 0.55923$ ,  $c = 2.25576$  nm,  $c/a = 4.034$ ,  $V = 0.6109$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.15655	0.3131	0.04957		tetrahedron Al <sub>4</sub>
Li2	12 <i>k</i>	. <i>m</i> .	0.166	0.332	0.7086	0.095	
Al3	12 <i>k</i>	. <i>m</i> .	0.16852	0.33704	0.60632		octahedron O <sub>6</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.5022	0.0044	0.14682		square pyramid Al <sub>3</sub> Li <sub>2</sub>
O5	6 <i>h</i>	<i>mm</i> 2	0.29673	0.59346	$\frac{1}{4}$	0.333	
Na6	6 <i>h</i>	<i>mm</i> 2	0.7182	0.4364	$\frac{1}{4}$	0.15	
Al7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0243		tetrahedron O <sub>4</sub>
Al8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.17575		
O9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.55751		tetrahedron Al <sub>4</sub>
O10	4 <i>e</i>	3 <i>m</i> .	0	0	0.14233		trigonal prism Al <sub>3</sub> Li <sub>3</sub>
Al11	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $wR_p = 0.069$ ,  $T = 4.2$  K

Remarks: Part of non-framework species not located. Short interatomic distances for partly occupied site(s). In table 1 of [1] the Wyckoff position of the Li site is misprinted as 6*h* instead of 12*k*.

References: [1] Tofield B.C., Farrington G.C. (1979), Nature (London) 278, 438-439.

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hP78

$\text{K}_{1.28}\text{Ga}_{11}\text{O}_{17.14}$	<i>hP78</i>	(194) $P6_3/mmc - k^4hf^3edcba$
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**K<sub>1.28</sub>Ga<sub>11</sub>O<sub>17.14</sub>** [1],  $\beta$  alumina(Ga)-K

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Ga in octahedral and tetrahedral voids) and K<sub>1+2x</sub>O<sub>1+x</sub> layers (K at BR and aBr, (K,O) near mO positions, the additional O between Ga displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked GaO<sub>6</sub> octahedra sharing vertices with single GaO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked GaO<sub>4</sub> tetrahedra to form a 3D-framework.

Ikawa H. et al. (1985) [1]

 $\text{Ga}_{10.98}\text{K}_{1.34}\text{O}_{17.14}$  $a = 0.5839$ ,  $c = 2.347$  nm,  $c/a = 4.02$ ,  $V = 0.6930$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1572	0.3144	0.5504		tetrahedron Ga <sub>4</sub>
Ga2	12 <i>k</i>	. <i>m</i> .	0.1612	0.3224	0.1752	0.047	single atom Ga
Ga3	12 <i>k</i>	. <i>m</i> .	0.16791	0.33582	0.10555	0.949	7-vertex polyhedron GaO <sub>6</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.505	0.01	0.6473		square pyramid Ga <sub>5</sub>
M5	6 <i>h</i>	<i>mm</i> 2	0.1136	0.2272	$\frac{1}{4}$	0.245	

O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0555	tetrahedron Ga <sub>4</sub>
Ga7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52443	tetrahedron O <sub>4</sub>
Ga8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67481	tetrahedron O <sub>4</sub>
O9	4e	3m.	0	0	0.1429	trigonal prism Ga <sub>6</sub>
O10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	colinear Ga <sub>2</sub>
K11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.725
K12	2b	-6m2	0	0	$\frac{1}{4}$	0.02
Ga13	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

M5 = 0.809K + 0.191O

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

Experimental: single crystal, diffractometer, X-rays, R = 0.039

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

References: [1] Ikawa H., Tsurumi T., Ishimori M., Urabe K., Udagawa S. (1985), J. Solid State Chem. 60, 51-61.

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hP80

Lu <sub>1.82</sub> Fe <sub>17.35</sub>	hP80	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>2,3</sup> j <sup>3</sup> gfedcb
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**Lu<sub>1.82</sub>Fe<sub>17.35</sub>** [1]; ThNi<sub>9.5</sub> [2]

Structural features: Kagomé-mesh Fe<sub>9</sub> layers and LuLu<sub>2-x</sub>(Fe<sub>2</sub>)<sub>2x</sub>Fe<sub>6</sub> layers (a Fe hexagon mesh, the hexagons of which are centered by a Lu atom or a Fe<sub>2</sub> dumbbell perpendicular to the layer) alternate along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks (partial disorder, splitting of the framework sites).

Givord D. et al. (1972) [1]

Fe<sub>17.35</sub>Lu<sub>1.83</sub>

*a* = 0.8388, *c* = 0.8287 nm, *c/a* = 0.988, *V* = 0.5050 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	12k	.m.	0.1656	0.3312	0.0000	0.29	
Fe2	12k	.m.	0.1656	0.3312	0.0233	0.71	
Fe3	12j	m..	0.0000	0.2925	$\frac{1}{4}$	0.08	
Fe4	12j	m..	0.3333	0.0213	$\frac{1}{4}$	0.20	
Fe5	12j	m..	0.3738	0.0408	$\frac{1}{4}$	0.72	
Fe6	6g	.2/m.	$\frac{1}{2}$	0	0		
Fe7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6060	0.900	
Fe8	4e	3m.	0	0	0.1100	0.275	
Lu9	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.10	
Lu10	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		
Lu11	2b	-6m2	0	0	$\frac{1}{4}$	0.725	

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

Experimental: single crystal, diffractometer, neutrons, R = 0.039

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

References: [1] Givord D., Lemaire R., Moreau J.M., Roudaut E. (1972), J. Less-Common Met. 29, 361-369. [2] Givord D., Givord F., Lemaire R., James W.J., Shah J.S. (1972), J. Less-Common Met. 29, 389-396.

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hP80

CsRbMn <sub>2</sub> Cl <sub>6</sub>	hP80	(194) $P6_3/mmc - k^2jih^3gfca$
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**CsRbMn<sub>2</sub>Cl<sub>6</sub>** [1], perovskite 4H

Structural features: Close-packed CsRb<sub>3</sub>Cl<sub>12</sub> and Cs<sub>3</sub>RbCl<sub>12</sub> layers in hc stacking; Mn in octahedral voids. Units of two face-linked MnCl<sub>6</sub> octahedra share vertices to form a 3D-framework. Substitution derivative of BaMnO<sub>3</sub> 4H of ideal composition [AA']B<sub>2</sub>X<sub>6</sub>.

Van Veen J.A.R. (1971) [1]

Cl<sub>6</sub>CsMn<sub>2</sub>Rb $a = 1.4418$ ,  $c = 1.2017$  nm,  $c/a = 0.833$ ,  $V = 2.1634$  nm<sup>3</sup>,  $Z = 8$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	12k	.m.	0.16667	0.33333	0.125		octahedron Cl <sub>6</sub>
Cl2	12k	.m.	0.25	0.5	0.0		colinear Mn <sub>2</sub>
Cl3	12j	m..	0.08333	0.41667	$\frac{1}{4}$		non-colinear Mn <sub>2</sub>
Cl4	12i	.2.	0.25	0	0		colinear Mn <sub>2</sub>
Cl5	6h	mm2	0.08333	0.16667	$\frac{1}{4}$		non-colinear Mn <sub>2</sub>
Cl6	6h	mm2	0.58333	0.16667	$\frac{1}{4}$		non-colinear Mn <sub>2</sub>
Rb7	6h	mm2	0.83333	0.66667	$\frac{1}{4}$		anticuboctahedron Cl <sub>12</sub>
Cs8	6g	.2/m.	$\frac{1}{2}$	0	0		cuboctahedron Cl <sub>12</sub>
Mn9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.625		octahedron Cl <sub>6</sub>
Cs10	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		anticuboctahedron Cl <sub>12</sub>
Rb11	2a	-3m.	0	0	0		cuboctahedron Cl <sub>12</sub>

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates.

References: [1] Van Veen J.A.R. (1971), Mater. Res. Bull. 6, 1269-1271.

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hP80

Ba <sub>1.17</sub> Al <sub>10.67</sub> O <sub>17.17</sub>	hP80	(194) $P6_3/mmc - k^4hf^4edca$
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**Ba<sub>1.17</sub>Al<sub>10.67</sub>O<sub>17.17</sub>** [1],  $\beta$  alumina-Ba

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Ba<sub>1-x</sub>O layers (Ba at BR positions) alternate along [001]; Ba vacancies are compensated for by two Ba in the spinel-type slabs and a triple Reidingen defect (partial Al migration). Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Groppi G. et al. (1995) [1]

Al<sub>10.69</sub>Ba<sub>1.16</sub>O<sub>17.16</sub> $a = 0.56016$ ,  $c = 2.2906$  nm,  $c/a = 4.089$ ,  $V = 0.6224$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1574	0.3148	0.5485		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.159	0.318	0.1769	0.157	trigonal bipyramid AlO <sub>4</sub>
Al3	12k	.m.	0.1636	0.3272	0.1034	0.843	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.505	0.01	0.6499		square pyramid Al <sub>5</sub>
O5	6h	mm2	0.106	0.212	$\frac{1}{4}$	0.157	tetrahedron Al <sub>2</sub> O <sub>2</sub>
Ba6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0306	0.157	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0555	0.843	



Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5231	0.843	
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6768		tetrahedron O <sub>4</sub>
O10	4e	3m.	0	0	0.1464		trigonal prism Al <sub>6</sub>
O11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Ba12	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.843	tricapped trigonal prism O <sub>3</sub> Al <sub>6</sub>
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, X-rays,  $wR_p = 0.150$

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

References: [1] Groppi G., Assandri F., Bellotto M., Cristiani C., Forzatti P. (1995), J. Solid State Chem. 114, 326-336.

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hP80

K <sub>2</sub> [SeO <sub>4</sub> ]	hP80	(194) $P6_3/mmc - l^3f^2$
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### K<sub>2</sub>SeO<sub>4</sub> α [1]

Structural features: K atoms and SeO<sub>4</sub> tetrahedra (orientational disorder) in a Ni<sub>2</sub>In-type (ht-Co<sub>2</sub>Ge) arrangement (K and Se displaced from the ideal positions).

Iwata Y. et al. (1984) [1]

K<sub>2</sub>O<sub>4</sub>Se

$a = 0.6077$ ,  $c = 0.8029$  nm,  $c/a = 1.321$ ,  $V = 0.2568$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
K1	24l	1	0.04	0.002	0.009	0.083	
O2	24l	1	0.155	0.386	0.216	0.25	
O3	24l	1	0.254	0.576	0.057	0.083	
Se4	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.224	0.5	
K5	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.702	0.5	

Experimental: single crystal, diffractometer, neutrons,  $R = 0.090$ ,  $T = 773$  K

Remarks: Phase stable at  $T > 745$  K. Short interatomic distances for partly occupied site(s).

References: [1] Iwata Y., Koyano N., Shibuya I., Hidaka M., Okazaki A. (1984), Annu. Rep. Res. React. Inst. Kyoto Univ. 17, 43-53.

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hP80

ZrCr <sub>2</sub> H <sub>3.8</sub>	hP80	(194) $P6_3/mmc - lk^2h^3f^2ea$
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### ZrCr<sub>2</sub>H<sub>3.8</sub> [1]

Structural features: Filled-up derivative of MgZn<sub>2</sub> with H in tetrahedral (Zr<sub>2</sub>Cr<sub>2</sub>, ZrCr<sub>3</sub> and Cr<sub>4</sub>) voids.

Irodova A.V., Suard E. (2000) [1]

Cr<sub>2</sub>D<sub>3.83</sub>Zr

$a = 0.54284$ ,  $c = 0.88826$  nm,  $c/a = 1.636$ ,  $V = 0.2267$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	24l	1	0.0405	0.3298	0.0643	0.304	tetrahedron D <sub>4</sub>
D2	12k	.m.	0.125	0.25	0.64062	0.044	tetrahedron D <sub>4</sub>
D3	12k	.m.	0.5417	0.0834	0.627	0.276	tetrahedron D <sub>4</sub>

Cr4	6h	mm2	0.162	0.324	$\frac{1}{4}$		20-vertex polyhedron D <sub>20</sub>
D5	6h	mm2	0.5332	0.0664	$\frac{1}{4}$	0.408	tetrahedron D <sub>4</sub>
D6	6h	mm2	0.7989	0.5978	$\frac{1}{4}$	0.22	tetrahedron D <sub>4</sub>
D7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.17188	0.102	tetrahedron D <sub>4</sub>
Zr8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5635		28-vertex polyhedron D <sub>28</sub>
D9	4e	3m.	0	0	0.1875	0.002	tetrahedron D <sub>4</sub>
Cr10	2a	-3m.	0	0	0		20-vertex polyhedron D <sub>20</sub>

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

Experimental: powder, diffractometer, neutrons,  $R_p = 0.041$ ,  $T = 300$  K

References: [1] Irodova A.V., Suard E. (2000), J. Alloys Compd. 299, 32-38.

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hP82

Pr <sub>0.83</sub> Al <sub>11.83</sub> O <sub>19</sub>	hP82	(194) $P6_3/mmc - k^4h^2f^3e^2a$
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**Pr<sub>0.83</sub>Al<sub>11.83</sub>O<sub>19</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and PrO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Pr atoms (split site); partial Al migration.

Haemers T.A.M. et al. (1993) [1]

Al<sub>11.83</sub>O<sub>19</sub>Pr<sub>0.83</sub>

$a = 0.55582$ ,  $c = 2.1999$  nm,  $c/a = 3.958$ ,  $V = 0.5886$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.148	0.296	0.671	0.056	4-vertex polyhedron AlO <sub>3</sub>
O2	12k	.m.	0.1573	0.3146	0.05182		tetrahedron Al <sub>4</sub>
Al3	12k	.m.	0.1685	0.337	0.6079	0.944	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.5042	0.0084	0.1506		square pyramid Al <sub>5</sub>
O5	6h	mm2	0.183	0.366	$\frac{1}{4}$		
Pr6	6h	mm2	0.706	0.412	$\frac{1}{4}$	0.278	
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0261		tetrahedron O <sub>4</sub>
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1903		octahedron O <sub>6</sub>
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5564		tetrahedron Al <sub>4</sub>
O10	4e	3m.	0	0	0.148		7-vertex polyhedron Al <sub>7</sub>
Al11	4e	3m.	0	0	0.2363	0.417	
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Experimental: powder, diffractometer, neutrons,  $R_p = 0.033$ ,  $T = 295$  K

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

References: [1] Haemers T.A.M., Ijdo D.J.W., Groen W.A., Hal H.A.M., Helmholdt R.B. (1993), Mater. Res. Bull. 28, 111-116.

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hP82

Na <sub>1.22</sub> Al <sub>11</sub> O <sub>17.11</sub>	hP82	(194) $P6_3/mmc - k^4h^2f^3edca$
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**Na<sub>1+x</sub>Al<sub>11</sub>O<sub>17+x/2</sub>** [1],  $\beta$  alumina-Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Na<sub>x</sub>O<sub>1+y</sub> layers (Na at BR and near mO positions, additional O at mO positions)

between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework. See Fig. III.47.

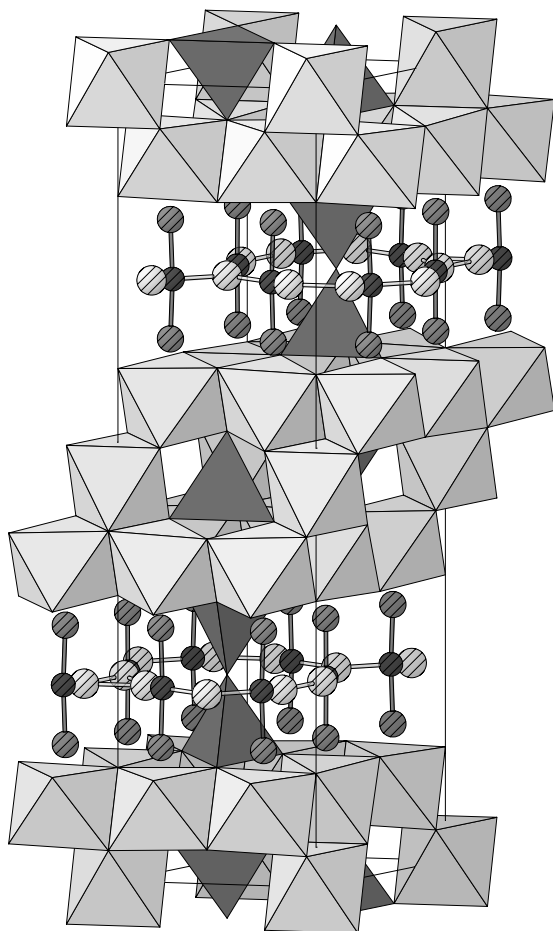


Fig. III.47.  $\text{Na}_{1+x}\text{Al}_{11}\text{O}_{17+x/2}$

Arrangement of  $\text{AlO}_4$  tetrahedra (dark),  $\text{AlO}_6$  octahedra (light) and interstitial partly occupied Na (light), Al (medium) and O (dark) sites.

Edström K. et al. (1991) [1]

$\text{Al}_{11}\text{Na}_{1.22}\text{O}_{17.11}$

$a = 0.55929$ ,  $c = 2.2526$  nm,  $c/a = 4.028$ ,  $V = 0.6102$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.15712	0.31424	0.54998		tetrahedron $\text{Al}_4$
Al2	12k	.m.	0.16045	0.3209	0.17523	0.037	
Al3	12k	.m.	0.16798	0.33596	0.1061	0.963	7-vertex polyhedron $\text{AlO}_6$
O4	12k	.m.	0.50305	0.0061	0.64632		square pyramid $\text{Al}_5$
Na5	6h	mm2	0.10298	0.20596	$\frac{1}{4}$	0.162	
O6	6h	mm2	0.16667	0.33333	$\frac{1}{4}$	0.037	
O7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05525		tetrahedron $\text{Al}_4$
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52482		tetrahedron $\text{O}_4$
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67576		tetrahedron $\text{O}_4$
O10	4e	3m.	0	0	0.14219		trigonal prism $\text{Al}_6$
O11	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear $\text{Al}_2$
Na12	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.734	coplanar triangle $\text{O}_3$

Al13    2a   -3m.    0    0    0    octahedron O<sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.019, T = 295 K

Remarks: Short interatomic distances for partly occupied site(s). The same data are also reported in [2].

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 210-216. [2] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 635-643.

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hP82

Ba<sub>0.78</sub>(Mn<sub>0.13</sub>Al<sub>0.87</sub>)<sub>2</sub>Al<sub>8.96</sub>O<sub>17.15</sub>    hP82    (194) *P6<sub>3</sub>/mmc* – k<sup>4</sup>h<sup>2</sup>f<sup>3</sup>edca

**Ba<sub>0.78</sub>Mn<sub>0.254</sub>Al<sub>10.706</sub>O<sub>17.153</sub>** [1], β alumina(Al,Mn)-Ba

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and outer tetrahedral, (Al,Mn) in inner tetrahedral voids) and Ba<sub>1/2+x</sub>O<sub>1+x</sub> layers (in part split framework O site, Ba at BR positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked (Al,Mn)O<sub>4</sub> tetrahedra to form a 3D-framework.

Inoue H. et al. (1996) [1]

Al<sub>10.70</sub>Ba<sub>0.78</sub>Mn<sub>0.25</sub>O<sub>17.15</sub>

*a* = 0.5591, *c* = 2.2659 nm, *c/a* = 4.053, *V* = 0.6134 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	<i>m.</i>	0.15683	0.31366	0.55013		tetrahedron Al <sub>4</sub>
Al2	12k	<i>m.</i>	0.16	0.32	0.1774	0.053	trigonal bipyramid AlO <sub>4</sub>
Al3	12k	<i>m.</i>	0.16691	0.33382	0.10528	0.94	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	<i>m.</i>	0.5039	0.0078	0.64734		square pyramid Al <sub>5</sub>
O5	6h	<i>mm2</i>	0.12	0.24	1/4	0.039	non-collinear Al <sub>2</sub>
O6	6h	<i>mm2</i>	0.7051	0.4102	1/4	0.267	
O7	4f	3 <i>m.</i>	1/3	2/3	0.05676		tetrahedron Al <sub>4</sub>
M8	4f	3 <i>m.</i>	1/3	2/3	0.52374		tetrahedron O <sub>4</sub>
Al9	4f	3 <i>m.</i>	1/3	2/3	0.67512		
O10	4e	3 <i>m.</i>	0	0	0.14207		trigonal prism Al <sub>6</sub>
O11	2d	-6 <i>m2</i>	1/3	2/3	3/4	0.235	
Ba12	2c	-6 <i>m2</i>	1/3	2/3	1/4	0.78	tricapped trigonal prism O <sub>3</sub> Al <sub>6</sub>
Al13	2a	-3 <i>m.</i>	0	0	0		octahedron O <sub>6</sub>

M8 = 0.873Al + 0.127Mn

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

Experimental: single crystal, diffractometer, X-rays, R = 0.029, T = 297 K

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

References: [1] Inoue H., Machida M., Eguchi K., Arai H. (1996), J. Mater. Chem. 6, 455-458.

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hP82

Li<sub>1.2</sub>Al<sub>11</sub>O<sub>17.1</sub>[H<sub>2</sub>O]<sub>0.8</sub>    hP82    (194) *P6<sub>3</sub>/mmc* – k<sup>4</sup>h<sup>2</sup>f<sup>4</sup>ea

**Li<sub>1.2</sub>Al<sub>11</sub>O<sub>17.1</sub>·0.8H<sub>2</sub>O** [1], β alumina-Li<sub>2</sub>H<sub>2</sub>O

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, partial disorder for the latter) and Li<sub>1+2x</sub>O<sub>1+x</sub>(H<sub>2</sub>O)<sub>y</sub> layers (split framework O site, Li above and below BR, H<sub>2</sub>O near mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub>

octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Bates J.B. et al. (1982) [1]

$\text{Al}_{11}\text{H}_{1.55}\text{LiO}_{17.77}$

$a = 0.5591$ ,  $c = 2.2715$  nm,  $c/a = 4.063$ ,  $V = 0.6149$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	12 <i>k</i>	. <i>m</i> .	0.1571	0.3142	0.1747	0.083	trigonal bipyramid $\text{AlO}_4$
O2	12 <i>k</i>	. <i>m</i> .	0.15731	0.31462	0.54964		tetrahedron $\text{Al}_4$
Al3	12 <i>k</i>	. <i>m</i> .	0.1683	0.3366	0.10488	0.917	7-vertex polyhedron $\text{AlO}_6$
O4	12 <i>k</i>	. <i>m</i> .	0.5029	0.0058	0.64609		square pyramid $\text{Al}_5$
O5	6 <i>h</i>	<i>mm</i> 2	0.0925	0.185	$\frac{1}{4}$	0.258	tetrahedron $\text{O}_2\text{Al}_2$
O6	6 <i>h</i>	<i>mm</i> 2	0.702	0.404	$\frac{1}{4}$	0.333	
O7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.05486		tetrahedron $\text{Al}_4$
Li8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.227	0.5	
Al9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.52443		tetrahedron $\text{O}_4$
Al10	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.67549		
O11	4 <i>e</i>	3 <i>m</i> .	0	0	0.14166		trigonal prism $\text{Al}_6$
Al12	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron $\text{O}_6$
H13	12 <i>k</i>	. <i>m</i> .	0.037	0.074	0.2134	0.258	

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

Experimental: single crystal, diffractometer, neutrons,  $R = 0.060$

Remarks: Part of non-framework species not located. The authors state that excess O is located near site O5 ( $\text{H}_2\text{O}$ ), between interstitial Al. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table I of [1] the  $x$ -coordinate of site Li is misprinted as  $\frac{1}{3}$  instead of  $\frac{2}{3}$  (from the description of the structure).

References: [1] Bates J.B., Dudney N.J., Brown G.M., Wang J.C., Frech R. (1982), J. Chem. Phys. 77, 4838-4856.

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hP82

$\text{Na}_{11}\text{Ba}_7\text{Ca}_{0.5}\text{N}_3$	hP82	(194) $P6_3/mmc - k^4\text{ihgfea}$
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**$\text{Na}_{22}\text{Ba}_{14}\text{CaN}_6$**  [1]

Structural features:  $\text{CaN}_6\text{Ba}_{14}$  clusters (a central Ca atom surrounded by a  $\text{N}_6$  octahedron, a  $\text{Ba}_8$  cube and a large  $\text{Ba}_6$  octahedron) in a matrix of Na atoms; disorder described as a superposition of rods in two different orientations.

Steinbrenner U., Simon A. (1997) [1]

$\text{Ba}_7\text{Ca}_{0.50}\text{N}_3\text{Na}_{11}$

$a = 1.255$ ,  $c = 1.252$  nm,  $c/a = 0.998$ ,  $V = 1.7077$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
N1	12 <i>k</i>	. <i>m</i> .	0.0964	0.1928	0.1189	0.5	
Ba2	12 <i>k</i>	. <i>m</i> .	0.14121	0.28242	0.58757	0.5	
Na3	12 <i>k</i>	. <i>m</i> .	0.1601	0.3202	0.5656	0.5	
Ba4	12 <i>k</i>	. <i>m</i> .	0.19085	0.3817	0.23226	0.5	
Na5	12 <i>i</i>	.2.	0.479	0	0	0.333	
Na6	6 <i>h</i>	<i>mm</i> 2	0.5677	0.1354	$\frac{1}{4}$		
Na7	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0	0.333	
Na8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0044		

Ba9	4e	3m.	0	0	0.2362	0.5	
Ca10	2a	-3m.	0	0	0	0.5	octahedron N <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.038, T = 128 K

Remarks: Short interatomic distances for partly occupied site(s). A slightly different model for disorder is proposed for data collected at 293 K.

References: [1] Steinbrenner U., Simon A. (1997), Z. Kristallogr. 212, 428-438.

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hP84

(Li<sub>0.5</sub>Zn<sub>0.5</sub>)<sub>2</sub>Mg<sub>7</sub>Zn<sub>12</sub>

hP84

(194) *P6<sub>3</sub>/mmc* – k<sup>3</sup>h<sup>7</sup>e<sup>3</sup>a

**MgLi<sub>0.11</sub>Zn<sub>1.89</sub>** [1], Laves phase 14H

Structural features: (Zn,Li)<sub>4</sub> tetrahedra (partial order ignored) share faces and vertices to form a 3D-framework. Laves-type slabs in h<sub>3</sub>c<sub>2</sub> stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Krypyakevich P.I., Melnik E.V. (1974) [1]

LiMg<sub>7</sub>Zn<sub>13</sub>

*a* = 0.5215, *c* = 5.989 nm, *c/a* = 11.484, *V* = 1.4106 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	12k	.m.	0.167	0.334	0.107		icosahedron LiZn <sub>5</sub> Mg <sub>6</sub>
Zn2	12k	.m.	0.167	0.334	0.536		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Zn3	12k	.m.	0.503	0.006	0.179		icosahedron Zn <sub>4</sub> Li <sub>2</sub> Mg <sub>6</sub>
Zn4	6h	mm2	0.174	0.348	1/4		icosahedron Zn <sub>4</sub> Li <sub>2</sub> Mg <sub>6</sub>
Mg5	4f	3m.	1/3	2/3	0.009		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Mg6	4f	3m.	1/3	2/3	0.063		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
M7	4f	3m.	1/3	2/3	0.141		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
M8	4f	3m.	1/3	2/3	0.214		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg9	4f	3m.	1/3	2/3	0.582		16-vertex Frank-Kasper Mg <sub>4</sub> Zn <sub>12</sub>
Mg10	4f	3m.	1/3	2/3	0.63		16-vertex Frank-Kasper Mg <sub>4</sub> Zn <sub>9</sub> Li <sub>3</sub>
Mg11	4f	3m.	1/3	2/3	0.724		16-vertex Frank-Kasper Zn <sub>9</sub> Li <sub>3</sub> Mg <sub>4</sub>
Zn12	4e	3m.	0	0	0.072		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg13	4e	3m.	0	0	0.151		16-vertex Frank-Kasper Zn <sub>9</sub> Li <sub>3</sub> Mg <sub>4</sub>
Mg14	4e	3m.	0	0	0.204		16-vertex Frank-Kasper Zn <sub>9</sub> Li <sub>3</sub> Mg <sub>4</sub>
Zn15	2a	-3m.	0	0	0		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>

M7 = 0.5Li + 0.5Zn; M8 = 0.5Li + 0.5Zn

Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.076

References: [1] Krypyakevich P.I., Melnik E.V. (1974), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1974, 847-850.

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hP84

MgLa<sub>0.4</sub>Gd<sub>0.6</sub>Al<sub>11</sub>O<sub>19</sub>

hP84

(194) *P6<sub>3</sub>/mmc* – k<sup>3</sup>j<sup>2</sup>f<sup>3</sup>e<sup>2</sup>da

**La<sub>0.4</sub>Gd<sub>0.6</sub>MgAl<sub>11</sub>O<sub>19</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and (La,Gd)O<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub> stacking; (Al,Mg) in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked (Al,Mg)O<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked (Al,Mg)O<sub>6</sub>

octahedra, (Al,Mg)O<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and (La,Gd) atoms (split site for Gd).

Salem Y. et al. (1990) [1]



$a = 0.5565$ ,  $c = 2.189$  nm,  $c/a = 3.934$ ,  $V = 0.5871$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1533	0.3066	0.0533		tetrahedron Al <sub>4</sub>
M2	12 <i>k</i>	. <i>m</i> .	0.1678	0.3356	0.6085		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.5053	0.0106	0.1515	0.94	non-coplanar triangle Al <sub>3</sub>
O4	12 <i>j</i>	. <i>m</i> ..	0.1638	0.3632	$\frac{1}{4}$	0.47	
Gd5	12 <i>j</i>	. <i>m</i> ..	0.6245	0.2972	$\frac{1}{4}$	0.077	
M6	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0273		tetrahedron O <sub>4</sub>
M7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1901		
O8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5578		tetrahedron Al <sub>4</sub>
O9	4 <i>e</i>	3 <i>m</i> .	0	0	0.1511		tetrahedron Al <sub>4</sub>
M10	4 <i>e</i>	3 <i>m</i> .	0	0	0.2419	0.5	
La11	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.43	
M12	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

M2 = 0.917Al + 0.083Mg; M6 = 0.917Al + 0.083Mg; M7 = 0.917Al + 0.083Mg; M10 = 0.917Al + 0.083Mg; M12 = 0.917Al + 0.083Mg

Experimental: single crystal, diffractometer, X-rays,  $R = 0.079$

Remarks: Composition La<sub>0.43</sub>Gd<sub>0.46</sub>Mg<sub>0.63</sub>Al<sub>11</sub>O<sub>18.46</sub> from electron microprobe analysis. No attempt was made to distinguish Mg and Al. Short interatomic distances for partly occupied site(s). Space groups (186) *P6<sub>3</sub>mc* and (190) *P-62c* were tested and rejected.

References: [1] Salem Y., Linares C., Jacquier B., Saine M.C., Gasperin M., Lejus A.M., Vivien D. (1990), J. Chem. Phys. 93, 7076-7084.

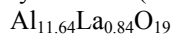
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hP84

La <sub>0.83</sub> Al <sub>11.83</sub> O <sub>19</sub>	hP84	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>4</sup> h <sup>2</sup> f <sup>3</sup> e <sup>2</sup> da
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**La<sub>0.83</sub>Al<sub>11.83</sub>O<sub>19</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers (partial vacancies ignored for the latter) in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (ideal and split site); partial Al migration.

Iyi N. et al. (1984) [1]



$a = 0.5561$ ,  $c = 2.207$  nm,  $c/a = 3.969$ ,  $V = 0.5911$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1561	0.3122	0.0518		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.161	0.322	0.686	0.048	trigonal bipyramid AlO <sub>3</sub> La
Al3	12 <i>k</i>	. <i>m</i> .	0.169	0.338	0.60772	0.917	7-vertex polyhedron AlO <sub>6</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.5023	0.0046	0.1501		square pyramid Al <sub>5</sub>
O5	6 <i>h</i>	<i>mm</i> 2	0.178	0.356	$\frac{1}{4}$		
La6	6 <i>h</i>	<i>mm</i> 2	0.718	0.436	$\frac{1}{4}$	0.115	
Al7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0271		tetrahedron O <sub>4</sub>

Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1899	octahedron O <sub>6</sub>
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5553	tetrahedron Al <sub>4</sub>
O10	4e	3m.	0	0	0.1481	7-vertex polyhedron Al <sub>7</sub>
Al11	4e	3m.	0	0	0.2389	0.425
La12	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.49
Al13	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.039

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

References: [1] Iyi N., Inoue Z., Takekawa S., Kimura S. (1984), J. Solid State Chem. 54, 70-77.

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hP84

Na <sub>1.45</sub> Al <sub>11</sub> O <sub>17.225</sub>	hP84	(194) $P6_3/mmc - k^4h^3f^3ea$
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**Na<sub>1.45</sub>Al<sub>11</sub>O<sub>17.225</sub>** [1], β alumina-Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, partial disorder for the latter) and Na<sub>1+2x</sub>O<sub>1+x</sub> layers (split framework O site, Na near BR and mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

England W.A. et al. (1982) [1]

Al<sub>11</sub>Na<sub>1.50</sub>O<sub>17</sub>

$a = 0.5601$ ,  $c = 2.254$  nm,  $c/a = 4.024$ ,  $V = 0.6124$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1574	0.3148	0.5506		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1616	0.3232	0.1736	0.042	
Al3	12k	.m.	0.168	0.336	0.1077	0.958	7-vertex polyhedron O <sub>6</sub> Al
O4	12k	.m.	0.5037	0.0074	0.6467		non-coplanar triangle Al <sub>3</sub>
Na5	6h	mm2	0.1004	0.2008	$\frac{1}{4}$	0.2	
Na6	6h	mm2	0.383	0.766	$\frac{1}{4}$	0.3	
O7	6h	mm2	0.6955	0.391	$\frac{1}{4}$	0.333	
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0559		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5237		tetrahedron O <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6736		
O11	4e	3m.	0	0	0.1407		
Al12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.065, T = 4.2 K

Remarks: Short interatomic distances for partly occupied site(s). We assume that in table 5 of [1] the x-coordinate of former O(5) ( standard uncertainty 0.0160) is misprinted as 0.9384 instead of 0.8384 (better agreement with the model, no impossibly short distances to fully occupied sites).

References: [1] England W.A., Jacobson A.J., Tofield B.C. (1982), Solid State Ionics 6, 21-27.

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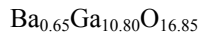
Ba <sub>0.65</sub> Ga <sub>10.80</sub> O <sub>16.84</sub>	hP84	(194) $P6_3/mmc - k^4h^3f^3ea$
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**Ba<sub>0.65</sub>Ga<sub>10.80</sub>O<sub>16.84</sub>** [1], β alumina(Ga)-Ba



Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Ga in octahedral and tetrahedral voids) and  $\text{Ba}_{1/2+x}\text{O}_{1+x}$  layers (split framework O site, Ba at BR positions, additional O at mO positions between Ga displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{GaO}_6$  octahedra sharing vertices with single  $\text{GaO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{GaO}_4$  tetrahedra to form a 3D-framework.

Samaras D. et al. (1986) [1]



$a = 0.5859$ ,  $c = 2.3192$  nm,  $c/a = 3.958$ ,  $V = 0.6895$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1558	0.3116	0.5522	0.94	tetrahedron Ga <sub>4</sub>
Ga2	12k	.m.	0.1585	0.317	0.1737	0.018	trigonal bipyramid GaO <sub>4</sub>
Ga3	12k	.m.	0.16641	0.33282	0.10729	0.982	7-vertex polyhedron GaO <sub>6</sub>
O4	12k	.m.	0.5071	0.0142	0.6507		square pyramid Ga <sub>5</sub>
O5	6h	mm2	0.1277	0.2554	<sup>1</sup> / <sub>4</sub>	0.07	non-collinear Ga <sub>2</sub>
Ba6	6h	mm2	0.3219	0.6438	<sup>1</sup> / <sub>4</sub>	0.216	
O7	6h	mm2	0.714	0.428	<sup>1</sup> / <sub>4</sub>	0.333	
O8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0579		tetrahedron Ga <sub>4</sub>
Ga9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5243	0.899	tetrahedron O <sub>4</sub>
Ga10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.67538		
O11	4e	3m.	0	0	0.146		trigonal prism Ga <sub>6</sub>
Ga12	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

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

References: [1] Samaras D., Kotrotsios G., Collomb A., Guitel J.C., Stergiou A.C. (1986), Solid State Ionics 21, 143-149.

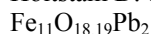
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hP84

$\text{Mg}_{0.10}\text{Mn}_{0.23}\text{Fe}_{10.67}\text{Pb}_2\text{O}_{18.33}$	hP84	(194) $P6_3/mmc - k^5hf^3ea$
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**Pb<sub>2</sub>(Mn,Mg)<sub>0.33</sub>Fe<sub>10.67</sub>O<sub>18.33</sub>** [1], plumboferrite

Structural features: Spinel-type slabs (six close-packed O layers in c stacking), where edge-linked  $\text{FeO}_6$  octahedra share vertices with single  $\text{FeO}_4$  tetrahedra, are interconnected via units of two face-linked  $\text{FeO}_6$  octahedra ( $\text{Fe}_2$  dumbbells) to form a 3D-framework; disordered arrangement of Pb atoms between the slabs.

Holtstam D. et al. (1995) [1]



$a = 0.5931$ ,  $c = 2.3551$  nm,  $c/a = 3.971$ ,  $V = 0.7175$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pb1	12k	.m.	0.04168	0.08336	0.24735	0.167	
O2	12k	.m.	0.1566	0.3133	0.0515		tetrahedron Fe <sub>4</sub>
Fe3	12k	.m.	0.16905	0.3381	0.60614		octahedron O <sub>6</sub>
O4	12k	.m.	0.5031	0.0062	0.1482		non-coplanar triangle Fe <sub>3</sub>
Pb5	12k	.m.	0.7147	0.4294	0.24425	0.167	
O6	6h	mm2	0.1871	0.3743	<sup>1</sup> / <sub>4</sub>	0.73	
Fe7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.02627		tetrahedron O <sub>4</sub>
Fe8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.18468		octahedron O <sub>6</sub>

O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5535	tetrahedron Fe <sub>4</sub>
O10	4e	3m.	0	0	0.1455	non-coplanar triangle Fe <sub>3</sub>
Fe11	2a	-3m.	0	0	0	octahedron O <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.039, T = 293 K

Remarks: Natural specimen from Jakobsberg, Filipstad, Sweden. Composition Pb<sub>2.03</sub>Fe<sub>10.59</sub>Mn<sub>0.23</sub>Ti<sub>0.03</sub>Si<sub>0.02</sub>Mg<sub>0.10</sub>O<sub>18.35</sub> from electron microprobe analysis. No attempt was made to locate Mn and Mg. Short interatomic distances for partly occupied site(s). Additional reflections could be indexed with a 9-fold supercell (new axes 2a+b, -a+b, 3c). One Fe site (0 0 1/4) missing with respect to magnetoplumbite.

References: [1] Holtstam D., Norrestam R., Sjödin A. (1995), Am. Mineral. 80, 1065-1072.

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hP86

[NH <sub>4</sub> ] <sub>1.3</sub> Al <sub>11</sub> O <sub>17.15</sub>	hP86	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>4</sup> h <sup>3</sup> f <sup>3</sup> eba
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(NH<sub>4</sub>)<sub>1.3</sub>Al<sub>11</sub>O<sub>17.15</sub> [1], β alumina-NH<sub>4</sub>

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, partial disorder for the latter) and (NH<sub>4</sub>)<sub>1+2x</sub>O<sub>1+x</sub> layers (split framework O site, NH<sub>4</sub> at aBR and BR and near mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Colomban P. et al. (1978) [1]

Al<sub>10.93</sub>H<sub>5.12</sub>N<sub>1.28</sub>O<sub>17</sub>

a = 0.5592, c = 2.2808 nm, c/a = 4.079, V = 0.6177 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1569	0.3138	0.5494		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1612	0.3224	0.1757	0.021	trigonal bipyramid AlO <sub>3</sub> (NH <sub>4</sub> )
Al3	12k	.m.	0.1679	0.3358	0.1049	0.968	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.5019	0.0038	0.6443		square pyramid Al <sub>5</sub>
(NH <sub>4</sub> )5	6h	mm2	0.0851	0.1702	$\frac{1}{4}$	0.092	
(NH <sub>4</sub> )6	6h	mm2	0.3206	0.6412	$\frac{1}{4}$	0.305	
O7	6h	mm2	0.6853	0.3706	$\frac{1}{4}$	0.333	
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0548		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5246		tetrahedron O <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6751		
O11	4e	3m.	0	0	0.1402		trigonal prism Al <sub>6</sub>
(NH <sub>4</sub> )12	2b	-6m2	0	0	$\frac{1}{4}$	0.09	
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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] Colomban P., Boilot J.P., Kahn A., Lucazeau G. (1978), Nouv. J. Chim. 2, 21-32.

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hP86

[NH <sub>4</sub> ] <sub>1.2</sub> Al <sub>11</sub> O <sub>17.1</sub>	hP86	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>4</sup> h <sup>3</sup> f <sup>3</sup> eca
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**(NH<sub>4</sub>)<sub>1.2</sub>Al<sub>11</sub>O<sub>17.1</sub>** [1],  $\beta$  alumina-NH<sub>4</sub>

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (NH<sub>4</sub>)<sub>1+2x</sub>O<sub>1+x</sub> layers (split framework O site, NH<sub>4</sub> at BR and near mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Iyi N. et al. (1991) [1]

Al<sub>10.96</sub>H<sub>5.22</sub>N<sub>1.31</sub>O<sub>17.09</sub>

$a = 0.5598$ ,  $c = 2.2876$  nm,  $c/a = 4.086$ ,  $V = 0.6208$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.157	0.314	0.54928		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.161	0.322	0.1757	0.037	
Al3	12k	.m.	0.1678	0.3356	0.1045	0.957	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.5019	0.0038	0.64427		square pyramid Al <sub>5</sub>
(NH <sub>4</sub> )5	6h	mm2	0.091	0.182	<sup>1</sup> / <sub>4</sub>	0.145	
O6	6h	mm2	0.146	0.292	<sup>1</sup> / <sub>4</sub>	0.03	
O7	6h	mm2	0.674	0.348	<sup>1</sup> / <sub>4</sub>	0.333	
O8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0547		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.52454		tetrahedron O <sub>4</sub>
Al10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.67448		
O11	4e	3m.	0	0	0.14		trigonal prism Al <sub>6</sub>
(NH <sub>4</sub> )12	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.87	coplanar triangle O <sub>3</sub>
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

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] Iyi N., Yajima Y., Kimura S. (1991), J. Solid State Chem. 92, 578-590.

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hP86

Ba <sub>0.79</sub> Al <sub>10.9</sub> O <sub>17.14</sub>	hP86	(194) $P6_3/mmc - k^4h^3f^3eda$
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**Ba<sub>0.79</sub>Al<sub>10.9</sub>O<sub>17.14</sub>** [1],  $\beta$  alumina-Ba

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Ba<sub>1/2+x</sub>O<sub>1+x</sub> layers (in part split framework O site, Ba near BR positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Iyi N. et al. (1984) [1]

Al<sub>10.90</sub>Ba<sub>0.74</sub>O<sub>17.28</sub>

$a = 0.5588$ ,  $c = 2.2769$  nm,  $c/a = 4.075$ ,  $V = 0.6157$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	.m.	0.1574	0.3148	0.1769	0.078	trigonal bipyramid AlO <sub>4</sub>
O2	12k	.m.	0.158	0.316	0.54953		tetrahedron Al <sub>4</sub>
Al3	12k	.m.	0.16744	0.33488	0.10462	0.905	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.5039	0.0078	0.64721		square pyramid Al <sub>5</sub>
O5	6h	mm2	0.119	0.238	<sup>1</sup> / <sub>4</sub>	0.092	non-collinear Al <sub>2</sub>

Ba6	6h	mm2	0.3283	0.6566	$\frac{1}{4}$	0.248	
O7	6h	mm2	0.71	0.42	$\frac{1}{4}$	0.27	
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05574		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52356		tetrahedron O <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67537		
O11	4e	3m.	0	0	0.1411		trigonal prism Al <sub>6</sub>
O12	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.19	
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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

References: [1] Iyi N., Inoue Z., Takekawa S., Kimura S. (1984), J. Solid State Chem. 52, 66-72.

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hP86

HCs<sub>2</sub>Rh<sub>6</sub>N[CO]<sub>14</sub> hP86 (194) P6<sub>3</sub>/mmc – k<sup>5</sup>h<sup>3</sup>edc

**Cs<sub>2</sub>[Rh<sub>6</sub>(μ-H)N(CO)<sub>14</sub>] [1]**

Structural features: Rh<sub>6</sub>N(CO)<sub>14</sub>H units (a central N atom surrounded by a Rh<sub>6</sub> trigonal prism capped by a CO unit above each prism edge and vertex, one of the three CO units above the vertical edges being replaced by an H atom) in a Mg-type (h.c.p.) arrangement.

Ciani G. et al. (1994) [1]

C<sub>14</sub>Cs<sub>2</sub>HNO<sub>14</sub>Rh<sub>6</sub>

*a* = 1.1089, *c* = 1.2308 nm, *c/a* = 1.110, *V* = 1.3107 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	.m.	0.1552	0.3104	0.559		single atom C
C2	12k	.m.	0.1911	0.3822	0.017		single atom O
Rh3	12k	.m.	0.25124	0.50248	0.1342		square pyramid C <sub>4</sub> N
O4	12k	.m.	0.5186	0.0372	0.122		single atom C
C5	12k	.m.	0.5409	0.0818	0.626		single atom O
Cs6	6h	mm2	0.0534	0.1068	$\frac{1}{4}$	0.216	
O7	6h	mm2	0.12	0.24	$\frac{1}{4}$	0.667	single atom C
C8	6h	mm2	0.179	0.358	$\frac{1}{4}$	0.667	single atom O
Cs9	4e	3m.	0	0	0.086	0.175	
Cs10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		trigonal prism O <sub>6</sub>
N11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Rh <sub>6</sub>
H12	6h	mm2	0.1899	0.3798	$\frac{1}{4}$	0.333	

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

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] Ciani G., Proserpio D.M., Sironi A., Martinengo S., Fumagalli A. (1994), J. Chem. Soc., Dalton Trans. 1974, 471-475.

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hP88

NaCd<sub>0.11</sub>Al<sub>11</sub>O<sub>17.11</sub> hP88 (194) P6<sub>3</sub>/mmc – k<sup>4</sup>h<sup>3</sup>f<sup>3</sup>edca

**NaCd<sub>0.11</sub>Al<sub>11</sub>O<sub>17.11</sub> [1], β alumina-Na,Cd**

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and  $(\text{Na,Cd})_x\text{O}_{1+y}$  layers (Na at BR and near mO, Cd on the opposite side of mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Edström K. et al. (1991) [1]



$a = 0.55921$ ,  $c = 2.2526$  nm,  $c/a = 4.028$ ,  $V = 0.6100$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1573	0.3146	0.54999		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.16365	0.3273	0.17496	0.037	
Al3	12k	.m.	0.16771	0.33542	0.10643	0.963	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.50311	0.00622	0.6464		square pyramid Al <sub>5</sub>
Na5	6h	mm2	0.10298	0.20596	<sup>1</sup> / <sub>4</sub>	0.095	
O6	6h	mm2	0.16667	0.33333	<sup>1</sup> / <sub>4</sub>	0.037	
Cd7	6h	mm2	0.21237	0.42474	<sup>1</sup> / <sub>4</sub>	0.035	
O8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.05545		tetrahedron Al <sub>4</sub>
Al9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.52479		tetrahedron O <sub>4</sub>
Al10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.67564		tetrahedron O <sub>4</sub>
O11	4e	3m.	0	0	0.14223		trigonal prism Al <sub>6</sub>
O12	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		colinear Al <sub>2</sub>
Na13	2c	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>	0.723	
Al14	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.024, T = 295 K

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

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 635-643.

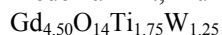
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hP88

$\text{Gd}_{4.5}(\text{Ti}_{0.58}\text{W}_{0.42})_3\text{O}_{14}$	hP88	(194) $P6_3/mmc - k^4h^3gf^2eca$
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### **Gd<sub>18</sub>Ti<sub>7</sub>W<sub>5</sub>O<sub>56</sub>** [1]

Structural features: (Ti,W)O<sub>6</sub> octahedra share vertices to form HTB-type slabs ((Ti,W) forms a Kagomé mesh); additional O in Gd<sub>4</sub> tetrahedra.

Tiedemann P., Müller Buschbaum H. (1985) [1]



$a = 0.7382$ ,  $c = 2.349$  nm,  $c/a = 3.182$ ,  $V = 1.1086$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.153	0.306	0.665		single atom Ti
Gd2	12k	.m.	0.1677	0.3354	0.1184		monocapped trigonal prism O <sub>7</sub>
O3	12k	.m.	0.214	0.428	0.013		non-colinear Ti <sub>2</sub>
O4	12k	.m.	0.529	0.058	0.08		single atom Ti
O5	6h	mm2	0.142	0.284	<sup>1</sup> / <sub>4</sub>		non-colinear Ti <sub>2</sub>
O6	6h	mm2	0.55	0.1	<sup>1</sup> / <sub>4</sub>		non-colinear Ti <sub>2</sub>
M7	6h	mm2	0.8401	0.6802	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
M8	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		octahedron O <sub>6</sub>
O9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.156		tetrahedron Gd <sub>4</sub>

Gd10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6411	octahedron O <sub>6</sub>
O11	4e	3m.	0	0	0.097	tetrahedron Gd <sub>4</sub>
Gd12	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.625 8-vertex polyhedron O <sub>8</sub>
Gd13	2a	-3m.	0	0	0	0.375 8-vertex polyhedron O <sub>8</sub>

M7 = 0.646Ti + 0.354W; M8 = 0.521Ti + 0.479W

Experimental: single crystal, diffractometer, X-rays, wR = 0.084

References: [1] Tiedemann P., Müller Buschbaum H. (1985), Z. Anorg. Allg. Chem. 526, 67-72.

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hP90

K <sub>1.3</sub> Al <sub>10.9</sub> O <sub>17</sub>	hP90	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>4</sup> h <sup>4</sup> f <sup>3</sup> ea
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**K<sub>1.3</sub>Al<sub>10.9</sub>O<sub>17</sub>** [1], β alumina-K; Ag<sub>0.95</sub>Al<sub>11</sub>O<sub>16.975</sub> [2], β alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids, partial disorder for the latter) and K<sub>x</sub>O layers (split O site, K near BR, aBR and mO positions) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Collin G. et al. (1977) [1]

Al<sub>10.93</sub>K<sub>1.30</sub>O<sub>17</sub>

*a* = 0.5602, *c* = 2.2734 nm, *c/a* = 4.058, *V* = 0.6179 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	.m.	0.1571	0.3142	0.5496		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.162	0.324	0.175	0.03	
Al3	12k	.m.	0.1678	0.3356	0.1052	0.958	
O4	12k	.m.	0.5027	0.0054	0.6454		
K5	6h	mm2	0.0293	0.0586	$\frac{1}{4}$	0.047	
K6	6h	mm2	0.1176	0.2352	$\frac{1}{4}$	0.125	
K7	6h	mm2	0.3113	0.6226	$\frac{1}{4}$	0.26	
O8	6h	mm2	0.6849	0.3698	$\frac{1}{4}$	0.333	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0552		tetrahedron Al <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5245		tetrahedron O <sub>4</sub>
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6749		
O12	4e	3m.	0	0	0.1411		
Al13	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

Remarks: The authors state that a slight deviation from charge balance may be compensated for by interstitial O. Short interatomic distances for partly occupied site(s).

References: [1] Collin G., Boilot J.P., Kahn A., Thery J., Comes R. (1977), J. Solid State Chem. 21, 283-292. [2] Boilot J.P., Colomban P., Collin G., Comes R. (1980), J. Phys. Chem. Solids 41, 47-54.

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hP90

Ag <sub>0.23</sub> Cd <sub>0.49</sub> Al <sub>11</sub> O <sub>17.11</sub>	hP90	(194) <i>P6<sub>3</sub>/mmc</i> – k <sup>4</sup> h <sup>4</sup> f <sup>3</sup> ea
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**Ag<sub>0.23</sub>Cd<sub>0.49</sub>Al<sub>11</sub>O<sub>17.11</sub>** [1], β alumina-Ag,Cd

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Ag,Cd)<sub>x</sub>O<sub>1+y</sub> layers (split framework O site, Ag near BR, Cd near mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Edström K. et al. (1991) [1]

Ag<sub>0.23</sub>Al<sub>11</sub>Cd<sub>0.50</sub>O<sub>17.11</sub>

$a = 0.55896$ ,  $c = 2.2434$  nm,  $c/a = 4.014$ ,  $V = 0.6070$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.15705	0.3141	0.55033		tetrahedron Al <sub>4</sub>
Al2	12 <i>k</i>	. <i>m</i> .	0.1593	0.3186	0.17657	0.037	
Al3	12 <i>k</i>	. <i>m</i> .	0.16798	0.33596	0.10696	0.963	7-vertex polyhedron AlO <sub>6</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.50276	0.00552	0.64701		square pyramid Al <sub>5</sub>
Cd5	6 <i>h</i>	<i>mm</i> 2	0.14404	0.28808	<sup>1</sup> / <sub>4</sub>	0.165	
O6	6 <i>h</i>	<i>mm</i> 2	0.16667	0.33333	<sup>1</sup> / <sub>4</sub>	0.037	
Ag7	6 <i>h</i>	<i>mm</i> 2	0.2946	0.5892	<sup>1</sup> / <sub>4</sub>	0.077	
O8	6 <i>h</i>	<i>mm</i> 2	0.72153	0.44306	<sup>1</sup> / <sub>4</sub>	0.333	
O9	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.05587		tetrahedron Al <sub>4</sub>
Al10	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5248		tetrahedron O <sub>4</sub>
Al11	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.67595		
O12	4 <i>e</i>	3 <i>m</i> .	0	0	0.14352		trigonal prism Al <sub>6</sub>
Al13	2 <i>a</i>	-3 <i>m</i> .	0	0	0		octahedron O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.041$ ,  $T = 295$  K

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

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 643-650.

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hP90

SrMg <sub>4</sub>	hP90	(194) $P6_3/mmc - k^5h^2gf^2e$
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**SrMg<sub>4</sub>** [1]

Structural features: Sr<sub>6</sub> octahedral clusters and Sr<sub>3</sub> trigonal clusters in a matrix of Mg atoms.

Wang F.E. et al. (1965) [1]

Mg<sub>4</sub>Sr

$a = 1.0511$ ,  $c = 2.8362$  nm,  $c/a = 2.698$ ,  $V = 2.7137$  nm<sup>3</sup>,  $Z = 18$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sr1	12 <i>k</i>	. <i>m</i> .	0.1369	0.2738	0.0625		7-capped pentagonal prism Mg <sub>13</sub> Sr <sub>4</sub>
Mg2	12 <i>k</i>	. <i>m</i> .	0.1677	0.3354	0.654		11-vertex polyhedron Mg <sub>7</sub> Sr <sub>4</sub>
Mg3	12 <i>k</i>	. <i>m</i> .	0.1772	0.3544	0.1897		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Mg4	12 <i>k</i>	. <i>m</i> .	0.2321	0.4642	0.5546		11-vertex polyhedron Mg <sub>8</sub> Sr <sub>3</sub>
Mg5	12 <i>k</i>	. <i>m</i> .	0.5	0.0	0.1177		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Sr6	6 <i>h</i>	<i>mm</i> 2	0.522	0.044	<sup>1</sup> / <sub>4</sub>		cuboctahedron Mg <sub>12</sub>
Mg7	6 <i>h</i>	<i>mm</i> 2	0.8989	0.7978	<sup>1</sup> / <sub>4</sub>		icosahedron Mg <sub>10</sub> Sr <sub>2</sub>
Mg8	6 <i>g</i>	.2/ <i>m</i> .	<sup>1</sup> / <sub>2</sub>	0	0		icosahedron Mg <sub>8</sub> Sr <sub>4</sub>
Mg9	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0373		pseudo Frank-Kasper Mg <sub>10</sub> Sr <sub>3</sub>
Mg10	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1427		7-vertex polyhedron Mg <sub>7</sub>

Mg11    4e   3m.    0    0    0.158    icosahedron Mg<sub>9</sub>Sr<sub>3</sub>

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

Remarks: An additional Mg site was detected in [2]. In table 3 of [1] the *x*-coordinate of former Sr(h) is misprinted as 0.0478 instead of -0.478, and the *z*-coordinate of former Mg(f2) as -0.1427 instead of 0.1427 (checked on interatomic distances).

References: [1] Wang F.E., Kanda F.A., Miskell C.F., King A.J. (1965), Acta Crystallogr. 18, 24-31. [2] Merlo F., Fornasini M.L. (1982), Acta Crystallogr. B 38, 1797-1798.

194  
hP90

La<sub>0.85</sub>Al<sub>11.5</sub>O<sub>18.5</sub>    hP90    (194) *P6<sub>3</sub>/mmc* – *lk<sup>2</sup>jh<sup>3</sup>e<sup>2</sup>ca*

**La<sub>0.85</sub>Al<sub>11.5</sub>O<sub>18.5</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers (partial vacancies ignored for the latter) in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (ideal and split site); split O sites.

Gasperin M. et al. (1984) [1]

Al<sub>11.53</sub>La<sub>0.85</sub>O<sub>18.62</sub>

*a* = 0.555, *c* = 2.2031 nm, *c/a* = 3.970, *V* = 0.5877 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24l	1	0.3121	0.1487	0.0518	0.5	
Al2	12k	.m.	0.1676	0.3352	0.1076	0.952	
O3	12k	.m.	0.5034	0.0068	0.6501		non-coplanar triangle Al <sub>3</sub>
O4	12j	m..	0.3623	0.1614	1/4	0.437	
La5	6h	mm2	0.283	0.566	1/4	0.1	
O6	4f	3m.	1/3	2/3	0.0554		tetrahedron Al <sub>4</sub>
Al7	4f	3m.	1/3	2/3	0.5269		
Al8	4f	3m.	1/3	2/3	0.6899		
O9	4e	3m.	0	0	0.1481		tetrahedron Al <sub>4</sub>
Al10	4e	3m.	0	0	0.2386	0.41	
La11	2c	-6m2	1/3	2/3	1/4	0.55	
Al12	2a	-3m.	0	0	0		

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

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

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

References: [1] Gasperin M., Saine M.C., Kahn A., Laville F., Lejus A.M. (1984), J. Solid State Chem. 54, 61-69.

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hP92

Mg<sub>13</sub>Zn<sub>30</sub>Sm<sub>3</sub>    hP92    (194) *P6<sub>3</sub>/mmc* – *k<sup>3</sup>i<sup>2</sup>h<sup>2</sup>fda*

**Mg<sub>28.3</sub>Zn<sub>65.2</sub>Sm<sub>6.5</sub>** [1]

Structural features: 3D-framework containing infinite columns of Zn-centered icosahedra.



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

 $\text{Mg}_{13}\text{Sm}_3\text{Zn}_{30}$  $a = 1.4619$ ,  $c = 0.8708$  nm,  $c/a = 0.596$ ,  $V = 1.6117$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	12k	.m.	0.11618	0.23236	0.5646		16-vertex Frank-Kasper $\text{Zn}_{12}\text{Mg}_4$
Mg2	12k	.m.	0.22819	0.45638	0.0531		pseudo Frank-Kasper $\text{Zn}_9\text{Mg}_2\text{Sm}_2$
Zn3	12k	.m.	0.56815	0.1363	0.08674		pseudo Frank-Kasper $\text{Zn}_6\text{Mg}_3\text{Sm}_2$
Zn4	12j	m..	0.06421	0.30371	$\frac{1}{4}$		icosahedron $\text{Zn}_5\text{Mg}_6\text{Sm}$
Zn5	12j	m..	0.40866	0.11808	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_5\text{Sm}$
Zn6	12i	.2.	0.35897	0	0		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn7	6h	mm2	0.06122	0.12244	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_6$
Sm8	6h	mm2	0.45834	0.91668	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Zn}_{14}\text{Mg}_4$
Zn9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1001		pseudo Frank-Kasper $\text{Zn}_4\text{Mg}_4\text{Sm}_3$
Mg10	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		8-vertex polyhedron $\text{Zn}_8$
Zn11	2a	-3m.	0	0	0		icosahedron $\text{Zn}_6\text{Mg}_6$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.020$ 

References: [1] Sugiyama K., Yasuda K., Ohsuna T., Hiraga K. (1998), Z. Kristallogr. 213, 537-543.

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hP92

$\text{Ag}_{1.22}\text{Al}_{11}\text{O}_{17.11}$	hP92	(194) $P6_3/mmc - k^4h^4f^3eda$
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 $\text{Ag}_{1.22}\text{Al}_{11}\text{O}_{17.11}$  [1],  $\beta$  alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and  $\text{Ag}_{1+2x}\text{O}_{1+x}$  layers (Ag near BR, aBR and mO positions, additional O in mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Edström K. et al. (1991) [1]

 $\text{Ag}_{1.22}\text{Al}_{11}\text{O}_{17.11}$  $a = 0.55914$ ,  $c = 2.243$  nm,  $c/a = 4.012$ ,  $V = 0.6073$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.15699	0.31398	0.5502		tetrahedron $\text{Al}_4$
Al2	12k	.m.	0.15959	0.31918	0.17572	0.037	
Al3	12k	.m.	0.168	0.336	0.1065	0.963	7-vertex polyhedron $\text{AlO}_6$
O4	12k	.m.	0.50288	0.00576	0.64646		square pyramid $\text{Al}_5$
Ag5	6h	mm2	0.02372	0.04744	$\frac{1}{4}$	0.134	
O6	6h	mm2	0.16667	0.33333	$\frac{1}{4}$	0.037	
Ag7	6h	mm2	0.22199	0.44398	$\frac{1}{4}$	0.105	
Ag8	6h	mm2	0.29524	0.59048	$\frac{1}{4}$	0.168	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05536		tetrahedron $\text{Al}_4$
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52495		tetrahedron $\text{O}_4$
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67573		tetrahedron $\text{O}_4$
O12	4e	3m.	0	0	0.14299		trigonal prism $\text{Al}_6$
O13	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear $\text{Al}_2$
Al14	2a	-3m.	0	0	0		octahedron $\text{O}_6$

Transformation from published data: origin shift  $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $R = 0.037$ ,  $T = 295$  K

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

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 643-650.

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hP92

$\text{BaFe}_{18}\text{O}_{27}$

hP92

(194)  $P6_3/mmc - k^4hgf^5e^2cb$

**BaFe<sub>18</sub>O<sub>27</sub>** [2], ferrite W-type

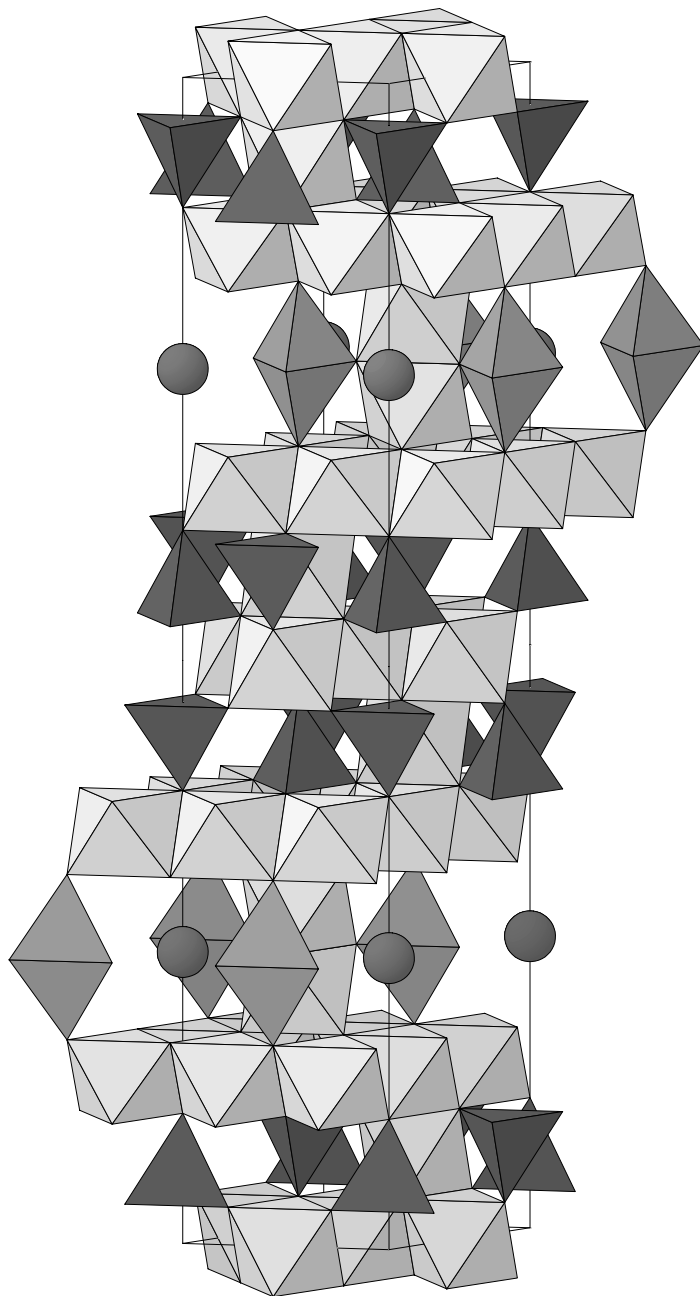


Fig. III.48. **BaFe<sub>18</sub>O<sub>27</sub>**

Arrangement of  $\text{FeO}_4$  tetrahedra (dark),  $\text{FeO}_5$  trigonal bipyramids (medium),  $\text{FeO}_6$  octahedra (light) and Ba atoms.

Structural features: Close-packed O<sub>4</sub> and BaO<sub>3</sub> layers in h<sub>3</sub>c<sub>4</sub> stacking; Fe in octahedral, tetrahedral and trigonal bipyramidal voids. Intergrowth of spinel-type slabs (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells), FeO<sub>5</sub> trigonal bipyramids and Ba atoms. See Fig. III.48.

Braun P.B. (1957) [1]

BaFe<sub>18</sub>O<sub>27</sub>

$a = 0.588$ ,  $c = 3.2845$  nm,  $c/a = 5.586$ ,  $V = 0.9835$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.16667	0.33334	0.036		tetrahedron Fe <sub>4</sub>
Fe2	12 <i>k</i>	. <i>m</i> .	0.16667	0.33334	0.14998		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.16667	0.33334	0.6791		non-coplanar triangle Fe <sub>3</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.5	0.0	0.1116		tetrahedron Fe <sub>4</sub>
O5	6 <i>h</i>	<i>mm</i> 2	0.5	0.0	$\frac{1}{4}$		coplanar triangle Fe <sub>3</sub>
Fe6	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		octahedron O <sub>6</sub>
Fe7	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0734		octahedron O <sub>6</sub>
O8	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1791		tetrahedron Fe <sub>4</sub>
O9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.536		tetrahedron Fe <sub>4</sub>
Fe10	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5927		tetrahedron O <sub>4</sub>
Fe11	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.708		octahedron O <sub>6</sub>
Fe12	4 <i>e</i>	3 <i>m</i> .	0	0	0.0564		tetrahedron O <sub>4</sub>
O13	4 <i>e</i>	3 <i>m</i> .	0	0	0.1116		tetrahedron Fe <sub>4</sub>
Fe14	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>
Ba15	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.146$

References: [1] Braun P.B. (1957), Philips Res. Rep. 12, 491-548. [2] Braun P.B. (1952), Nature (London) 170, 708.

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hP92

K <sub>16</sub> Na <sub>9</sub> Tl <sub>18</sub> Cd <sub>3</sub>	hP92	(194) $P6_3/mmc - k^5h^2gf^2ed$
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**K<sub>16</sub>Na<sub>9</sub>Tl<sub>18</sub>Cd<sub>3</sub>** [1]

Structural features: Tl<sub>6</sub>(Tl<sub>2</sub>Cd<sub>3</sub>) pentacapped trigonal prisms (Cd above the rectangular prism faces) and Tl<sub>5</sub> trigonal bipyramids in a matrix of K and Na atoms.

Huang D.P., Corbett J.D. (1999) [1]

Cd<sub>3</sub>K<sub>16</sub>Na<sub>9</sub>Tl<sub>18</sub>

$a = 1.1136$ ,  $c = 2.9352$  nm,  $c/a = 2.636$ ,  $V = 3.1523$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
K1	12 <i>k</i>	. <i>m</i> .	0.129	0.258	0.5589		16-vertex Frank-Kasper Tl <sub>6</sub> K <sub>6</sub> Na <sub>4</sub>
Tl2	12 <i>k</i>	. <i>m</i> .	0.1586	0.3172	0.69658		icosahedron Cd <sub>2</sub> Tl <sub>2</sub> Na <sub>2</sub> K <sub>6</sub>
Na3	12 <i>k</i>	. <i>m</i> .	0.163	0.326	0.1527		icosahedron CdTl <sub>5</sub> K <sub>6</sub>
Tl4	12 <i>k</i>	. <i>m</i> .	0.2339	0.4678	0.05443		icosahedron Tl <sub>4</sub> Na <sub>3</sub> K <sub>5</sub>
K5	12 <i>k</i>	. <i>m</i> .	0.5374	0.0748	0.1247		15-vertex Frank-Kasper Tl <sub>6</sub> Na <sub>3</sub> K <sub>6</sub>
Cd6	6 <i>h</i>	<i>mm</i> 2	0.1042	0.2084	$\frac{1}{4}$		icosahedron Na <sub>2</sub> Tl <sub>6</sub> Cd <sub>2</sub> K <sub>2</sub>
K7	6 <i>h</i>	<i>mm</i> 2	0.4556	0.9112	$\frac{1}{4}$		7-capped pentagonal prism Cd <sub>2</sub> K <sub>5</sub> Tl <sub>6</sub> Na <sub>4</sub>
Na8	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		icosahedron Tl <sub>6</sub> K <sub>6</sub>
Tl9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1398		icosahedron Tl <sub>3</sub> Na <sub>3</sub> K <sub>6</sub>

Tl10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5303	icosahedron $\text{Ti}_3\text{Na}_3\text{K}_6$
Tl11	4e	3m.	0	0	0.1587	icosahedron $\text{Na}_3\text{Ti}_3\text{Cd}_3\text{K}_3$
K12	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	15-vertex Frank-Kasper $\text{Ti}_6\text{K}_9$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.026$ ,  $T = 296$  K

References: [1] Huang D.P., Corbett J.D. (1999), Inorg. Chem. 38, 316-320.

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hP94

$\text{Na}_{0.47}\text{Li}_{0.75}\text{Al}_{11}\text{O}_{17.11}$	hP94	(194) $P6_3/mmc - k^4h^4f^4ea$
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$\text{Na}_{0.47}\text{Li}_{0.75}\text{Al}_{11}\text{O}_{17.11}$  [1],  $\beta$  alumina-Li,Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and  $(\text{Li,Na})_{1+2x}\text{O}_{1+x}$  layers (split framework O site, Li and (Li,Na) near BR, Na near mO positions, additional O at mO positions between Al displaced into interstitial Al site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Edström K. et al. (1997) [1]

$\text{Al}_{11}\text{Li}_{0.75}\text{Na}_{1.31}\text{O}_{17.11}$

$a = 0.559$ ,  $c = 2.2656$  nm,  $c/a = 4.053$ ,  $V = 0.6131$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.15703	0.31406	0.54976		tetrahedron $\text{Al}_4$
Al2	12k	.m.	0.1601	0.3202	0.1762	0.037	
Al3	12k	.m.	0.16788	0.33576	0.10538	0.963	7-vertex polyhedron $\text{AlO}_6$
O4	12k	.m.	0.50299	0.00598	0.64592		square pyramid $\text{Al}_5$
Na5	6h	mm2	0.0942	0.1884	$\frac{1}{4}$	0.421	
O6	6h	mm2	0.1667	0.3334	$\frac{1}{4}$	0.037	
M7	6h	mm2	0.2968	0.5936	$\frac{1}{4}$	0.172	
O8	6h	mm2	0.688	0.376	$\frac{1}{4}$	0.333	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0552		tetrahedron $\text{Al}_4$
Li10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2043	0.142	
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5246		tetrahedron $\text{O}_4$
Al12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67552		
O13	4e	3m.	0	0	0.14148		trigonal prism $\text{Al}_6$
Al14	2a	-3m.	0	0	0		octahedron $\text{O}_6$

$M7 = 0.91\text{Li} + 0.09\text{Na}$

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.036$ ,  $T = 30$  K

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

References: [1] Edström K., Gustafsson T., Thomas J.O., Farrington G.C. (1997), Acta Crystallogr. B 53, 631-638.

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hP94

$\text{NaMg}_2\text{Al}_{15}\text{O}_{25}$	hP94	(194) $P6_3/mmc - k^4hgf^5e^2dcb$
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$\text{NaMg}_2\text{Al}_{15}\text{O}_{25}$  [1]

Structural features: Spinel-type slabs (six close-packed O layers in c stacking, (Al,Mg) in octahedral and tetrahedral voids) and NaO layers (Na delocalized within a hexagon mesh) alternate along [001]. Infinite slabs of edge-linked (Al,Mg)O<sub>6</sub> octahedra sharing vertices with single (Al,Mg)O<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked (Al,Mg)O<sub>4</sub> tetrahedra to form a 3D-framework.

Bettman M., Terner L.L. (1971) [1]

Al<sub>14.99</sub>Mg<sub>2.01</sub>Na<sub>1.93</sub>O<sub>25</sub>

$a = 0.563$ ,  $c = 3.185$  nm,  $c/a = 5.657$ ,  $V = 0.8743$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.0334		tetrahedron Al <sub>4</sub>
M2	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.1474		octahedron O <sub>6</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.167	0.334	0.6765		non-coplanar triangle Al <sub>3</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.5	0.0	0.1109		tetrahedron Al <sub>4</sub>
Na5	6 <i>h</i>	<i>mm</i> 2	0.167	0.334	$\frac{1}{4}$	0.16	
M6	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0		octahedron O <sub>6</sub>
M7	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0701		octahedron O <sub>6</sub>
O8	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1765		non-coplanar triangle Al <sub>3</sub>
O9	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5334		tetrahedron Al <sub>4</sub>
M10	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.5932		tetrahedron O <sub>4</sub>
M11	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6972		tetrahedron O <sub>4</sub>
M12	4 <i>e</i>	3. <i>m</i> .	0	0	0.0577		tetrahedron O <sub>4</sub>
O13	4 <i>e</i>	3. <i>m</i> .	0	0	0.1109		tetrahedron Al <sub>4</sub>
O14	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Na15	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.49	
Na16	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$	0.96	

M2 = 0.882Al + 0.118Mg; M6 = 0.882Al + 0.118Mg; M7 = 0.882Al + 0.118Mg; M10 = 0.882Al + 0.118Mg; M11 = 0.882Al + 0.118Mg; M12 = 0.882Al + 0.118Mg

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

Experimental: single crystal, precession photographs, X-rays

Remarks: Structure studied jointly on single crystal and powder diffraction data. No attempt was made to locate Mg. We assigned an approximate value to the Al/Mg ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Bettman M., Terner L.L. (1971), Inorg. Chem. 10, 1442-1446.

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hP94

Ba(Zn <sub>0.5</sub> Fe <sub>0.5</sub> ) <sub>4</sub> Fe <sub>14</sub> O <sub>27</sub>	hP94	(194) $P6_3/mmc - k^4hg^6e^2b$
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**BaZn<sub>2</sub>Fe<sub>16</sub>O<sub>27</sub>** [2], ferrite W-type

Structural features: Close-packed O<sub>4</sub> and BaO<sub>3</sub> layers in h<sub>3</sub>c<sub>4</sub> stacking; Fe in octahedral and tetrahedral, (Fe,Zn) in tetrahedral voids. Intergrowth of spinel-type slabs (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single (Fe,Zn)O<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells), FeO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and Ba atoms.

Collomb A., Vallet Regi M. (1987) [1]

BaFe<sub>16.26</sub>O<sub>27</sub>Zn<sub>1.74</sub>

$a = 0.59109$ ,  $c = 3.2985$  nm,  $c/a = 5.580$ ,  $V = 0.9981$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.1637	0.3274	0.6789		non-coplanar triangle Fe <sub>3</sub>

Fe2	12k	.m.	0.1644	0.3288	0.15	octahedron O <sub>6</sub>
O3	12k	.m.	0.1806	0.3612	0.0352	tetrahedron ZnFe <sub>3</sub>
O4	12k	.m.	0.5126	0.0252	0.6098	tetrahedron Fe <sub>4</sub>
O5	6h	mm2	0.5167	0.0334	$\frac{1}{4}$	
Fe6	6g	.2/m.	$\frac{1}{2}$	0	0	octahedron O <sub>6</sub>
Fe7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0751	octahedron O <sub>6</sub>
O8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1794	tetrahedron Fe <sub>4</sub>
Fe9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2434	0.5 octahedron O <sub>6</sub>
O10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5363	tetrahedron Fe <sub>4</sub>
M11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.593	tetrahedron O <sub>4</sub>
Fe12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7077	octahedron O <sub>6</sub>
M13	4e	3m.	0	0	0.0571	tetrahedron O <sub>4</sub>
O14	4e	3m.	0	0	0.1124	tetrahedron ZnFe <sub>3</sub>
Ba15	2b	-6m2	0	0	$\frac{1}{4}$	anticuboctahedron O <sub>12</sub>

M11 = 0.79Fe + 0.21Zn; M13 = 0.66Zn + 0.34Fe

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

Experimental: powder, diffractometer, neutrons, wR = 0.029, T = 698 K

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

References: [1] Collomb A., Vallet Regi M. (1987), Mater. Res. Bull. 22, 753-760. [2] Deschizeaux Cheruy M.N., Vallet Regi M., Joubert J.C. (1985), J. Solid State Chem. 57, 234-239.

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hP94

Sr <sub>9</sub> Mg <sub>38</sub>	hP94	(194) $P6_3/mmc - k^5h^2gf^3e$
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#### Sr<sub>9</sub>Mg<sub>38</sub> [1]

Structural features: Sr<sub>6</sub> octahedral clusters and Sr<sub>3</sub> trigonal clusters in a matrix of Mg atoms.

Merlo F., Fornasini M.L. (1982) [1]

Mg<sub>38</sub>Sr<sub>9</sub>

$a = 1.0500$ ,  $c = 2.8251$  nm,  $c/a = 2.691$ ,  $V = 2.6974$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sr1	12k	.m.	0.1362	0.2724	0.5621		7-capped pentagonal prism Mg <sub>13</sub> Sr <sub>4</sub>
Mg2	12k	.m.	0.1674	0.3348	0.1533		icosahedron Mg <sub>8</sub> Sr <sub>4</sub>
Mg3	12k	.m.	0.1743	0.3486	0.6898		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Mg4	12k	.m.	0.2337	0.4674	0.0547		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Mg5	12k	.m.	0.5037	0.0074	0.1170		pseudo Frank-Kasper Mg <sub>10</sub> Sr <sub>3</sub>
Mg6	6h	mm2	0.0989	0.1978	$\frac{1}{4}$		icosahedron Mg <sub>10</sub> Sr <sub>2</sub>
Sr7	6h	mm2	0.4688	0.9376	$\frac{1}{4}$		pseudo Frank-Kasper Mg <sub>16</sub> Sr <sub>2</sub>
Mg8	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Mg <sub>8</sub> Sr <sub>4</sub>
Mg9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1465		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>
Mg10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5378		pseudo Frank-Kasper Mg <sub>10</sub> Sr <sub>3</sub>
Mg11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6426		7-vertex polyhedron Mg <sub>7</sub>
Mg12	4e	3m.	0	0	0.1575		icosahedron Mg <sub>9</sub> Sr <sub>3</sub>

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

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

Remarks: Supersedes a structure proposal in [2] where site Mg8 was not detected (SrMg<sub>4</sub>). In [2] the x-coordinate of former Sr(h) is misprinted as -0.478 instead of 0.0478 and the z-coordinate of former Mg(f2) as 0.1427 instead of -0.1427 (see [1] and [3]).

References: [1] Merlo F., Fornasini M.L. (1982), Acta Crystallogr. B 38, 1797-1798. [2] Wang F.E., Kanda F.A., Miskell C.F., King A.J. (1965), Acta Crystallogr. 18, 24-31. [3] (1975), Structure Reports 30A, 24.

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hP96

$\text{Mg}(\text{Cu}_{0.54}\text{Al}_{0.46})_2$	hP96	(194) $P6_3/mmc - k^3\text{hgf}^8\text{e}^4$
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**Mg(Cu<sub>0.535</sub>Al<sub>0.465</sub>)<sub>2</sub> 16H** [1], Laves phase 16H

Structural features: (Cu,Al)<sub>4</sub> tetrahedra share faces and vertices to form a 3D-framework. Laves-type slabs in h<sub>2</sub>ch<sub>2</sub>chc stacking. Tetrahedrally close-packed structure (Frank-Kasper phase).

Kitano Y. et al. (1977) [1]

Al<sub>0.92</sub>Cu<sub>1.08</sub>Mg

$a = 0.510$ ,  $c = 6.67$  nm,  $c/a = 13.078$ ,  $V = 1.5024$  nm<sup>3</sup>,  $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.16667	0.33333	0.0625		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M2	12k	.m.	0.16667	0.33333	0.1875		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M3	12k	.m.	0.5	0.0	0.125		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M4	6h	mm2	0.83333	0.66667	<sup>1</sup> / <sub>4</sub>		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M5	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M6	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.03125		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M7	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.09375		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
M8	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.15625		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>
Mg9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.22656		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.53906		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg11	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.58594		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg12	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.66406		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg13	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.71094		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg14	4e	3m.	0	0	0.02344		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg15	4e	3m.	0	0	0.10156		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
Mg16	4e	3m.	0	0	0.14844		16-vertex Frank-Kasper Cu <sub>12</sub> Mg <sub>4</sub>
M17	4e	3m.	0	0	0.21875		icosahedron Cu <sub>6</sub> Mg <sub>6</sub>

M1 = 0.54Cu + 0.46Al; M2 = 0.54Cu + 0.46Al; M3 = 0.54Cu + 0.46Al; M4 = 0.54Cu + 0.46Al; M5 = 0.54Cu + 0.46Al; M6 = 0.54Cu + 0.46Al; M7 = 0.54Cu + 0.46Al; M8 = 0.54Cu + 0.46Al; M17 = 0.54Cu + 0.46Al

Experimental: foil, electron diffraction

Remarks: Idealized coordinates. We assigned an approximate value to the Cu/Al ratio of sites M based on the nominal composition.

References: [1] Kitano Y., Komura Y., Kajiwara H. (1977), Trans. Jpn. Inst. Met. 18, 39-45.

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hP96

$\text{Ag}_{1.25}\text{Al}_{11}\text{O}_{17.125}$	hP96	(194) $P6_3/mmc - k^4\text{h}^5\text{f}^3\text{e}^a$
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**Ag<sub>1.25</sub>Al<sub>11</sub>O<sub>17.125</sub>** [1], β alumina-Ag

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Ag<sub>1+2x</sub>O<sub>1+x</sub> layers (split framework O site, Ag near BR, aBR and mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Boilot J.P. et al. (1980) [1]

$\text{Ag}_{1.25}\text{Al}_{11.07}\text{O}_{17.13}$

$a = 0.5598$ ,  $c = 2.2479$  nm,  $c/a = 4.016$ ,  $V = 0.6101$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1568	0.3136	0.5504		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.1594	0.3188	0.1721	0.038	
Al3	12k	.m.	0.1682	0.3364	0.1065	0.973	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.503	0.006	0.6467		square pyramid Al <sub>5</sub>
Ag5	6h	mm2	0.0242	0.0484	$\frac{1}{4}$	0.145	
O6	6h	mm2	0.137	0.274	$\frac{1}{4}$	0.042	
Ag7	6h	mm2	0.2273	0.4546	$\frac{1}{4}$	0.14	
Ag8	6h	mm2	0.2991	0.5982	$\frac{1}{4}$	0.132	
O9	6h	mm2	0.7019	0.4038	$\frac{1}{4}$	0.333	
O10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0551		tetrahedron Al <sub>4</sub>
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5249		tetrahedron O <sub>4</sub>
Al12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6757		
O13	4e	3m.	0	0	0.1432		trigonal prism Al <sub>6</sub>
Al14	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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

References: [1] Boilot J.P., Colomban P., Collin G., Comes R. (1980), J. Phys. Chem. Solids 41, 47-54.

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hP96

$\text{Li}(\text{Li}_{0.5}\text{Zn}_{0.5})_6\text{Mg}_8\text{Zn}_9$	hP96	(194) $P6_3/mmc - k^4j^2h^2f^2e$
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**Mg<sub>2</sub>LiZn<sub>3</sub>** [1], Laves phase 4H

Structural features: Laves-type slabs in hc stacking. Tetrahedrally close-packed structure (Frank-Kasper phase). Ordering variant of MgNi<sub>2</sub>.

Mel'nyk E.V., Kripyakevich P.I. (1974) [1]

$\text{Li}_4\text{Mg}_8\text{Zn}_{12}$

$a = 1.046$ ,  $c = 1.705$  nm,  $c/a = 1.630$ ,  $V = 1.6155$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	12k	.m.	0.16667	0.33333	0.125		icosahedron Zn <sub>2</sub> Li <sub>4</sub> Mg <sub>6</sub>
Mg2	12k	.m.	0.16667	0.33333	0.65625		16-vertex Frank-Kasper Li <sub>5</sub> Zn <sub>7</sub> Mg <sub>4</sub>
Zn3	12k	.m.	0.25	0.5	0.0		icosahedron Li <sub>3</sub> Zn <sub>3</sub> Mg <sub>6</sub>
Mg4	12k	.m.	0.5	0.00001	0.09375		16-vertex Frank-Kasper Zn <sub>7</sub> Li <sub>5</sub> Mg <sub>4</sub>
M5	12j	m..	0.08333	0.41667	$\frac{1}{4}$		icosahedron Zn <sub>4</sub> Li <sub>2</sub> Mg <sub>6</sub>
M6	12i	.2.	0.25	0	0		icosahedron Zn <sub>4</sub> Li <sub>2</sub> Mg <sub>6</sub>
Zn7	6h	mm2	0.08333	0.16667	$\frac{1}{4}$		icosahedron Zn <sub>4</sub> Li <sub>2</sub> Mg <sub>6</sub>
Zn8	6h	mm2	0.58333	0.16667	$\frac{1}{4}$		icosahedron Li <sub>4</sub> Zn <sub>2</sub> Mg <sub>6</sub>
Mg9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.15625		16-vertex Frank-Kasper Zn <sub>6</sub> Li <sub>6</sub> Mg <sub>4</sub>
Li10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.625		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Mg11	4e	3m.	0	0	0.09375		16-vertex Frank-Kasper Zn <sub>6</sub> Li <sub>6</sub> Mg <sub>4</sub>

M5 = 0.5Li + 0.5Zn; M6 = 0.5Li + 0.5Zn

Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.119



Remarks: Idealized coordinates.

References: [1] Mel'nyk E.V., Kripyakevich P.I. (1974), Sov. Phys. Crystallogr. 19, 398-399 (Kristallografiya 19, 645-648).

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hP96

$(\text{Sr}_{0.67}\text{Eu}_{0.33})_3\text{Mg}_{13}$	hP96	(194) $P6_3/mmc - k^5h^2gf^3ed$
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**$(\text{Sr}_{0.67}\text{Eu}_{0.33})_3\text{Mg}_{13}$  [1]**

Structural features:  $(\text{Sr},\text{Eu})_6$  octahedral clusters and  $(\text{Sr},\text{Eu})_3$  trigonal clusters in a matrix of Mg atoms.

Erassme J., Lueken H. (1987) [1]

$\text{Eu}_{0.99}\text{Mg}_{13}\text{Sr}_{2.01}$

$a = 1.0465$ ,  $c = 2.8166$  nm,  $c/a = 2.691$ ,  $V = 2.6714$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.13680	0.27360	0.56229		7-capped pentagonal prism $\text{Mg}_{13}\text{Sr}_4$
Mg2	12k	.m.	0.1669	0.3338	0.1536		icosahedron $\text{Mg}_8\text{Sr}_4$
Mg3	12k	.m.	0.1757	0.3514	0.6902		pseudo Frank-Kasper $\text{Mg}_{10}\text{Sr}_3$
Mg4	12k	.m.	0.2323	0.4646	0.0545		icosahedron $\text{Mg}_9\text{Sr}_3$
Mg5	12k	.m.	0.5034	0.0068	0.1179		pseudo Frank-Kasper $\text{Mg}_{10}\text{Sr}_3$
Mg6	6h	mm2	0.0988	0.1976	$\frac{1}{4}$		icosahedron $\text{Mg}_{10}\text{Sr}_2$
M7	6h	mm2	0.46938	0.9388	$\frac{1}{4}$		7-capped pentagonal prism $\text{Mg}_{15}\text{Sr}_2$
Mg8	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron $\text{Mg}_8\text{Sr}_4$
Mg9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1491		icosahedron $\text{Mg}_9\text{Sr}_3$
Mg10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5375		pseudo Frank-Kasper $\text{Mg}_{10}\text{Sr}_3$
Mg11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6438		square prism (cube) $\text{Mg}_8$
Mg12	4e	3m.	0	0	0.1582		icosahedron $\text{Mg}_9\text{Sr}_3$
Mg13	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper $\text{Mg}_8\text{Sr}_3$

M1 = 0.69Sr + 0.31Eu; M7 = 0.63Sr + 0.37Eu

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

Experimental: single crystal, diffractometer, X-rays, R = 0.026, T = 294 K

References: [1] Erassme J., Lueken H. (1987), Acta Crystallogr. B 43, 244-250.

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hP96

$\text{K}_9\text{Na}_{23}\text{Tl}_{15.3}$	hP96	(194) $P6_3/mmc - k^5h^2gf^3ed$
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**$\text{K}_9\text{Na}_{23}\text{Tl}_{15.3}$  [1]**

Structural features:  $\text{Tl}_5$  trigonal bipyramids,  $\text{Tl}_4$  tetrahedra and  $\text{Tl}_3$  linear chains (partial vacancies on the central site) in a matrix of Na and K atoms.

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

$\text{K}_9\text{Na}_{23}\text{Tl}_{15.31}$

$a = 1.1235$ ,  $c = 3.0133$  nm,  $c/a = 2.682$ ,  $V = 3.2940$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	12k	.m.	0.1319	0.2638	0.5598		7-capped pentagonal prism $\text{Na}_8\text{Tl}_5\text{K}_4$
Na2	12k	.m.	0.1669	0.3338	0.154		icosahedron $\text{Tl}_4\text{Na}_4\text{K}_4$
Na3	12k	.m.	0.1777	0.3554	0.6897		pseudo Frank-Kasper $\text{Tl}_5\text{Na}_5\text{K}_3$
Tl4	12k	.m.	0.23598	0.47196	0.05511		icosahedron $\text{Na}_6\text{Tl}_3\text{K}_3$
Na5	12k	.m.	0.504	0.008	0.1164		pseudo Frank-Kasper $\text{Tl}_4\text{Na}_6\text{K}_3$

Tl6	6h	mm2	0.0973	0.1946	$\frac{1}{4}$		icosahedron Na <sub>6</sub> Tl <sub>4</sub> K <sub>2</sub>
K7	6h	mm2	0.4555	0.911	$\frac{1}{4}$		7-capped pentagonal prism Tl <sub>5</sub> Na <sub>10</sub> K <sub>2</sub>
Na8	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Tl <sub>4</sub> Na <sub>4</sub> K <sub>4</sub>
Tl9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1436		icosahedron Na <sub>6</sub> Tl <sub>3</sub> K <sub>3</sub>
Na10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5396		pseudo Frank-Kasper Tl <sub>4</sub> Na <sub>6</sub> K <sub>3</sub>
Tl11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.646		square prism (cube) TlNa <sub>7</sub>
Tl12	4e	3m.	0	0	0.1638		icosahedron Tl <sub>3</sub> Na <sub>6</sub> K <sub>3</sub>
Tl13	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.31	pseudo Frank-Kasper Tl <sub>2</sub> Na <sub>6</sub> K <sub>3</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.042, T = 296 K

References: [1] Dong Z.C., Corbett J.D. (1996), Inorg. Chem. 35, 3107-3112.

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hP96

La<sub>0.85</sub>Al<sub>11.6</sub>O<sub>18.7</sub> hP96 (194)  $P6_3/mmc - 1k^2j^2f^3e^2ca$

**La<sub>0.85</sub>Al<sub>11.6</sub>O<sub>18.7</sub>** [1], magnetoplumbite family

Structural features: Close-packed O<sub>4</sub> and LaO<sub>3</sub> layers (partial vacancies ignored for the latter) in h<sub>3</sub>c<sub>2</sub> stacking; Al in octahedral and tetrahedral voids. Intergrowth of spinel-type (edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra) and so-called R slabs containing units of two face-linked AlO<sub>6</sub> octahedra, AlO<sub>4</sub> tetrahedra (statistical occupation of two face-sharing tetrahedra) and La atoms (ideal and split site); split O sites.

Gasperin M. et al. (1984) [1]

Al<sub>11.60</sub>La<sub>0.85</sub>O<sub>18.64</sub>

$a = 0.5546$ ,  $c = 2.2008$  nm,  $c/a = 3.968$ ,  $V = 0.5862$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.3115	0.1496	0.0518	0.5	
Al2	12k	.m.	0.1675	0.335	0.1076	0.96	
O3	12k	.m.	0.503	0.006	0.6502		non-coplanar triangle Al <sub>3</sub>
La4	12j	m..	0.2744	0.5601	$\frac{1}{4}$	0.048	
O5	12j	m..	0.3224	0.1211	$\frac{1}{4}$	0.44	
O6	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0554		tetrahedron Al <sub>4</sub>
Al7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5269		
Al8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6898		
O9	4e	3m.	0	0	0.148		tetrahedron Al <sub>4</sub>
Al10	4e	3m.	0	0	0.2384	0.42	
La11	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.56	
Al12	2a	-3m.	0	0	0		

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

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

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

References: [1] Gasperin M., Saine M.C., Kahn A., Laville F., Lejus A.M. (1984), J. Solid State Chem. 54, 61-69.

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hP98

Au<sub>12</sub>(Au<sub>0.58</sub>Cd<sub>0.42</sub>)<sub>36</sub>Cd hP98 (194)  $P6_3/mmc - j^5h^6c$

**Au<sub>2</sub>Cd** [2]; (CuSb) ε [3]

Structural features: Distorted close-packed layers in h stacking. Substitution derivative of Mg (h.c.p) with 7-fold translation unit in (001).

Watanabe Y., Iwasaki H. (1982) [1]

$\text{Au}_{32.70}\text{Cd}_{16.30}$

$a = 2.0433$ ,  $c = 0.4818$  nm,  $c/a = 0.236$ ,  $V = 1.7421$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	12j	$m..$	0.0467	0.3800	$1/4$		anticuboctahedron $\text{Au}_8\text{Cd}_4$
M2	12j	$m..$	0.0480	0.2381	$1/4$		anticuboctahedron $\text{Au}_7\text{Cd}_5$
Au3	12j	$m..$	0.1903	0.5239	$1/4$		anticuboctahedron $\text{Cd}_6\text{Au}_6$
Au4	12j	$m..$	0.3340	0.0954	$1/4$		anticuboctahedron $\text{Cd}_7\text{Au}_5$
M5	12j	$m..$	0.4770	0.0954	$1/4$		anticuboctahedron $\text{Au}_5\text{Cd}_7$
M6	6h	$mm2$	0.0473	0.0946	$1/4$		anticuboctahedron $\text{Au}_8\text{Cd}_4$
M7	6h	$mm2$	0.1909	0.3818	$1/4$		anticuboctahedron $\text{Au}_8\text{Cd}_4$
M8	6h	$mm2$	0.4757	0.9514	$1/4$		anticuboctahedron $\text{Au}_8\text{Cd}_4$
M9	6h	$mm2$	0.6188	0.2376	$1/4$		anticuboctahedron $\text{Au}_8\text{Cd}_4$
M10	6h	$mm2$	0.7625	0.5250	$1/4$		anticuboctahedron $\text{Au}_{10}\text{Cd}_2$
M11	6h	$mm2$	0.9045	0.8090	$1/4$		anticuboctahedron $\text{Au}_{12}$
Cd12	2c	$-6m2$	$1/3$	$2/3$	$1/4$		anticuboctahedron $\text{Au}_{12}$

M1 = 0.74Cd + 0.26Au; M2 = 0.92Au + 0.08Cd; M5 = 0.92Au + 0.08Cd; M6 = 0.91Au + 0.09Cd; M7 = 0.65Cd + 0.35Au; M8 = 0.65Cd + 0.35Au; M9 = 0.91Au + 0.09Cd; M10 = 0.91Cd + 0.09Au; M11 = 0.91Cd + 0.09Au

Experimental: single crystal, precession photographs, X-rays,  $R = 0.084$

Remarks: Average structure. A refinement in 5D superspace is reported in [4]. A single site with mixed occupation was reported for  $\varepsilon(\text{CuSb})$  in [3]. The modulated structure of  $\varepsilon(\text{CuSb})$  is studied in [5].

References: [1] Watanabe Y., Iwasaki H. (1982), J. Appl. Crystallogr. 15, 174-181. [2] Hirabayashi M., Yamaguchi S., Hiraga K., Ino N., Sato H., Toth R.S. (1970), J. Phys. Chem. Solids 31, 77-94. [3] Yamaguchi S., Hirabayashi M. (1972), J. Phys. Soc. Jpn. 33, 708-717. [4] Yamamoto A. (1983), Acta Crystallogr. B 39, 17-20. [5] Motai K., Watanabe Y., Hashimoto S. (1993), Acta Crystallogr. B 49, 655-661.

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hP98

$\text{Na}_{0.47}\text{Li}_{0.75}\text{Al}_{11}\text{O}_{17.11}$	hP98	(194) $P6_3/mmc - k^4h^4f^5ea$
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**$\text{Na}_{0.47}\text{Li}_{0.75}\text{Al}_{11}\text{O}_{17.11}$**  [1],  $\beta$  alumina-Li,Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and  $(\text{Li,Na})_{1+2x}\text{O}_{1+x}$  layers (split framework O site, Li and (Li,Na) near BR, Na near mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Edström K. et al. (1997) [1]

$\text{Al}_{11}\text{Li}_{0.75}\text{Na}_{1.31}\text{O}_{17.11}$

$a = 0.55929$ ,  $c = 2.2652$  nm,  $c/a = 4.050$ ,  $V = 0.6136$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	$.m.$	0.15713	0.31426	0.54976		tetrahedron $\text{Al}_4$
Al2	12k	$.m.$	0.1595	0.319	0.1764	0.037	
Al3	12k	$.m.$	0.16796	0.33592	0.10547	0.963	7-vertex polyhedron $\text{AlO}_6$
O4	12k	$.m.$	0.50294	0.00588	0.64604		square pyramid $\text{Al}_5$

Na5	6h	mm2	0.0907	0.1814	$\frac{1}{4}$	0.421	
O6	6h	mm2	0.1667	0.3334	$\frac{1}{4}$	0.037	
M7	6h	mm2	0.3006	0.6012	$\frac{1}{4}$	0.172	
O8	6h	mm2	0.6949	0.3898	$\frac{1}{4}$	0.333	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05525		tetrahedron Al <sub>4</sub>
Li10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2043	0.128	
Li11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2271	0.014	
Al12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52461		tetrahedron O <sub>4</sub>
Al13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67561		
O14	4e	3m.	0	0	0.14151		trigonal prism Al <sub>6</sub>
Al15	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

M7 = 0.91Li + 0.09Na

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

Experimental: single crystal, diffractometer, X-rays, R = 0.033, T = 298 K

Remarks: The structure was analyzed jointly on X-ray and neutron single-crystal diffraction data. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s).

References: [1] Edström K., Gustafsson T., Thomas J.O., Farrington G.C. (1997), Acta Crystallogr. B 53, 631-638.

194  
hP98

Na<sub>0.26</sub>Cd<sub>0.48</sub>Al<sub>11</sub>O<sub>17.11</sub>

hP98

(194) *P6<sub>3</sub>/mmc* – k<sup>5</sup>h<sup>3</sup>f<sup>3</sup>eda

**Na<sub>0.26</sub>Cd<sub>0.48</sub>Al<sub>11</sub>O<sub>17.11</sub>** [1], β alumina-Cd,Na

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Na,Cd)<sub>x</sub>O<sub>1+y</sub> layers (in part split framework O site, Na near BR, Cd near mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with single AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Catti M. et al. (1987) [1]

Al<sub>11</sub>Cd<sub>0.48</sub>Na<sub>0.26</sub>O<sub>17.11</sub>

*a* = 0.559, *c* = 2.2423 nm, *c/a* = 4.011, *V* = 0.6068 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Al1	12k	.m.	0.156	0.312	0.175	0.032	
Cd2	12k	.m.	0.156	0.312	0.2425	0.08	
O3	12k	.m.	0.1568	0.3136	0.55014		tetrahedron Al <sub>4</sub>
Al4	12k	.m.	0.1678	0.3356	0.10693	0.968	7-vertex polyhedron AlO <sub>6</sub>
O5	12k	.m.	0.503	0.006	0.64711		
O6	6h	mm2	0.18	0.36	$\frac{1}{4}$	0.037	
Na7	6h	mm2	0.379	0.758	$\frac{1}{4}$	0.086	
O8	6h	mm2	0.729	0.458	$\frac{1}{4}$	0.25	
O9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0558		tetrahedron Al <sub>4</sub>
Al10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52477		tetrahedron O <sub>4</sub>
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67581		
O12	4e	3m.	0	0	0.1433		
O13	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.25	
Al14	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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

References: [1] Catti M., Cazzanelli E., Ivaldi G., Mariotto G. (1987), Phys. Rev. B: Condens. Matter 36, 9451-9460.

194  
hP100

$\text{Mg}_{0.4}\text{Mn}_{0.6}\text{Fe}_{16}\text{Pb}_2\text{O}_{27}$	hP100	(194) $P6_3/mmc - k^4h^3gf^6e^2$
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**Pb<sub>2</sub>(Mn,Mg)Fe<sub>16</sub>O<sub>27</sub>** [1], lindqvistite

Structural features: Spinel-type slabs (six close-packed O layers in c stacking) of edge-linked (Fe,Mg)O<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra are interconnected via units of two face-linked FeO<sub>6</sub> octahedra (Fe<sub>2</sub> dumbbells) to form a 3D-framework; partly disordered arrangement of Pb and (Pb,Mg) between the slabs.

Holtstam D., Norrestam R. (1993) [1]

$\text{Fe}_{16.20}\text{Mg}_{0.98}\text{O}_{27}\text{Pb}_{1.82}$

$a = 0.5951$ ,  $c = 3.3358$  nm,  $c/a = 5.605$ ,  $V = 1.0231$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	.m.	0.1644	0.3288	0.1485		octahedron O <sub>6</sub>
O2	12k	.m.	0.1649	0.3298	0.6783		non-coplanar triangle Fe <sub>3</sub>
O3	12k	.m.	0.1758	0.3516	0.0359		tetrahedron Fe <sub>4</sub>
O4	12k	.m.	0.5117	0.0234	0.6097		tetrahedron Fe <sub>4</sub>
Pb5	6h	mm2	0.0473	0.0946	$\frac{1}{4}$	0.333	
M6	6h	mm2	0.3731	0.7462	$\frac{1}{4}$	0.333	
O7	6h	mm2	0.521	0.042	$\frac{1}{4}$		single atom Pb
M8	6g	.2/m.	$\frac{1}{2}$	0	0		octahedron O <sub>6</sub>
M9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0736		octahedron O <sub>6</sub>
O10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1773		non-coplanar triangle Fe <sub>3</sub>
O11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5337		tetrahedron Fe <sub>4</sub>
Fe12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.592		tetrahedron O <sub>4</sub>
Fe13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7043		octahedron O <sub>6</sub>
Fe14	4e	3m.	0	0	0.0555		tetrahedron O <sub>4</sub>
O15	4e	3m.	0	0	0.1138		tetrahedron Fe <sub>4</sub>

M1 = 0.95Fe + 0.05Mg; M6 = 0.82Pb + 0.18Mg; M8 = 0.90Fe + 0.10Mg; M9 = 0.90Fe + 0.10Mg

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.041$ ,  $T = 293$  K

Remarks: Natural specimen from Jakobsberg, Filipstad, Sweden. Composition  $\text{Pb}_{2.04}\text{Mn}_{1.27}\text{Mg}_{0.71}\text{Zn}_{0.04}\text{Fe}_{14.84}\text{Al}_{0.02}\text{Ti}_{0.03}\text{Si}_{0.05}\text{O}_{26.51}$  from electron microprobe analysis. No attempt was made to distinguish Fe and Mn. Short interatomic distances for partly occupied site(s). Average structure; additional reflections could be indexed with a 3-fold supercell (new axes  $2a+b$ ,  $-a+b$ ,  $c$ ).

References: [1] Holtstam D., Norrestam R. (1993), Am. Mineral. 78, 1304-1312.

194  
hP102

$\text{Ag}_{1.12}\text{Cd}_{0.05}\text{Al}_{11}\text{O}_{17.11}$	hP102	(194) $P6_3/mmc - k^4h^6f^3ea$
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**Ag<sub>1.12</sub>Cd<sub>0.05</sub>Al<sub>11</sub>O<sub>17.11</sub>** [1],  $\beta$  alumina-Ag,Cd

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and (Ag,Cd)<sub>x</sub>O<sub>1+y</sub> layers (split framework O site, Ag near BR, aBR and mO, Cd near

mO positions, additional O at mO positions between Al displaced to interstitial site) alternate along [001]. Infinite slabs of edge-linked  $\text{AlO}_6$  octahedra sharing vertices with single  $\text{AlO}_4$  tetrahedra are interconnected via units of two vertex-linked  $\text{AlO}_4$  tetrahedra to form a 3D-framework.

Edström K. et al. (1991) [1]

$\text{Ag}_{1.12}\text{Al}_{11}\text{Cd}_{0.05}\text{O}_{17.11}$

$a = 0.56032$ ,  $c = 2.2504$  nm,  $c/a = 4.016$ ,  $V = 0.6119$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.15711	0.31422	0.55018		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.15975	0.3195	0.17627	0.037	
Al3	12k	.m.	0.16798	0.33596	0.10656	0.963	7-vertex polyhedron AlO <sub>6</sub>
O4	12k	.m.	0.50287	0.00574	0.64652		square pyramid Al <sub>5</sub>
Ag5	6h	mm2	0.0229	0.0458	$\frac{1}{4}$	0.119	
Cd6	6h	mm2	0.15431	0.30862	$\frac{1}{4}$	0.016	
O7	6h	mm2	0.16667	0.33333	$\frac{1}{4}$	0.037	
Ag8	6h	mm2	0.22199	0.44398	$\frac{1}{4}$	0.087	
Ag9	6h	mm2	0.29492	0.58984	$\frac{1}{4}$	0.168	
O10	6h	mm2	0.69708	0.39416	$\frac{1}{4}$	0.333	
O11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05543		tetrahedron Al <sub>4</sub>
Al12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5249		tetrahedron O <sub>4</sub>
Al13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67574		
O14	4e	3m.	0	0	0.14301		trigonal prism Al <sub>6</sub>
Al15	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

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

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

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 643-650.

194  
hP106

$\text{H}_3\text{Cs}_5[\text{SO}_4]_4[\text{H}_2\text{O}]_{0.5}$	hP106	(194) $P6_3/mmc - I^2k^2h^2f^3e^2b$
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**Cs<sub>5</sub>H<sub>3</sub>(SO<sub>4</sub>)<sub>4</sub>·xH<sub>2</sub>O** [1]

Structural features: SO<sub>4</sub> tetrahedra (partial orientational disorder) arranged in triangle-mesh layers (AABBAACC stacking).

Merinov B.V. (1997) [1]

$\text{Cs}_5\text{H}_{3.54}\text{O}_{16.52}\text{S}_4$

$a = 0.62455$ ,  $c = 2.969$  nm,  $c/a = 4.754$ ,  $V = 1.0029$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.396	0.1578	0.1755	0.13	
O2	24l	1	0.5758	0.267	0.1328	0.17	
O3	12k	.m.	0.1293	0.2586	0.0536		single atom S
O4	12k	.m.	0.5432	0.0864	0.2044	0.74	non-coplanar triangle O <sub>2</sub> S
O5	6h	mm2	0.28	0.56	$\frac{1}{4}$	0.08	
O6	6h	mm2	0.391	0.782	$\frac{1}{4}$	0.08	
Cs7	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.13243		
Cs8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.53064		
S9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6796		
S10	4e	3m.	0	0	0.0668		non-coplanar triangle O <sub>3</sub>

O11	4e	3m.	0	0	0.1192	single atom S
Cs12	2b	-6m2	0	0	$\frac{1}{4}$	
H13	24l	1	0.154	0.04	0.132	0.05
H14	24l	1	0.45	0.065	0.23	0.06
H15	12k	.m.	0.115	0.23	0.62	0.17
H16	12k	.m.	0.15	0.3	0.616	0.03
H17	12k	.m.	0.21	0.42	0.63	0.08
H18	12j	m..	0.07	0.43	$\frac{1}{4}$	0.06
H19	12j	m..	0.13	0.38	$\frac{1}{4}$	0.03

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

Remarks: Homogeneity range  $\text{Cs}_5\text{H}_3(\text{SO}_4)_4 \cdot x\text{H}_2\text{O}$ ,  $0 < x < \sim 1$  at rt. 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] Merinov B.V. (1997), Kristallografiya 42, 982-993.

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hP108

$\text{K}_{2.5}\text{Na}_{1.5}\text{Ca}_{1.5}\text{Mg}(\text{Al}_{0.25}\text{Si}_{0.75})_{36}\text{O}_{72}[\text{H}_2\text{O}]_{27}$	hP108	(194) $P6_3/mmc - I^2k^2:jih^2$
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**(Ca,Mg,Na<sub>2</sub>,K<sub>2</sub>)<sub>4.5</sub>Al<sub>9</sub>Si<sub>27</sub>O<sub>72</sub>·27H<sub>2</sub>O** [1], erionite-(Na), zeolite ERI-Na hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001].

Staples L.W., Gard J.A. (1959) [1]

Al<sub>9</sub>O<sub>72</sub>Si<sub>27</sub>

$a = 1.326$ ,  $c = 1.512$  nm,  $c/a = 1.140$ ,  $V = 2.3023$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.0	0.237	0.106		tetrahedron O <sub>4</sub>
O2	24l	1	0.017	0.35	0.162		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.106	0.212	0.128		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.123	0.246	0.633		non-colinear Si <sub>2</sub>
M5	12j	m..	0.088	0.421	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O6	12i	.2.	0.262	0	0		non-colinear Si <sub>2</sub>
O7	6h	mm2	0.217	0.434	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O8	6h	mm2	0.45	0.9	$\frac{1}{4}$		non-colinear Si <sub>2</sub>

M1 = 0.75Si + 0.25Al; M5 = 0.75Si + 0.25Al

Experimental: powder, film, X-rays, R = 0.340

Remarks: Natural specimen from Durkee opal mine, Baker County, Oregon. Composition  $\text{Ca}_{1.46}\text{Mg}_{0.77}\text{K}_{2.02}\text{Na}_{1.31}\text{Si}_{26.80}\text{Al}_{8.57}\text{O}_{70.3} \cdot 27.4\text{H}_2\text{O}$  from chemical analysis. Non-framework species not located. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Staples L.W., Gard J.A. (1959), Mineral. Mag. J. Mineral. Soc. 32, 261-281.

194  
hP110

$\text{Ba}_2\text{NbS}_5$	hP110	(194) $P6_3/mmc - k^6hf^6eba$
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**Ba<sub>2</sub>NbS<sub>4</sub>(S<sub>2</sub>)<sub>0.5</sub>** [1]

Structural features: Close-packed  $\text{BaS}_3$  layers and partly disordered Ba-rich layers in CBdBABdBCBCdCACdCB stacking (d = disordered layer); Nb in octahedral ( $\text{S}_6$ ) voids between ordered layers. Units of two and three face-sharing  $\text{NbS}_6$  octahedra ( $\text{Nb}_2$  dumbbells and linear  $\text{Nb}_3$  chains). One S dumbbell for eight single S anions.

Swinnea J.S. et al. (1985) [1]



$a = 0.6909$ ,  $c = 4.925$  nm,  $c/a = 7.128$ ,  $V = 2.0360$  nm<sup>3</sup>,  $Z = 10$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	12k	.m.	0.0563	0.1126	0.1438	0.299	
S2	12k	.m.	0.1641	0.3282	0.5293		non-colinear $\text{Nb}_2$
S3	12k	.m.	0.1646	0.3292	0.1924		
S4	12k	.m.	0.166	0.332	0.0878		single atom Nb
S5	12k	.m.	0.2448	0.4896	0.6404	0.37	
S6	12k	.m.	0.5832	0.1664	0.1406	0.19	
S7	6h	mm2	0.4952	0.9904	$\frac{1}{4}$		non-colinear $\text{Nb}_2$
Ba8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0287		anticuboctahedron $\text{S}_{12}$
Ba9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1385	0.8	single atom S
S10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1916	0.5	
Nb11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2138		
Ba12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5809		
Ba13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7001		
Nb14	4e	3m.	0	0	0.0668		octahedron $\text{S}_6$
Ba15	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron $\text{S}_{12}$
Nb16	2a	-3m.	0	0	0		octahedron $\text{S}_6$

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

Remarks: Short interatomic distances:  $d(\text{Nb11-S10}) = 0.109$  nm. Short interatomic distances for partly occupied site(s). Different supercells are reported in [2].

References: [1] Swinnea J.S., Steinfink H., Rendon Diazmiron L.E., Banos Lopez L. (1985), J. Solid State Chem. 56, 249-254. [2] Saeki M., Onoda N., Ohta M. (1993), Mater. Res. Bull. 28, 279-285.

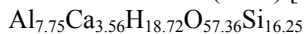
194  
hP110

$\text{Ca}_{3.9}(\text{Al}_{0.32}\text{Si}_{0.68})_{24}\text{O}_{48}[\text{H}_2\text{O}]_{24}$  hP110 (194)  $P6_3/mmc - 1k^3j^2ihfe$

**$\text{Ca}_{3.9}\text{Al}_{7.8}\text{Si}_{16.2}\text{O}_{48} \cdot 24\text{H}_2\text{O}$**  [1], gmelinite-(Ca), zeolite GME-Ca hydrated

Structural features:  $(\text{Si,Al})\text{O}_4$  tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to  $[001]$  and by 8-rings perpendicular to  $[001]$ ; Ca near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and near 8-rings in the large channels,  $\text{H}_2\text{O}$  delocalized over three sites.

Sacerdoti M. et al. (1995) [1]



$a = 1.3807$ ,  $c = 0.9792$  nm,  $c/a = 0.709$ ,  $V = 1.6166$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.4428	0.1085	0.0882		tetrahedron $\text{O}_4$
Ca2	12k	.m.	0.1053	0.211	0.051	0.12	
O3	12k	.m.	0.2124	0.425	0.543		non-colinear $\text{Si}_2$
O4	12k	.m.	0.5728	0.146	0.045		non-colinear $\text{Si}_2$
$(\text{OH}_2)_5$	12j	m..	0.181	0.556	$\frac{1}{4}$	0.5	



O6	12j	<i>m.</i>	0.4211	0.0795	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O7	12i	.2.	0.3547	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )8	6h	<i>mm</i> 2	0.1623	0.325	$\frac{1}{4}$	0.4	non-colinear Ca <sub>2</sub>
Ca9	4f	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.09	0.53	
(OH <sub>2</sub> )10	4e	3 <i>m.</i>	0	0	0.04	0.24	

M1 = 0.677Si + 0.323Al

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

Remarks: Natural specimen from San Giorgio Pelena, Vicenza, Italy, ion-exchanged with CaCl<sub>2</sub> solution. Composition Na<sub>0.01</sub>K<sub>0.01</sub>Ca<sub>3.53</sub>Sr<sub>0.01</sub>Al<sub>7.30</sub>Si<sub>16.75</sub>O<sub>48</sub>·22.89H<sub>2</sub>O from electron microprobe analysis. Main part of H<sub>2</sub>O 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] Sacerdoti M., Passaglia E., Carnevali R. (1995), Zeolites 15, 276-281.

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hP114

K <sub>2</sub> Na <sub>2</sub> CaMg <sub>3</sub> (Al <sub>0.36</sub> Si <sub>0.64</sub> ) <sub>36</sub> O <sub>72</sub> [H <sub>2</sub> O] <sub>27</sub>	hP114	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – <i>l</i> <sup>2</sup> <i>k</i> <sup>2</sup> <i>j</i> <i>h</i> <sup>2</sup> <i>fb</i>
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**K<sub>2</sub>Na<sub>2</sub>CaMg<sub>3</sub>Al<sub>13</sub>Si<sub>23</sub>O<sub>72</sub>·27H<sub>2</sub>O** [1], erionite-(Mg), zeolite ERI-Mg,K hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; Ca at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), H<sub>2</sub>O in large (erionite-type) cages.

Kawahara A., Curien H. (1969) [1]

Al<sub>13</sub>Ca<sub>2</sub>H<sub>8</sub>O<sub>76</sub>Si<sub>23</sub>

*a* = 1.315, *c* = 1.502 nm, *c/a* = 1.142, *V* = 2.2493 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24 <i>l</i>	1	0.0	0.2328	0.1064		tetrahedron O <sub>4</sub>
O2	24 <i>l</i>	1	0.3475	0.0273	0.164		non-colinear Si <sub>2</sub>
O3	12 <i>k</i>	<i>m.</i>	0.0987	0.1974	0.6223		non-colinear Si <sub>2</sub>
O4	12 <i>k</i>	<i>m.</i>	0.1255	0.251	0.137		non-colinear Si <sub>2</sub>
M5	12 <i>j</i>	<i>m.</i>	0.4255	0.0938	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O6	12 <i>i</i>	.2.	0.2672	0	0		non-colinear Si <sub>2</sub>
O7	6 <i>h</i>	<i>mm</i> 2	0.5419	0.0838	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O8	6 <i>h</i>	<i>mm</i> 2	0.7716	0.5432	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )9	4 <i>f</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0702		15-vertex polyhedron O <sub>15</sub>
Ca10	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>

M1 = 0.639Si + 0.361Al; M5 = 0.639Si + 0.361Al

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

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.170

Remarks: Natural specimen from Mazé, Niigata, Japan. Composition Ca<sub>0.7</sub>Mg<sub>2.4</sub>Na<sub>1.3</sub>K<sub>2.1</sub>Al<sub>13.1</sub>Si<sub>23.6</sub>O<sub>72</sub>·27.6H<sub>2</sub>O from chemical analysis. Main part of cations and H<sub>2</sub>O not located. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table V of [1] the *z*-coordinate of former OH1 is misprinted as 0.702 instead of 0.0702 (from the orthorhombic description in table IV).

References: [1] Kawahara A., Curien H. (1969), Bull. Soc. Fr. Mineral. Cristallogr. 92, 250-256.

194  
hP114

ScFe <sub>2</sub> H <sub>2.9</sub>	hP114	(194) $P6_3/mmc - I^2k^3h^2gf^2e$
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**ScFe<sub>2</sub>H<sub>2.9</sub> [1]**

Structural features: Filled-up derivative of MgNi<sub>2</sub> with H in tetrahedral (Sc<sub>2</sub>Fe<sub>2</sub>) and trigonal (ScFe<sub>2</sub>) voids.

Yartys' V.A. et al. (1986) [1]

D<sub>2.92</sub>Fe<sub>2</sub>Sc $a = 0.5256$ ,  $c = 1.6595$  nm,  $c/a = 3.157$ ,  $V = 0.3970$  nm<sup>3</sup>,  $Z = 8$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
D1	24l	1	0.01	0.38	0.09	0.012	non-coplanar triangle D <sub>3</sub>
D2	24l	1	0.028	0.308	0.15	0.333	non-coplanar triangle D <sub>3</sub>
D3	12k	.m.	0.15	0.3	0.7	0.4	non-coplanar triangle D <sub>2</sub>
D4	12k	.m.	0.194	0.388	0.555	0.25	non-coplanar triangle D <sub>3</sub>
D5	12k	.m.	0.198	0.396	0.022	0.408	single atom D
Fe6	6h	mm2	0.1777	0.3554	$\frac{1}{4}$		coplanar square D <sub>4</sub>
D7	6h	mm2	0.578	0.156	$\frac{1}{4}$	0.4	non-coplanar D <sub>2</sub>
Fe8	6g	.2/m.	$\frac{1}{2}$	0	0		coplanar square D <sub>4</sub>
Fe9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1318		hexagonal prism D <sub>12</sub>
Sc10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6477		21-vertex polyhedron D <sub>21</sub>
Sc11	4e	3m.	0	0	0.0895		pseudo Frank-Kasper D <sub>24</sub>

Experimental: powder, diffractometer, neutrons,  $R_p = 0.077$ 

Remarks: In table 2 of [1] the  $c$ -parameter is misprinted as 1.695 nm instead of 1.6595 nm (given elsewhere; checked on interatomic distances).

References: [1] Yartys' V.A., Burnasheva V.V., Fadeeva N.V., Sarin V.A., Fykin L.E., Semenenko K.N. (1986), Russ. J. Inorg. Chem. 31, 175-179 (Zh. Neorg. Khim. 31, 311-317).

194  
hP114

Zn <sub>17</sub> U <sub>2</sub>	hP114	(194) $P6_3/mmc - Ik^4jgf^3e^2dc$
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**U<sub>2</sub>Zn<sub>17</sub> [1]**

Structural features: Kagomé-mesh Zn<sub>3</sub> layers alternate with (U,Zn<sub>2</sub>)Zn<sub>2</sub> layers (a Zn hexagon mesh, the hexagons of which are centered by a U atom or a Zn<sub>2</sub> dumbbell perpendicular to the layer) along [001]. Intergrowth of CaCu<sub>5</sub>- and Zr<sub>4</sub>Al<sub>3</sub>-type blocks in the ratio 2:1.

Makarov E.S., Vinogradov S.I. (1956) [1]

U<sub>2</sub>Zn<sub>17</sub> $a = 0.899$ ,  $c = 2.635$  nm,  $c/a = 2.931$ ,  $V = 1.8443$  nm<sup>3</sup>,  $Z = 6$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Zn1	24l	1	0.0	0.33333	0.08333		pseudo Frank-Kasper Zn <sub>11</sub> U <sub>2</sub>
Zn2	12k	.m.	0.16667	0.33333	0.0		icosahedron Zn <sub>9</sub> U <sub>3</sub>
Zn3	12k	.m.	0.16667	0.33333	0.16667		icosahedron Zn <sub>10</sub> U <sub>2</sub>
Zn4	12k	.m.	0.16667	0.33333	0.66667		icosahedron Zn <sub>9</sub> U <sub>3</sub>
Zn5	12k	.m.	0.5	0.0	0.16667		icosahedron Zn <sub>9</sub> U <sub>3</sub>
Zn6	12j	m..	0.0	0.33333	$\frac{1}{4}$		pseudo Frank-Kasper Zn <sub>11</sub> U <sub>2</sub>
Zn7	6g	.2/m.	$\frac{1}{2}$	0	0		icosahedron Zn <sub>10</sub> U <sub>2</sub>
Zn8	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.034		14-vertex Frank-Kasper Zn <sub>13</sub> U

Zn9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.132	14-vertex Frank-Kasper Zn <sub>13</sub> U
U10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.58333	pseudo Frank-Kasper Zn <sub>19</sub>
U11	4e	3m.	0	0	0.08333	pseudo Frank-Kasper Zn <sub>19</sub>
Zn12	4e	3m.	0	0	0.201	14-vertex Frank-Kasper Zn <sub>13</sub> U
U13	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	sixcapped hexagonal prism Zn <sub>18</sub>
U14	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	pseudo Frank-Kasper Zn <sub>20</sub>

Transformation from published data (*P*-6m2): origin shift 0 0  $\frac{3}{4}$

Experimental: powder, film, X-rays

Remarks: Idealized coordinates. Structure doubtful. According to [2] the sample may contain a mixture of phases with Th<sub>2</sub>Ni<sub>17</sub>- and Th<sub>2</sub>Zn<sub>17</sub>-type structures. The description in space group (187) *P*-6m2 in [1] does not take into consideration all symmetry elements of the proposed structure. In [1] the Wyckoff position of the 14th Zn site is misprinted as 6g instead of 2g.

References: [1] Makarov E.S., Vinogradov S.I. (1956), Sov. Phys. Crystallogr. 1, 499-505 (Kristallografiya 1, 634-643). [2] Johnson Q., Smith G.S., Wood D.H. (1969), Acta Crystallogr. B 25, 464-469.

194  
hP116

Cd <sub>0.61</sub> Al <sub>11</sub> O <sub>17.11</sub>	hP116	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – k <sup>5,2</sup> j <sup>2</sup> h <sup>2</sup> f <sup>3</sup> eda
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**Cd<sub>0.61</sub>Al<sub>11</sub>O<sub>17.11</sub>** [1], β alumina-Cd

Structural features: Spinel-type slabs (four close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and Cd<sub>1/2+x</sub>O<sub>1+x</sub> layers (Cd delocalized around mO positions, additional O at mO positions between Al displaced into interstitial site) alternate along [001]. Infinite slabs of edge-linked AlO<sub>6</sub> octahedra sharing vertices with AlO<sub>4</sub> tetrahedra are interconnected via units of two vertex-linked AlO<sub>4</sub> tetrahedra to form a 3D-framework.

Edström K. et al. (1991) [1]

Al<sub>11</sub>Cd<sub>0.62</sub>O<sub>17.11</sub>

*a* = 0.55869, *c* = 2.237 nm, *c/a* = 4.004, *V* = 0.6047 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12k	.m.	0.15714	0.31428	0.55028		tetrahedron Al <sub>4</sub>
Al2	12k	.m.	0.16019	0.32038	0.1754	0.037	
Cd3	12k	.m.	0.16383	0.32766	0.23876	0.023	
Al4	12k	.m.	0.16795	0.3359	0.10711	0.963	7-vertex polyhedron AlO <sub>6</sub>
O5	12k	.m.	0.50234	0.00468	0.64684		square pyramid Al <sub>5</sub>
Cd6	12j	m..	0.20185	0.49443	$\frac{1}{4}$	0.004	
Cd7	12j	m..	0.26417	0.59612	$\frac{1}{4}$	0.011	
Cd8	6h	mm2	0.13956	0.27912	$\frac{1}{4}$	0.129	
O9	6h	mm2	0.16667	0.33333	$\frac{1}{4}$	0.037	
O10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.05578		tetrahedron Al <sub>4</sub>
Al11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52501		tetrahedron O <sub>4</sub>
Al12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.67632		tetrahedron O <sub>4</sub>
O13	4e	3m.	0	0	0.14368		trigonal prism Al <sub>6</sub>
O14	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Al <sub>2</sub>
Al15	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.029, T = 295 K

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

References: [1] Edström K., Thomas J.O., Farrington G.C. (1991), Acta Crystallogr. B 47, 635-643.

194  
hP118

$\text{Na}_{9.7}(\text{Al}_{0.27}\text{Si}_{0.73})_{36}\text{O}_{72}$	<i>hP118</i>	(194) $P6_3/mmc - I^2k^3jigf$
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**$\text{Na}_{9.7}\text{Al}_{9.7}\text{Si}_{26.3}\text{O}_{72}$**  [1], zeolite EAB-Na

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an EAB-type zeolite framework (6-rings in ABBACC stacking) with channels delimited by 8-rings perpendicular to [001]; Na at and near the centers of 6-rings.

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

$\text{Al}_{9.68}\text{Na}_{7.96}\text{O}_{72}\text{Si}_{26.32}$

$a = 1.306$ ,  $c = 1.561$  nm,  $c/a = 1.195$ ,  $V = 2.3058$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.008	0.321	0.094		non-colinear Si <sub>2</sub>
M2	24 <i>l</i>	1	0.423	0.088	0.161		tetrahedron O <sub>4</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.113	0.226	0.006		non-colinear Si <sub>2</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.237	0.474	0.656		non-colinear Si <sub>2</sub>
O5	12 <i>k</i>	. <i>m</i> .	0.548	0.096	0.131		non-colinear Si <sub>2</sub>
O6	12 <i>j</i>	. <i>m</i> ..	0.377	0.027	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
M7	12 <i>i</i>	.2.	0.246	0	0		tetrahedron O <sub>4</sub>
Na8	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0	0.66	colinear O <sub>2</sub>
Na9	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.599		non-coplanar triangle O <sub>3</sub>

M2 = 0.731Si + 0.269Al; M7 = 0.731Si + 0.269Al

Experimental: powder, diffractometer, X-rays,  $R_B = 0.057$ ,  $T = 623$  K

Remarks: We assigned an approximate value to the Al/Si ratio of sites M based on the chemical analysis.

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

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hP118

$\text{K}_{9.7}(\text{Al}_{0.27}\text{Si}_{0.73})_{36}\text{O}_{72}$	<i>hP118</i>	(194) $P6_3/mmc - I^2k^3jihf$
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**$\text{K}_{9.7}\text{Al}_{9.7}\text{Si}_{26.3}\text{O}_{72}$**  [1], zeolite EAB-Na

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an EAB-type zeolite framework (6-rings in ABBACC stacking) with channels delimited by 8-rings perpendicular to [001]; K above the centers of 6- and 8-rings.

Cartlidge S. et al. (1984) [1]

$\text{Al}_{9.68}\text{K}_{9.08}\text{O}_{72}\text{Si}_{26.32}$

$a = 1.307$ ,  $c = 1.51$  nm,  $c/a = 1.155$ ,  $V = 2.2339$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.0126	0.3247	0.0904		non-colinear Si <sub>2</sub>
M2	24 <i>l</i>	1	0.4275	0.0934	0.1452		tetrahedron O <sub>4</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.1105	0.2211	0.5103		non-colinear Si <sub>2</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.2349	0.4698	0.6175		non-colinear Si <sub>2</sub>
O5	12 <i>k</i>	. <i>m</i> .	0.5342	0.0684	0.1219		non-colinear Si <sub>2</sub>
O6	12 <i>j</i>	. <i>m</i> ..	0.3878	0.0547	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
M7	12 <i>i</i>	.2.	0.2421	0	0		tetrahedron O <sub>4</sub>
K8	6 <i>h</i>	<i>mm</i> 2	0.172	0.344	$\frac{1}{4}$		non-colinear O <sub>2</sub>

K9       $4f$     $3m.$        $\frac{1}{3}$        $\frac{2}{3}$       0.0043    0.77    non-coplanar triangle O<sub>3</sub>

M2 = 0.731Si + 0.269Al; M7 = 0.731Si + 0.269Al

Experimental: powder, diffractometer, X-rays,  $wR_p = 0.180$ ,  $T = 493$  K

Remarks: We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. Refinement of the occupancy of site K8 showed no significant deviation from unity.

References: [1] Cartlidge S., Keller E.B., Meier W.M. (1984), Zeolites 4, 226-230.

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hP118

$\text{Na}_8(\text{Al}_{0.33}\text{Si}_{0.67})_{24}\text{O}_{48}[\text{H}_2\text{O}]_{24}$

hP118

(194)  $P6_3/mmc - 1k^{4:2}j^{2:1}ihf$

**Na<sub>7.8</sub>Al<sub>7.8</sub>Si<sub>16.2</sub>O<sub>48</sub>·24H<sub>2</sub>O** [2], gmelinite-(Na), zeolite GME-Na hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; Na near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and near 8-rings in the large channels, H<sub>2</sub>O delocalized over three sites. See Fig. III.49.

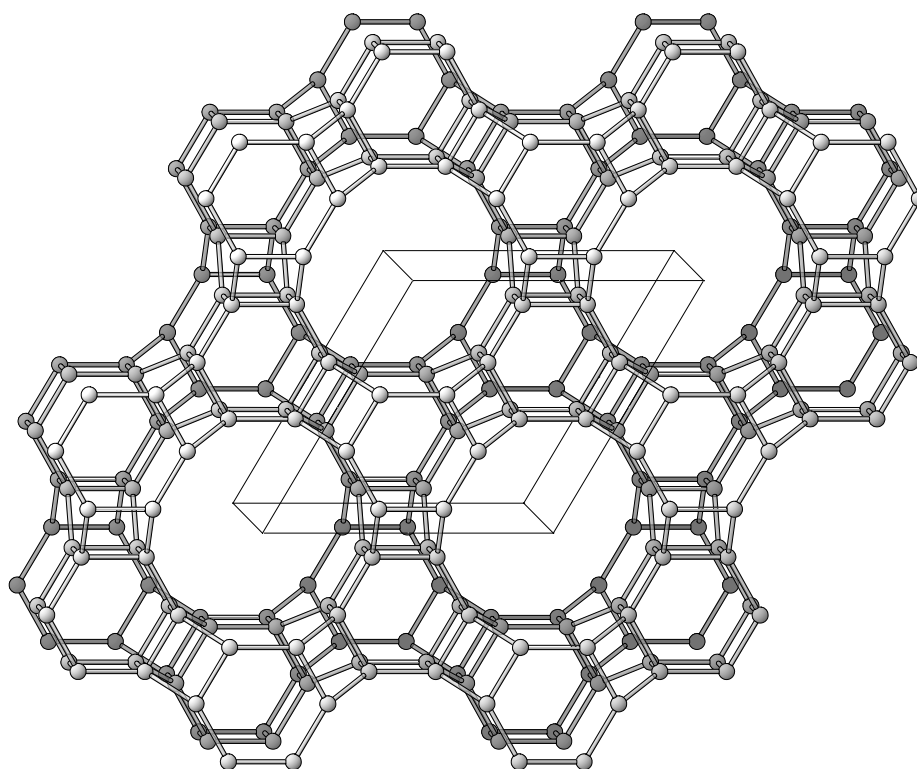


Fig. III.49. **Na<sub>7.8</sub>Al<sub>7.8</sub>Si<sub>16.2</sub>O<sub>48</sub>·24H<sub>2</sub>O**

GME-type (Si,Al) framework.

Sacerdoti M. et al. (1995) [1]

$\text{Al}_{7.80}\text{H}_{28.80}\text{Na}_{8.08}\text{O}_{62.40}\text{Si}_{16.20}$

$a = 1.3766$ ,  $c = 1.0076$  nm,  $c/a = 0.732$ ,  $V = 1.6536$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.4412	0.1058	0.0942		tetrahedron O <sub>4</sub>
(OH <sub>2</sub> )2	12k	.m.	0.0815	0.163	0.617	0.36	single atom Na
Na3	12k	.m.	0.1204	0.241	0.071	0.34	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O4	12k	.m.	0.2085	0.4171	0.5598		non-colinear Si <sub>2</sub>
O5	12k	.m.	0.5747	0.1495	0.0607		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )6	12j	m..	0.1965	0.549	<sup>1</sup> / <sub>4</sub>	0.5	single atom (OH <sub>2</sub> )
O7	12j	m..	0.411	0.0658	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O8	12i	.2.	0.3557	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )9	6h	mm2	0.1693	0.339	<sup>1</sup> / <sub>4</sub>	0.68	non-colinear Na <sub>2</sub>
Na10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0727		9-vertex polyhedron (OH <sub>2</sub> ) <sub>6</sub> O <sub>3</sub>

M1 = 0.675Si + 0.325Al

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

Remarks: Composition Na<sub>7.75</sub>K<sub>0.05</sub>Ca<sub>0.04</sub>Sr<sub>0.02</sub>Al<sub>7.69</sub>Si<sub>16.26</sub>O<sub>48</sub>·22.13H<sub>2</sub>O from electron microprobe analysis. We assigned an approximate value to the Al/Si ratio of site M based on the nominal composition. Main part of H<sub>2</sub>O 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] Sacerdoti M., Passaglia E., Carnevali R. (1995), Zeolites 15, 276-281. [2] Galli E., Passaglia E., Zanazzi P.F. (1982), Neues Jahrb. Mineral., Monatsh. 1982, 145-155.

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hP124

Cu <sub>18</sub> [NO <sub>3</sub> ] <sub>0.55</sub> Cl <sub>3.95</sub> [OH] <sub>31.5</sub> [H <sub>2</sub> O] <sub>2</sub>	hP124	(194) <i>P6<sub>3</sub>/mmc</i> – l <sup>2</sup> kjih <sup>5</sup> gda
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**Cu<sub>36</sub>(NO<sub>3</sub>)<sub>1.1</sub>(OH)<sub>63</sub>Cl<sub>7.9</sub>·4H<sub>2</sub>O** [1], buttgenbachite

Structural features: Cu(OH)<sub>4</sub> squares share vertices to form a 3D-framework; NO<sub>3</sub> trigonal units (in part replaced by Cl atoms) in large channels parallel to [001].

Hibbs D.E. et al. (2003) [1]

Cl<sub>3.95</sub>Cu<sub>18</sub>H<sub>34</sub>N<sub>0.55</sub>O<sub>35.15</sub>

*a* = 1.578, *c* = 0.91 nm, *c/a* = 0.577, *V* = 1.9624 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	24l	1	0.0703	0.326	0.1082		non-coplanar triangle Cu <sub>3</sub>
(OH)2	24l	1	0.4509	0.0811	0.0901		non-colinear Cu <sub>2</sub>
(OH)3	12k	.m.	0.0765	0.153	0.0959		non-coplanar triangle Cu <sub>2</sub> Cl
Cu4	12j	m..	0.359	0.0162	<sup>1</sup> / <sub>4</sub>		coplanar square (OH) <sub>4</sub>
Cu5	12i	.2.	0.2024	0	0		coplanar square (OH) <sub>4</sub>
Cu6	6h	mm2	0.1673	0.3346	<sup>1</sup> / <sub>4</sub>		square pyramid (OH) <sub>4</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )7	6h	mm2	0.251	0.502	<sup>1</sup> / <sub>4</sub>	0.167	single atom Cu
(OH)8	6h	mm2	0.4439	0.8878	<sup>1</sup> / <sub>4</sub>		6-vertex polyhedron (OH <sub>2</sub> ) <sub>2</sub> Cu <sub>4</sub>
O9	6h	mm2	0.6213	0.2426	<sup>1</sup> / <sub>4</sub>	0.55	single atom N
Cl10	6h	mm2	0.8615	0.723	<sup>1</sup> / <sub>4</sub>		trigonal prism Cu <sub>6</sub>
Cu11	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		coplanar square (OH) <sub>4</sub>
M12	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		coplanar triangle O <sub>3</sub>
Cl13	2a	-3m.	0	0	0	0.5	octahedron (OH) <sub>6</sub>

M12 = 0.55N + 0.45Cl

Experimental: single crystal, manual diffractometer, X-rays, R = 0.085, T = 293 K

Remarks: Natural specimen from Toughnut mine, Arizona. Refinement on diffraction data from [2], where the mineral was erroneously called connellite. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hibbs D.E., Leverett P., Williams P.A. (2003), Mineral. Mag. 67, 47-60. [2] McLean W.J., Anthony J.W. (1972), Am. Mineral. 57, 426-438.

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hP124

$K_{7.4}(Al_{0.31}Si_{0.69})_{24}O_{48}[H_2O]_{24}$	hP124	(194) $P6_3/mmc - lk^4j^2ih^2f$
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**$K_{7.4}Al_{7.4}Si_{16.6}O_{48} \cdot 24H_2O$**  [1], zeolite GME-K hydrated

Structural features: (Si,Al) $O_4$  tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; K near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and near 8-rings in the large channels,  $H_2O$  delocalized over four sites.

Sacerdoti M. et al. (1995) [1]

$Al_{7.44}H_{25.68}K_{7.72}O_{60.84}Si_{16.56}$

$a = 1.3687$ ,  $c = 1.0256$  nm,  $c/a = 0.749$ ,  $V = 1.6639$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.434	0.0999	0.0988		tetrahedron $O_4$
K2	12k	.m.	0.1013	0.203	0.077	0.31	
(OH <sub>2</sub> )3	12k	.m.	0.1369	0.274	0.175	0.2	coplanar triangle (OH <sub>2</sub> ) <sub>2</sub> K
O4	12k	.m.	0.2139	0.4279	0.5653		non-colinear $Si_2$
O5	12k	.m.	0.5646	0.1293	0.0726		non-colinear $Si_2$
(OH <sub>2</sub> )6	12j	m..	0.162	0.55	$1/4$	0.5	
O7	12j	m..	0.3949	0.0564	$1/4$		non-colinear $Si_2$
O8	12i	.2.	0.3453	0	0		non-colinear $Si_2$
(OH <sub>2</sub> )9	6h	mm2	0.1783	0.357	$1/4$	0.34	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )10	6h	mm2	0.9153	0.831	$1/4$	0.4	
K11	4f	3m.	$1/3$	$2/3$	0.066		

$M1 = 0.69Si + 0.31Al$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.053$

Remarks: Composition  $K_{7.22}Na_{0.63}Al_{7.32}Si_{16.55}O_{48} \cdot 20.06H_2O$  from electron microprobe analysis. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. Main part of  $H_2O$  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] Sacerdoti M., Passaglia E., Carnevali R. (1995), Zeolites 15, 276-281.

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hP124

$Mg_2Co_3Sn_{10}$	hP124	(194) $P6_3/mmc - lk^6hf^3e^2d$
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**$Mg_2Co_3Sn_{10+x}$**  [1]

Structural features: Slabs of edge- and vertex-linked  $CoSn_8$  square antiprisms share vertices with slabs of vertex-linked  $CoSn_6$  trigonal prisms to form a 3D-framework; Mg in voids in the prism slabs.

Schreyer M. et al. (2004) [1]

$Co_3Mg_2Sn_{10.01}$

$a = 0.949$ ,  $c = 3.3555$  nm,  $c/a = 3.536$ ,  $V = 2.6171$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	24l	1	0.34559	0.00736	0.11719	0.673	14-vertex Frank-Kasper Co <sub>2</sub> Sn <sub>10</sub> Mg <sub>2</sub>
Sn2	12k	.m.	0.14607	0.29214	0.02504		pseudo Frank-Kasper Co <sub>3</sub> Sn <sub>10</sub>
Co3	12k	.m.	0.15837	0.31674	0.55566		square antiprism Sn <sub>8</sub>
Co4	12k	.m.	0.16556	0.33112	0.17667		tricapped trigonal prism Sn <sub>6</sub> Mg <sub>3</sub>
Mg5	12k	.m.	0.1729	0.3458	0.6992		icosahedron Co <sub>2</sub> Sn <sub>9</sub> Mg
Sn6	12k	.m.	0.55298	0.10596	0.70689		14-vertex Frank-Kasper Co <sub>2</sub> Sn <sub>9</sub> Mg <sub>3</sub>
Sn7	12k	.m.	0.55473	0.10946	0.03574		pseudo Frank-Kasper Co <sub>2</sub> Sn <sub>11</sub>
Sn8	6h	mm2	0.10926	0.21852	<sup>1</sup> / <sub>4</sub>		14-vertex polyhedron Co <sub>2</sub> Mg <sub>4</sub> Sn <sub>8</sub>
Sn9	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.04903		16-vertex Frank-Kasper MgSn <sub>15</sub>
Mg10	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.136		pseudo Frank-Kasper Sn <sub>10</sub> Co <sub>3</sub>
Sn11	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.65418		10-vertex polyhedron Mg <sub>3</sub> Sn <sub>7</sub>
Sn12	4e	3m.	0	0	0.07531		pseudo Frank-Kasper Co <sub>3</sub> Sn <sub>10</sub>
Sn13	4e	3m.	0	0	0.161		16-vertex Frank-Kasper Co <sub>3</sub> Sn <sub>10</sub> Mg <sub>3</sub>
Sn14	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		bicapped hexagonal prism Mg <sub>6</sub> Sn <sub>8</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 293 K

Remarks: Homogeneity range Mg<sub>2</sub>Co<sub>3</sub>Sn<sub>10+x</sub>, 0 < x < 0.15.

References: [1] Schreyer M., Kraus G., Fässler T. (2004), Z. Anorg. Allg. Chem. 630, 2520-2526.

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hP126

Rb <sub>5</sub> Ta <sub>14.6</sub> O <sub>39</sub>	hP126	(194) P6 <sub>3</sub> /mmc – k <sup>9</sup> hfdB
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#### Rb<sub>10</sub>Ta<sub>29.2</sub>O<sub>78</sub> [1]

Structural features: TaO<sub>6</sub> octahedra share edges and vertices to form a 3D-framework with channels perpendicular to [001]. Two kinds of double HTB-type (Ta forms a Kagomé mesh) layer (common vertices in the former, common edges and vertices in the latter) interconnected via additional TaO<sub>6</sub> octahedra; additional Ta in trigonal prismatic voids. See Fig. III.50.

Fallon G.D., Gatehouse B.M. (1980) [1]

O<sub>39</sub>Rb<sub>4.98</sub>Ta<sub>14.60</sub>

a = 0.7503, c = 3.6348 nm, c/a = 4.844, V = 1.7721 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1192	0.2385	0.7081	0.33	non-coplanar triangle Ta <sub>3</sub>
O2	12k	.m.	0.1243	0.2487	0.1446		non-colinear Ta <sub>2</sub>
O3	12k	.m.	0.1262	0.2525	0.5816		non-colinear Ta <sub>2</sub>
O4	12k	.m.	0.1419	0.2839	0.0215		non-coplanar triangle Ta <sub>3</sub>
Ta5	12k	.m.	0.167	0.334	0.5343		octahedron O <sub>6</sub>
Ta6	12k	.m.	0.1722	0.3444	0.1965		octahedron O <sub>6</sub>
O7	12k	.m.	0.5404	0.0809	0.6861		non-colinear Ta <sub>2</sub>
O8	12k	.m.	0.5517	0.1034	0.036		non-colinear Ta <sub>2</sub>
Rb9	12k	.m.	0.6962	0.3925	0.1389		non-colinear Ta <sub>2</sub>
O10	6h	mm2	0.1922	0.3844	<sup>1</sup> / <sub>4</sub>		
Rb11	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0816		non-coplanar hexagon O <sub>6</sub>
Ta12	4e	3m.	0	0	0.1178		octahedron O <sub>6</sub>
Rb13	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>
Ta14	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>	0.6	trigonal prism O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>



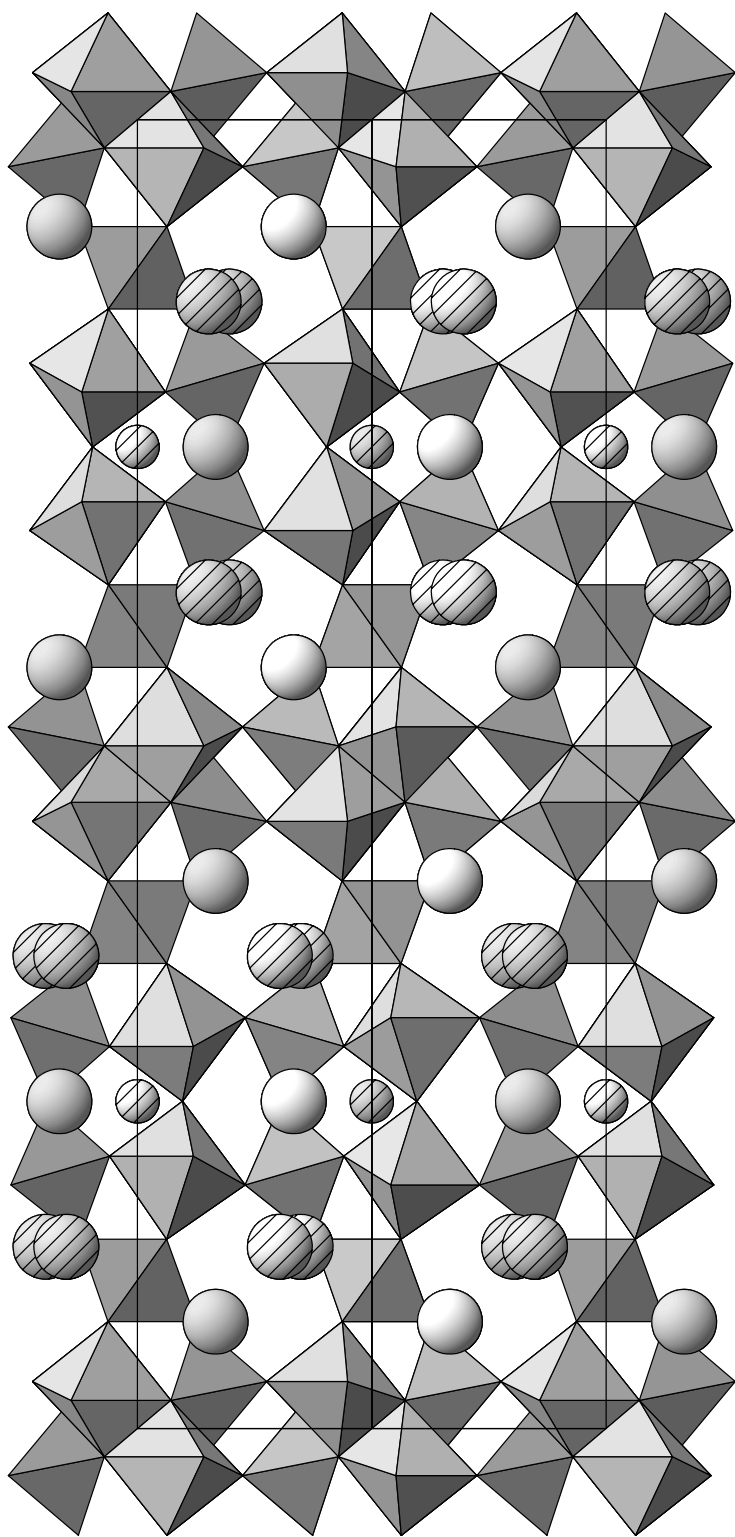


Fig. III.50.  $\text{Rb}_{10}\text{Ta}_{29.2}\text{O}_{78}$

Arrangement of  $\text{TaO}_6$  octahedra, Rb (large) and additional Ta (small) atoms viewed along  $[110]$  (atoms in partly occupied sites are hatched).

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.039$

Remarks: Short interatomic distances for partly occupied site(s). A slightly different arrangement of non-framework Ta atoms is proposed in [2].

References: [1] Fallon G.D., Gatehouse B.M. (1980), J. Solid State Chem. 34, 193-198. [2] Michel C., Guyomarc'h A., Raveau B. (1978), J. Solid State Chem. 25, 251-261.

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hP126

$\text{Rb}_5\text{VNb}_{14}\text{O}_{39}$	<i>hP126</i>	(194) $P6_3/mmc - k^9\text{hfd}b$
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**$\text{Rb}_5(\text{VO})\text{Nb}_{14}\text{O}_{38}$  [1]**

Structural features:  $\text{NbO}_6$  octahedra share edges and vertices to form a 3D-framework with channels perpendicular to [001]. Two kinds of double HTB-type (Nb forms a Kagomé mesh) layer (common vertices in the former, common edges and vertices in the latter) interconnected via additional  $\text{NbO}_6$  octahedra; V in trigonal prismatic voids.

Haddad A., Jouini T. (1997) [1]

$\text{Nb}_{14}\text{O}_{39}\text{Rb}_5\text{V}$

$a = 0.7515$ ,  $c = 3.6354$  nm,  $c/a = 4.838$ ,  $V = 1.7780$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.119	0.238	0.708		non-coplanar triangle Nb <sub>2</sub> V
O2	12 <i>k</i>	. <i>m</i> .	0.1239	0.2478	0.58216		non-coplanar Nb <sub>2</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.1244	0.2488	0.1451		non-coplanar Nb <sub>2</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.1422	0.2844	0.02313		non-coplanar triangle Nb <sub>3</sub>
Nb5	12 <i>k</i>	. <i>m</i> .	0.16753	0.33506	0.53429		octahedron O <sub>6</sub>
Nb6	12 <i>k</i>	. <i>m</i> .	0.17192	0.34384	0.19667		octahedron O <sub>6</sub>
O7	12 <i>k</i>	. <i>m</i> .	0.5409	0.0818	0.6883		non-coplanar Nb <sub>2</sub>
O8	12 <i>k</i>	. <i>m</i> .	0.5498	0.0996	0.0366		non-coplanar Nb <sub>2</sub>
Rb9	12 <i>k</i>	. <i>m</i> .	0.6422	0.2844	0.13679	0.333	
O10	6 <i>h</i>	<i>mm</i> 2	0.1909	0.3818	$\frac{1}{4}$		non-coplanar Nb <sub>2</sub>
Rb11	4 <i>f</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.07604		
Nb12	4 <i>e</i>	3 <i>m</i> .	0	0	0.11808		octahedron O <sub>6</sub>
Rb13	2 <i>d</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		trigonal prism O <sub>6</sub>
V14	2 <i>b</i>	-6 <i>m</i> 2	0	0	$\frac{1}{4}$		tricapped trigonal prism O <sub>9</sub>

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

Experimental: single crystal, diffractometer, X-rays,  $R = 0.029$ ,  $T = 293$  K

Remarks: Short interatomic distances for partly occupied site(s). In table 2 of [1] the *z*-coordinate of former Rb(1) is misprinted as 0.13679 instead of -0.13679 (checked on interatomic distances).

References: [1] Haddad A., Jouini T. (1997), J. Solid State Chem. 134, 10-16.

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hP132

$\text{Rb}_5\text{Ta}_{14.6}\text{O}_{39}$	<i>hP132</i>	(194) $P6_3/mmc - k^9\text{hf}^2\text{e}^2\text{d}$
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**$\text{Rb}_{10}\text{Ta}_{29.2}\text{O}_{78}$  [1]**

Structural features:  $\text{TaO}_6$  octahedra share edges and vertices to form a 3D-framework with channels perpendicular to [001]. Two kinds of double HTB-type (Ta forms a Kagomé mesh) layer (common vertices in the former, common edges and vertices in the latter) interconnected via additional  $\text{TaO}_6$  octahedra; additional Ta in voids.

Michel C. et al. (1978) [1]

$\text{O}_{39}\text{Rb}_5\text{Ta}_{14.60}$

$a = 0.7505$ ,  $c = 3.637$  nm,  $c/a = 4.846$ ,  $V = 1.7741$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.111	0.222	0.581		non-colinear Ta <sub>2</sub>
O2	12k	.m.	0.115	0.23	0.706		non-colinear Ta <sub>2</sub>
O3	12k	.m.	0.128	0.256	0.147		non-colinear Ta <sub>2</sub>
O4	12k	.m.	0.132	0.264	0.026		non-coplanar triangle Ta <sub>3</sub>
Ta5	12k	.m.	0.1658	0.3316	0.1953		octahedron O <sub>6</sub>
Ta6	12k	.m.	0.1666	0.3332	0.535		octahedron O <sub>6</sub>
O7	12k	.m.	0.539	0.078	0.684		non-colinear Ta <sub>2</sub>
O8	12k	.m.	0.554	0.108	0.037		non-colinear Ta <sub>2</sub>
Rb9	12k	.m.	0.71	0.42	0.1377	0.333	
O10	6h	mm2	0.168	0.336	<sup>1</sup> / <sub>4</sub>		non-colinear Ta <sub>2</sub>
Rb11	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0882		9-vertex polyhedron O <sub>9</sub>
Ta12	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.23	0.15	
Ta13	4e	3m.	0	0	0.1158		octahedron O <sub>6</sub>
Ta14	4e	3m.	0	0	0.249	0.15	
Rb15	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). A slightly different arrangement of non-framework Ta atoms is proposed in [2].

References: [1] Michel C., Guyomarc'h A., Raveau B. (1978), J. Solid State Chem. 25, 251-261. [2] Fallon G.D., Gatehouse B.M. (1980), J. Solid State Chem. 34, 193-198.

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hP132

$\text{Na}_8(\text{Ga}_{0.22}\text{Si}_{0.78})_{36}\text{O}_{72}$	hP132	(194) $P6_3/mmc - l^2kj^3ih^3g$
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**Na<sub>4</sub>Ga<sub>4</sub>Si<sub>14</sub>O<sub>36</sub>** [1], zeolite MAZ(Ga)-Na

Structural features: (Si,Ga)O<sub>4</sub> tetrahedra share vertices to form a MAZ-type zeolite framework with gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and channels delimited by 12-rings and 8-rings parallel to [001]; Na in both kinds of channel.

Newsam J.M. et al. (1985) [1]

$\text{Ga}_{7.90}\text{Na}_{7.08}\text{O}_{72}\text{Si}_{26.93}$

$a = 1.8043$ ,  $c = 0.7662$  nm,  $c/a = 0.425$ ,  $V = 2.1602$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.1047	0.4376	0.0749		non-colinear Si <sub>2</sub>
M2	24l	1	0.3584	0.0919	0.0468	0.962	tetrahedron O <sub>4</sub>
O3	12k	.m.	0.1658	0.3316	0.0014		non-colinear Si <sub>2</sub>
Na4	12j	m..	0.074	0.238	<sup>1</sup> / <sub>4</sub>	0.22	
M5	12j	m..	0.1594	0.4898	<sup>1</sup> / <sub>4</sub>	0.978	tetrahedron O <sub>4</sub>
O6	12j	m..	0.3859	0.0975	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O7	12i	.2.	0.2744	0	0		non-colinear Si <sub>2</sub>
O8	6h	mm2	0.2578	0.5156	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O9	6h	mm2	0.4226	0.8452	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>

Na10	6h	mm2	0.546	0.092	$\frac{1}{4}$	0.37	non-colinear Na <sub>2</sub>
Na11	6g	.2/m.	$\frac{1}{2}$	0	0	0.37	octahedron Na <sub>2</sub> O <sub>4</sub>

M2 = 0.78Si + 0.22Ga; M5 = 0.76Si + 0.24Ga

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

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.059

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

References: [1] Newsam J.M., Jarman R.H., Jacobson A.J. (1985), Mater. Res. Bull. 20, 125-136.

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hP134

Cu<sub>18</sub>[NO<sub>3</sub>]<sub>0.75</sub>Cl<sub>3.25</sub>[OH]<sub>32</sub>[H<sub>2</sub>O]<sub>2.75</sub>

hP134

(194) *P6<sub>3</sub>/mmc* – l<sup>2</sup>k<sup>2</sup>j<sup>4</sup>gfca

**Cu<sub>36</sub>(NO<sub>3</sub>)<sub>1.5</sub>(OH)<sub>64</sub>Cl<sub>6.5</sub>·5.5H<sub>2</sub>O** [1], buttgenbachite

Structural features: Cu(OH)<sub>4</sub> squares share vertices to form a 3D-framework; NO<sub>3</sub> trigonal units and part of the Cl atoms in large channels parallel to [001].

Hibbs D.E. et al. (2003) [1]

Cl<sub>3.25</sub>Cu<sub>18</sub>H<sub>37.50</sub>N<sub>0.75</sub>O<sub>37</sub>

*a* = 1.575, *c* = 0.9161 nm, *c/a* = 0.582, *V* = 1.9680 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH)1	24l	1	0.0806	0.4502	0.0899		non-colinear Cu <sub>2</sub>
(OH)2	24l	1	0.3264	0.07	0.1082		non-coplanar triangle Cu <sub>3</sub>
(OH)3	12k	.m.	0.0749	0.1498	0.595		non-coplanar triangle Cu <sub>2</sub> (OH <sub>3</sub> )
O4	12k	.m.	0.2897	0.5794	0.076	0.375	single atom N
Cu5	12j	m..	0.0168	0.3592	$\frac{1}{4}$		coplanar square (OH) <sub>4</sub>
Cu6	12i	.2.	0.2012	0	0		coplanar square (OH) <sub>4</sub>
Cl7	6h	mm2	0.1384	0.2768	$\frac{1}{4}$		trigonal prism Cu <sub>6</sub>
(OH)8	6h	mm2	0.5547	0.1094	$\frac{1}{4}$		6-vertex polyhedron Cu <sub>4</sub> (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )9	6h	mm2	0.749	0.498	$\frac{1}{4}$	0.25	single atom Cu
Cu10	6h	mm2	0.8323	0.6646	$\frac{1}{4}$		square pyramid (OH) <sub>4</sub> (OH <sub>2</sub> )
Cu11	6g	.2/m.	$\frac{1}{2}$	0	0		coplanar square (OH) <sub>4</sub>
N12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.076	0.375	coplanar triangle O <sub>3</sub>
Cl13	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.25	colinear N <sub>2</sub>
(OH <sub>3</sub> )14	2a	-3m.	0	0	0		octahedron (OH) <sub>6</sub>

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

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.048, T = 293 K

Remarks: Natural specimen from Likasi, Congo. Refinement on diffraction data from [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hibbs D.E., Leverett P., Williams P.A. (2003), Mineral. Mag. 67, 47-60. [2] Fanfani L., Nunzi A., Zanazzi P.F., Zanzari A.R. (1973), Mineral. Mag. 39, 264-270.

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hP140

Ba<sub>3</sub>Fe<sub>20</sub>(Fe<sub>0.67</sub>Co<sub>0.33</sub>)<sub>6</sub>O<sub>41</sub>

hP140

(194) *P6<sub>3</sub>/mmc* – k<sup>7</sup>hf<sup>8</sup>e<sup>3</sup>cba

**Ba<sub>3</sub>Fe<sub>24</sub>Co<sub>2</sub>O<sub>41</sub>** [1], ferrite Z-type

Structural features: Close-packed O<sub>4</sub> and BaO<sub>3</sub> layers in h<sub>3</sub>c<sub>2</sub>h<sub>4</sub>c<sub>2</sub> stacking; Fe in octahedral, tetrahedral and trigonal bipyramidal voids. Intergrowth of spinel-type slabs (edge-linked FeO<sub>6</sub> octahedra sharing vertices with single FeO<sub>4</sub> tetrahedra), R (units of two face-linked FeO<sub>6</sub> octahedra, FeO<sub>5</sub> trigonal

bipyramids and Ba atoms) and T slabs (units of three face-linked FeO<sub>6</sub> octahedra, FeO<sub>4</sub> tetrahedra and Ba atoms).

Braun P.B. (1957) [1]

Ba<sub>3</sub>Fe<sub>26</sub>O<sub>41</sub>

$a = 0.5885$ ,  $c = 5.23$  nm,  $c/a = 8.887$ ,  $V = 1.5686$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12k	.m.	0.1667	0.3334	0.021		non-collinear Fe <sub>2</sub>
O2	12k	.m.	0.1667	0.3334	0.1144		tetrahedron Fe <sub>4</sub>
Fe3	12k	.m.	0.1667	0.3334	0.1867		octahedron O <sub>6</sub>
O4	12k	.m.	0.1667	0.3334	0.5722		non-coplanar triangle Fe <sub>3</sub>
O5	12k	.m.	0.1667	0.3334	0.705		non-coplanar triangle Fe <sub>3</sub>
Fe6	12k	.m.	0.5	0.0	0.0912		octahedron O <sub>6</sub>
O7	12k	.m.	0.5	0.0	0.162		tetrahedron Fe <sub>4</sub>
O8	6h	mm2	0.5	0.0	$\frac{1}{4}$		coplanar triangle Fe <sub>3</sub>
Fe9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0359		tetrahedron O <sub>4</sub>
O10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.07		tetrahedron Fe <sub>4</sub>
Fe11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1393		octahedron O <sub>6</sub>
O12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.205		tetrahedron Fe <sub>4</sub>
Ba13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52735		anticuboctahedron O <sub>12</sub>
O14	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6144		tetrahedron Fe <sub>4</sub>
Fe15	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6505		tetrahedron O <sub>4</sub>
Fe16	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.7232		octahedron O <sub>6</sub>
Fe17	4e	3m.	0	0	0.0543		7-vertex polyhedron O <sub>6</sub> Fe
Fe18	4e	3m.	0	0	0.1263		tetrahedron O <sub>4</sub>
O19	4e	3m.	0	0	0.166		tetrahedron Fe <sub>4</sub>
Fe20	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O <sub>5</sub>
Ba21	2b	-6m2	0	0	$\frac{1}{4}$		anticuboctahedron O <sub>12</sub>
Fe22	2a	-3m.	0	0	0		8-vertex polyhedron O <sub>6</sub> Fe <sub>2</sub>

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

Experimental: single crystal, diffractometer and Weissenberg photographs, X-rays,  $R = 0.174$

Remarks: No attempt was made to distinguish Co and Fe in [1]. Co was located (mainly in site Fe3) in [2] (neutron diffraction), however, large differences in the positional coordinates were obtained for different refinements.

References: [1] Braun P.B. (1957), Philips Res. Rep. 12, 491-548. [2] Takada Y., Tachibana T., Nakagawa T., Yamamoto T.A., Shimada T., Kawano S. (2003), Mater. Res. Soc. Symp. Proc. 746, 49-54.

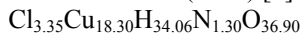
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hP140

Cu <sub>18.3</sub> [NO <sub>3</sub> ] <sub>1.3</sub> [OH] <sub>31.95</sub> Cl <sub>3.35</sub> [H <sub>2</sub> O] <sub>1.05</sub>	hP140	(194) $P6_3/mmc - I^2k^3j^3h^3g^3fca$
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**Cu<sub>36.6</sub>(NO<sub>3</sub>)<sub>2.6</sub>(OH)<sub>63.9</sub>Cl<sub>6.7</sub>·2.1H<sub>2</sub>O** [1], buttgenbachite

Structural features: Cu(OH)<sub>4</sub> squares share vertices to form a 3D-framework; additional Cu in compressed trigonal antiprismatic voids, NO<sub>3</sub> trigonal units (2-fold orientational disorder) and part of Cl atoms in large channels parallel to [001].

Fanfani L. et al. (1973) [1]



$a = 1.575$ ,  $c = 0.9161$  nm,  $c/a = 0.582$ ,  $V = 1.9680$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.081	0.4507	0.088		non-collinear Cu <sub>2</sub>
M2	24l	1	0.3256	0.0697	0.1094		non-coplanar triangle Cu <sub>3</sub>
M3	12k	.m.	0.0743	0.1486	0.5961		non-coplanar triangle Cu <sub>3</sub>
O4	12k	.m.	0.2877	0.5754	0.0748	0.47	non-coplanar triangle NO <sub>2</sub>
O5	12k	.m.	0.3773	0.7546	0.0335	0.18	non-coplanar triangle NO <sub>2</sub>
Cu6	12j	m..	0.0166	0.3589	$\frac{1}{4}$		non-coplanar square (OH) <sub>4</sub>
Cu7	12i	.2.	0.2012	0	0		coplanar square (OH) <sub>4</sub>
Cl8	6h	mm2	0.1382	0.2764	$\frac{1}{4}$		trigonal prism Cu <sub>6</sub>
M9	6h	mm2	0.5546	0.1092	$\frac{1}{4}$		non-collinear Cu <sub>2</sub>
Cu10	6h	mm2	0.8324	0.6648	$\frac{1}{4}$		non-coplanar square (OH) <sub>4</sub>
Cu11	6g	.2/m.	$\frac{1}{2}$	0	0		coplanar square (OH) <sub>4</sub>
N12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0557	0.65	non-coplanar triangle O <sub>3</sub>
Cl13	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.35	collinear N <sub>2</sub>
Cu14	2a	-3m.	0	0	0	0.3	octahedron (OH) <sub>6</sub>

M1 = 0.968OH + 0.032OH<sub>2</sub>; M2 = 0.968OH + 0.032OH<sub>2</sub>; M3 = 0.968OH + 0.032OH<sub>2</sub>; M9 = 0.968OH + 0.032OH<sub>2</sub>

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

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.055

Remarks: Natural specimen from Likasi, Congo. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space groups (186) *P6<sub>3</sub>mc* and (190) *P-62c* were tested and rejected.

References: [1] Fanfani L., Nunzi A., Zanazzi P.F., Zanzari A.R. (1973), Mineral. Mag. 39, 264-270.

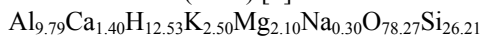
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hP140

$\text{K}_{2.5}\text{Na}_{0.5}\text{Ca}_{1.4}\text{Mg}_{2.1}(\text{Al}_{0.27}\text{Si}_{0.73})_{36}\text{O}_{72}[\text{H}_2\text{O}]_7$	<i>hP140</i>	(194) <i>P6<sub>3</sub>/mmc</i> – $\text{l}^2\text{kj}^3\text{ih}^3\text{gf}^2$
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**K<sub>2.5</sub>Na<sub>0.5</sub>Ca<sub>1.4</sub>Mg<sub>2.1</sub>Al<sub>10</sub>Si<sub>26</sub>O<sub>72</sub>·7H<sub>2</sub>O** [1], mazzite, zeolite MAZ-K,Mg,Ca residual water

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form a MAZ-type zeolite framework with gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and channels delimited by 12-rings and 8-rings parallel to [001]; K and H<sub>2</sub>O in the large channels, Ca in the smaller channels, Mg near the centers of planar 6-rings. See Fig. III.51.

Rinaldi R. et al. (1975) [1]



$a = 1.8007$ ,  $c = 0.7608$  nm,  $c/a = 0.423$ ,  $V = 2.1364$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.1104	0.4379	0.073		non-collinear Si <sub>2</sub>
M2	24l	1	0.3565	0.0934	0.0472		tetrahedron O <sub>4</sub>
O3	12k	.m.	0.164	0.328	0.5054		non-collinear Si <sub>2</sub>
K4	12j	m..	0.0773	0.2246	$\frac{1}{4}$	0.125	
M5	12j	m..	0.1572	0.4908	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O6	12j	m..	0.3875	0.0985	$\frac{1}{4}$		non-collinear Si <sub>2</sub>
O7	12i	.2.	0.2461	0	0		non-collinear Si <sub>2</sub>

O8	6h	mm2	0.2628	0.5256	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O9	6h	mm2	0.4225	0.845	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
M10	6h	mm2	0.5574	0.1148	$\frac{1}{4}$	0.833	non-colinear Ca <sub>2</sub>
M11	6g	.2/m.	$\frac{1}{2}$	0	0	0.3	square prism (cube) (OH <sub>2</sub> ) <sub>2</sub> O <sub>6</sub>
Mg12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1681	0.5	
(OH <sub>2</sub> )13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6453	0.567	single atom (OH <sub>2</sub> )

M2 = 0.728Si + 0.272Al; M5 = 0.728Si + 0.272Al; M10 = 0.80OH<sub>2</sub> + 0.20K; M11 = 0.778Ca + 0.167Na + 0.055Mg

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.026, T = 293 K

Remarks: Natural specimen from Mont Semiol, Montbrison, Loire, France, dehydrated. Composition K<sub>2.5</sub>Na<sub>0.3</sub>Ca<sub>1.4</sub>Mg<sub>2.1</sub>Al<sub>9.9</sub>Si<sub>26.5</sub>O<sub>72</sub>·xH<sub>2</sub>O from electron microprobe analysis. We assigned an approximate value to the Al/Si ratio of sites M2 and M5 based on the chemical analysis. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

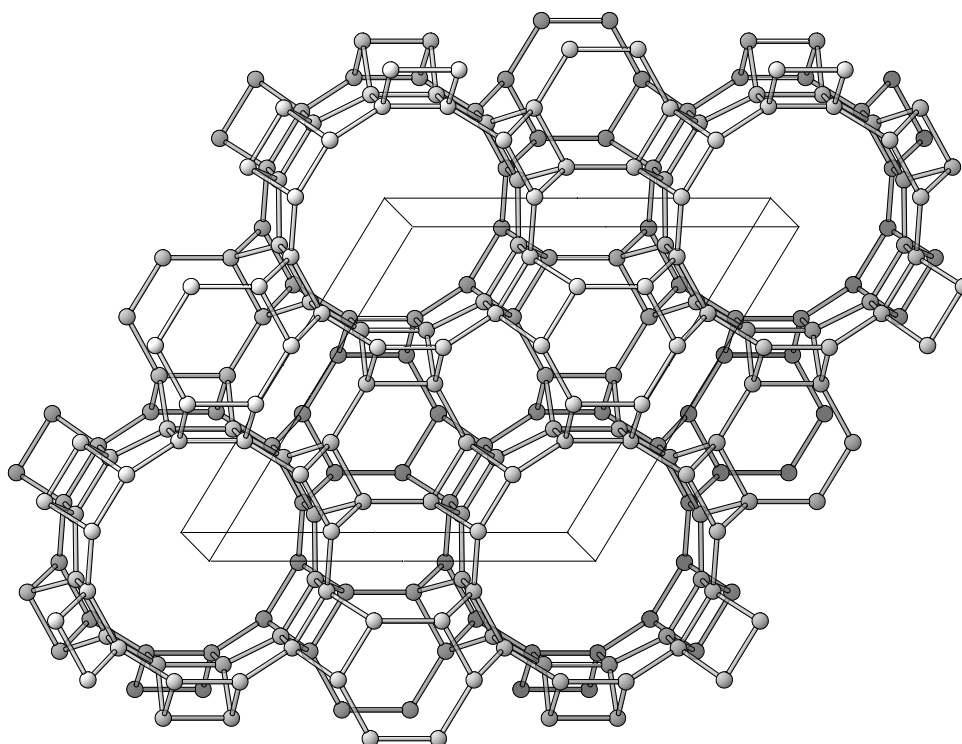


Fig. III.51. **K<sub>2.5</sub>Na<sub>0.3</sub>Ca<sub>1.4</sub>Mg<sub>2.1</sub>Al<sub>9.9</sub>Si<sub>26.5</sub>O<sub>72</sub>·7H<sub>2</sub>O**

MAZ-type (Si,Al) framework.

References: [1] Rinaldi R., Pluth J.J., Smith J.V. (1975), Acta Crystallogr. B 31, 1603-1608.

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Tl<sub>5</sub>Nb<sub>14.6</sub>O<sub>39</sub>

hP142

(194) *P6<sub>3</sub>/mmc* – k<sup>10</sup>h<sup>2</sup>feb

**Tl<sub>10</sub>Nb<sub>29.2</sub>O<sub>78</sub>** [1]

Structural features: NbO<sub>6</sub> octahedra share edges and vertices to form a 3D-framework with channels perpendicular to [001]. Two kinds of double HTB-type (Nb forms a Kagomé mesh) layer (common vertices in the former, common edges and vertices in the latter) interconnected via additional NbO<sub>6</sub> octahedra; additional Nb in trigonal prismatic voids.

Marini A. et al. (1979) [1]

Nb<sub>14.60</sub>O<sub>39</sub>Tl<sub>4.99</sub>

$a = 0.7532$ ,  $c = 3.642$  nm,  $c/a = 4.835$ ,  $V = 1.7893$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.114	0.228	0.146		non-collinear Nb <sub>2</sub>
O2	12 <i>k</i>	. <i>m</i> .	0.114	0.228	0.582		non-collinear Nb <sub>2</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.128	0.256	0.707		non-collinear Nb <sub>2</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.156	0.312	0.021		non-coplanar triangle Nb <sub>3</sub>
Nb5	12 <i>k</i>	. <i>m</i> .	0.16542	0.3308	0.1962		octahedron O <sub>6</sub>
Nb6	12 <i>k</i>	. <i>m</i> .	0.166	0.332	0.535		octahedron O <sub>6</sub>
Tl7	12 <i>k</i>	. <i>m</i> .	0.3153	0.6306	0.0691	0.333	
O8	12 <i>k</i>	. <i>m</i> .	0.54	0.08	0.684		non-collinear Nb <sub>2</sub>
O9	12 <i>k</i>	. <i>m</i> .	0.555	0.11	0.032		non-collinear Nb <sub>2</sub>
Tl10	12 <i>k</i>	. <i>m</i> .	0.7213	0.4426	0.1395	0.333	
O11	6 <i>h</i>	<i>mm</i> 2	0.165	0.33	<sup>1</sup> / <sub>4</sub>		non-collinear Nb <sub>2</sub>
Tl12	6 <i>h</i>	<i>mm</i> 2	0.6332	0.2664	<sup>1</sup> / <sub>4</sub>	0.333	
Nb13	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2349	0.15	
Nb14	4 <i>e</i>	3 <i>m</i> .	0	0	0.1158		octahedron O <sub>6</sub>
Nb15	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.3	tricapped trigonal prism O <sub>9</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.080

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). In Table I of [1] the chemical formula is misprinted as Tl<sub>10</sub>Nb<sub>29.2</sub>O<sub>78</sub>·10H<sub>2</sub>O instead of Tl<sub>10</sub>Nb<sub>29.2</sub>O<sub>78</sub> (given elsewhere, the authors state that the Tl-compounds do not fix H<sub>2</sub>O). In Table 3 of [1] the Wyckoff position of former Nb(IV) is misprinted as 4*e* instead of 2*b*.

References: [1] Marini A., Michel C., Raveau B. (1979), Rev. Chim. Miner. 16, 73-79.

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hP142

Zn<sub>58</sub>Gd<sub>13</sub> hP142 (194) *P*6<sub>3</sub>/*mmc* – lk<sup>5</sup>jñ<sup>3</sup>gfdba

**Gd<sub>2</sub>Zn<sub>9</sub>** [1]; Gd<sub>2</sub>Cd<sub>9</sub> [4]; Pu<sub>2</sub>Zn<sub>9</sub> [3]

Structural features: GdZn<sub>14</sub>, GdZn<sub>17</sub> and GdZn<sub>18</sub> polyhedra share atoms to form a dense 3D-framework. See Fig. III.52.

Cromer D.T., Larson A.C. (1972) [1]

Gd<sub>13</sub>Zn<sub>58</sub>

$a = 1.431$ ,  $c = 1.405$  nm,  $c/a = 0.982$ ,  $V = 2.4917$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	24 <i>l</i>	1	0.3633	0.0362	0.1012		icosahedron Zn <sub>8</sub> Gd <sub>4</sub>
Zn2	12 <i>k</i>	. <i>m</i> .	0.0973	0.1946	0.1599		icosahedron Zn <sub>8</sub> Gd <sub>4</sub>
Gd3	12 <i>k</i>	. <i>m</i> .	0.2065	0.4130	0.0515		pseudo Frank-Kasper Zn <sub>18</sub>
Zn4	12 <i>k</i>	. <i>m</i> .	0.2374	0.4748	0.6606		bicapped square prism Zn <sub>6</sub> Gd <sub>4</sub>
Zn5	12 <i>k</i>	. <i>m</i> .	0.5628	0.1256	0.6395		pseudo Frank-Kasper Zn <sub>10</sub> Gd <sub>3</sub>



Zn6	12k	.m.	0.6011	0.2022	0.0527	pseudo Frank-Kasper Zn <sub>10</sub> Gd <sub>3</sub>
Zn7	12j	m..	0.0833	0.3666	$\frac{1}{4}$	icosahedron Zn <sub>8</sub> Gd <sub>4</sub>
Zn8	12i	.2.	0.1902	0	0	tricapped trigonal prism Zn <sub>6</sub> Gd <sub>3</sub>
Zn9	6h	mm2	0.2692	0.5384	$\frac{1}{4}$	icosahedron Zn <sub>10</sub> Gd <sub>2</sub>
Gd10	6h	mm2	0.5414	0.0828	$\frac{1}{4}$	17-vertex polyhedron Zn <sub>17</sub>
Gd11	6h	mm2	0.8715	0.7430	$\frac{1}{4}$	17-vertex polyhedron Zn <sub>17</sub>
Zn12	6g	.2/m.	$\frac{1}{2}$	0	0	square prism (cube) Zn <sub>8</sub>
Zn13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0949	icosahedron Zn <sub>9</sub> Gd <sub>3</sub>
Zn14	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	15-vertex Frank-Kasper Zn <sub>12</sub> Gd <sub>3</sub>
Zn15	2b	-6m2	0	0	$\frac{1}{4}$	pseudo Frank-Kasper Zn <sub>6</sub> Gd <sub>5</sub>
Gd16	2a	-3m.	0	0	0	14-vertex polyhedron Zn <sub>14</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.083

Remarks: Phase referred to as  $\eta$ -(GdZn). Supersedes a refinement in space group (186)  $P6_3mc$  [2], which does not take into consideration all symmetry elements. Additional reflections observed for Pu<sub>2</sub>Zn<sub>9</sub> in [3] could be indexed with a 2-fold supercell. In table 3 of [1] the z-coordinate of former Zn(6) is misprinted as 0 instead of  $\frac{1}{4}$  (checked on interatomic distances). In [2] (Gd<sub>13</sub>Zn<sub>58</sub>) the z-coordinate of Zn(13) is misprinted as 0.3148 instead of 0.362 (see [5]).

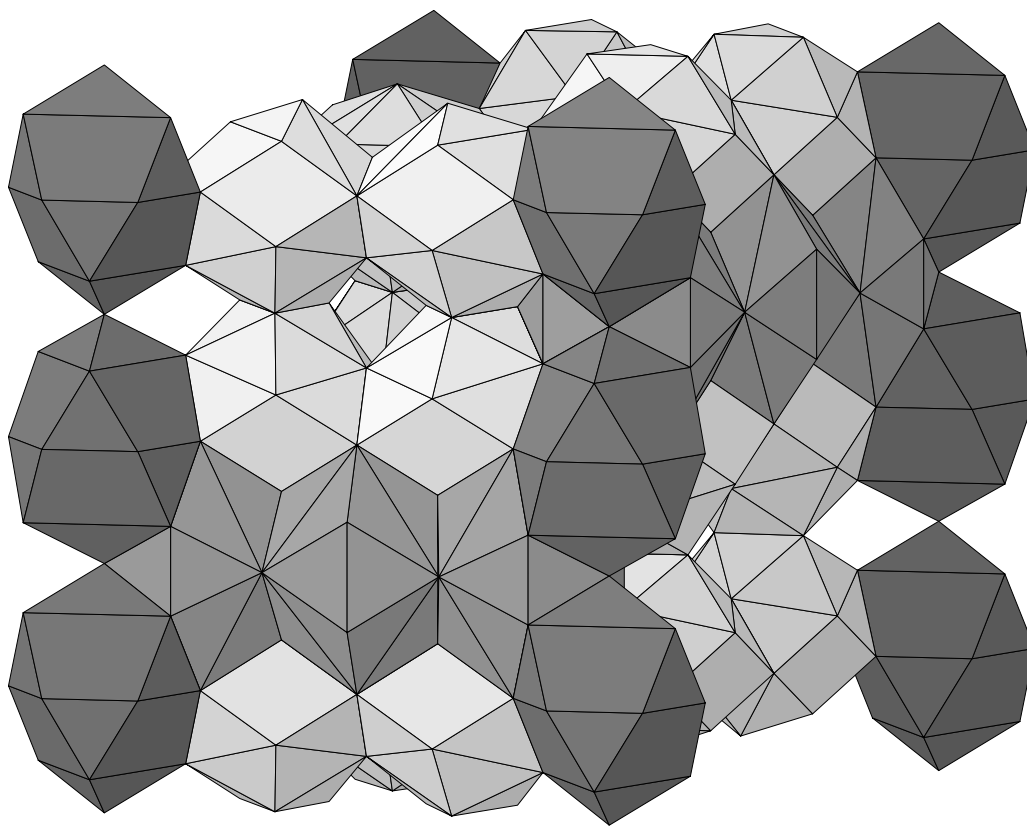


Fig. III.52. **Gd<sub>2</sub>Zn<sub>9</sub>**

Arrangement of GdZn<sub>14</sub> (dark), GdZn<sub>17</sub> (medium) and GdZn<sub>18</sub> (light) polyhedra.

References: [1] Cromer D.T., Larson A.C. (1972), Acta Crystallogr. B 28, 1016-1022. [2] Wang F.E. (1967), Acta Crystallogr. 22, 579-584. [3] Larson A.C., Cromer D.T. (1967), Acta Crystallogr. 23, 70-77.

[4] Bruzzzone G., Fornasini M.L., Merlo F. (1971), J. Less-Common Met. 25, 295-301. [5] Bruzzzone G., Fornasini M.L., Merlo F. (1970), J. Less-Common Met. 22, 253-264.

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hP142

$\text{Ca}_4(\text{Al}_{0.33}\text{Si}_{0.67})_{24}\text{O}_{48}[\text{H}_2\text{O}]_{24}$	hP142	(194) $P6_3/mmc - \text{Ik}^6_2\text{ihf}$
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**(Ca,Na)<sub>4</sub>Al<sub>8</sub>Si<sub>16</sub>O<sub>48</sub>·24H<sub>2</sub>O** [1], gmelinite-(Ca), zeolite GME-Ca hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; Ca near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings), H<sub>2</sub>O delocalized over six sites.

Fischer K. (1966) [1]

$\text{Al}_{7.99}\text{Ca}_4\text{H}_{13.20}\text{O}_{54.60}\text{Si}_{16.01}$

$a = 1.375$ ,  $c = 1.005$  nm,  $c/a = 0.731$ ,  $V = 1.6455$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.441	0.106	0.093		
(OH <sub>2</sub> )2	12k	.m.	0.08	0.16	0.61	0.1	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )3	12k	.m.	0.1	0.2	0.06	0.1	single atom (OH <sub>2</sub> )
O4	12k	.m.	0.202	0.404	0.563		
(OH <sub>2</sub> )5	12k	.m.	0.22	0.44	0.51	0.1	
(OH <sub>2</sub> )6	12k	.m.	0.57	0.14	0.03	0.1	
O7	12k	.m.	0.575	0.15	0.064		
(OH <sub>2</sub> )8	12j	m..	0.2	0.54	$\frac{1}{4}$	0.1	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O9	12j	m..	0.411	0.067	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O10	12i	.2.	0.354	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )11	6h	mm2	0.17	0.34	$\frac{1}{4}$	0.1	tetrahedron (OH <sub>2</sub> ) <sub>4</sub>
Ca12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0735		

$\text{M1} = 0.667\text{Si} + 0.333\text{Al}$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.145$

Remarks: Natural specimen from Nova Scotia. Approximate composition, small amounts of Na ignored. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. We assigned an arbitrary small value to the occupancies of the (OH<sub>2</sub>) sites. Short interatomic distances: d(O4-(OH<sub>2</sub>)5) = 0.068 nm and d(O7-(OH<sub>2</sub>)6) = 0.036 nm. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space groups (186)  $P6_3mc$  and (190)  $P-62c$  were tested and rejected ( $R = 0.19$ ).

References: [1] Fischer K. (1966), Neues Jahrb. Mineral., Monatsh. 1966, 1-13.

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hP144

$\text{LaMo}_2\text{O}_5$	hP144	(194) $P6_3/mmc - \text{Ik}^7_1\text{if}^6_2\text{e}$
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**LaMo<sub>2</sub>O<sub>5</sub>** [1]

Structural features: Mo<sub>6</sub>O<sub>18</sub> units (a Mo<sub>6</sub> octahedron surrounded by an O<sub>12</sub> cuboctahedron and a large O<sub>6</sub> octahedron) and slabs of condensed Mo<sub>3</sub>O<sub>13</sub> units (a central layer of Mo<sub>3</sub> triangles sharing edges and vertices) are interconnected to form infinite composite slabs; disorder caused by an interchange of Mo sheets and layers of La atoms.

Hibble S.J. et al. (1998) [1]

LaMo<sub>2</sub>O<sub>5</sub> $a = 0.8373$ ,  $c = 1.9151$  nm,  $c/a = 2.287$ ,  $V = 1.1627$  nm<sup>3</sup>,  $Z = 12$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.0	0.3277	0.2422	0.5	monocapped square prism O <sub>5</sub> Mo <sub>4</sub> non-coplanar triangle Mo <sub>3</sub> non-coplanar triangle Mo <sub>3</sub>
Mo2	12 <i>k</i>	. <i>m</i> .	0.1052	0.2104	0.058		
O3	12 <i>k</i>	. <i>m</i> .	0.1137	0.2274	0.6243		
O4	12 <i>k</i>	. <i>m</i> .	0.2256	0.4513	0.1135		
Mo5	12 <i>k</i>	. <i>m</i> .	0.2291	0.4582	0.6843	0.5	non-collinear Mo <sub>2</sub>
La6	12 <i>k</i>	. <i>m</i> .	0.5122	0.0244	0.1541	0.5	
O7	12 <i>k</i>	. <i>m</i> .	0.5618	0.1238	0.113	0.5	
Mo8	12 <i>k</i>	. <i>m</i> .	0.5623	0.1246	0.6786	0.5	
O9	12 <i>i</i>	.2.	0.3339	0	0		tetrahedron O <sub>3</sub> La
La10	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.015	0.5	
O11	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.249	0.5	
La12	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5098	0.5	
O13	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6028	0.5	
O14	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.7358	0.5	
La15	4 <i>e</i>	3 <i>m</i> .	0	0	0.2387	0.5	

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>Experimental: powder, diffractometer, neutrons, time-of-flight,  $wR_p = 0.029$ ,  $T = 300$  KRemarks: Short interatomic distances for partly occupied site(s). An ordered model was refined in space group (186)  $P6_3mc$  ( $wR_p = 0.086$ ). A refinement on diffraction data collected at 18 K is reported in [2].

References: [1] Hibble S.J., Cooper S.P., Hannon A.C., Patat S., McCarroll W.H. (1998), Inorg. Chem. 37, 6839-6846. [2] Hibble S.J., Cooper S.P., Patat S., Hannon A.C. (1999), Acta Crystallogr. B 55, 683-697.

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hP146

Zn <sub>58.7</sub> Y <sub>12.65</sub>	hP146	(194) $P6_3/mmc - 1k^5:jih^3gfedba$
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**Y<sub>2</sub>Zn<sub>9</sub>** [1]Structural features: Derivative of Gd<sub>2</sub>Zn<sub>9</sub> with part of Y atoms replaced by Zn<sub>2</sub> dumbbells parallel to [001].

Cromer D.T., Larson A.C. (1972) [1]

Y<sub>12.62</sub>Zn<sub>58.68</sub> $a = 1.424$ ,  $c = 1.400$  nm,  $c/a = 0.983$ ,  $V = 2.4586$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	24 <i>l</i>	1	0.3661	0.0341	0.1005		icosahedron Zn <sub>8</sub> Y <sub>4</sub>
Zn2	12 <i>k</i>	. <i>m</i> .	0.0984	0.1968	0.1581		16-vertex Frank-Kasper Zn <sub>16</sub> bicapped square prism Zn <sub>6</sub> Y <sub>4</sub> pseudo Frank-Kasper Zn <sub>10</sub> Y <sub>3</sub> pseudo Frank-Kasper Zn <sub>10</sub> Y <sub>3</sub>
Y3	12 <i>k</i>	. <i>m</i> .	0.2062	0.4124	0.0517		
Zn4	12 <i>k</i>	. <i>m</i> .	0.2369	0.4738	0.6585		
Zn5	12 <i>k</i>	. <i>m</i> .	0.5629	0.1258	0.6426		
Zn6	12 <i>k</i>	. <i>m</i> .	0.6009	0.2018	0.0521		icosahedron Zn <sub>8</sub> Y <sub>4</sub>
Zn7	12 <i>j</i>	. <i>m</i> ..	0.0860	0.3673	<sup>1</sup> / <sub>4</sub>		
Zn8	12 <i>i</i>	.2.	0.1958	0	0		icosahedron Zn <sub>10</sub> Y <sub>2</sub>
Zn9	6 <i>h</i>	<i>mm</i> 2	0.2701	0.5402	<sup>1</sup> / <sub>4</sub>		
Y10	6 <i>h</i>	<i>mm</i> 2	0.5425	0.0850	<sup>1</sup> / <sub>4</sub>		7-capped pentagonal prism Zn <sub>17</sub>

Y11	6h	mm2	0.8723	0.7446	$\frac{1}{4}$		
Zn12	6g	.2/m.	$\frac{1}{2}$	0	0		square prism (cube) Zn <sub>8</sub>
Zn13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0952		icosahedron Zn <sub>9</sub> Y <sub>3</sub>
Zn14	4e	3m.	0	0	0.0938	0.34	
Zn15	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		15-vertex Frank-Kasper Zn <sub>12</sub> Y <sub>3</sub>
Zn16	2b	-6m2	0	0	$\frac{1}{4}$		colinear Zn <sub>2</sub>
Y17	2a	-3m.	0	0	0	0.62	colinear Zn <sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.066

Remarks: Phase referred to as  $\eta$ -(YZn). Short interatomic distances for partly occupied site(s).

References: [1] Cromer D.T., Larson A.C. (1972), Acta Crystallogr. B 28, 1016-1022.

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hP150

Ba <sub>11</sub> Ti <sub>9</sub> Fe <sub>8</sub> O <sub>41</sub>	hP150	(194) $P6_3/mmc - k^7hf^{10}e^4da$
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### Ba<sub>11</sub>Fe<sub>8</sub>Ti<sub>9</sub>O<sub>41</sub> [1]

Structural features: Perovskite-type slabs (ten close-packed BaO<sub>3</sub> layers in hc<sub>2</sub>hc<sub>2</sub>hc<sub>2</sub>h stacking; Ti in octahedral voids) and partly disordered slabs (two BaO<sub>3</sub>/O<sub>4</sub> and a central O<sub>4</sub> layer in chc stacking, Fe in octahedral and tetrahedral voids) alternate along [001].

Siegrist T. et al. (2000) [1]

Ba<sub>11</sub>Fe<sub>8</sub>O<sub>41</sub>Ti<sub>11</sub>

$a = 0.57506$ ,  $c = 6.1413$  nm,  $c/a = 10.679$ ,  $V = 1.7588$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	.m.	0.1649	0.3298	0.09572		non-colinear Ti <sub>2</sub>
O2	12k	.m.	0.16575	0.3315	0.633		non-colinear Ti <sub>2</sub>
O3	12k	.m.	0.1658	0.3316	0.01847		non-colinear Ti <sub>2</sub>
O4	12k	.m.	0.16895	0.3379	0.71143		tetrahedron Fe <sub>3</sub> Ti
Fe5	12k	.m.	0.50856	0.01712	0.23342	0.5	
O6	12k	.m.	0.5138	0.0276	0.17222		coplanar triangle FeTi <sub>2</sub>
O7	12k	.m.	0.5178	0.0356	0.55696		non-colinear Ti <sub>2</sub>
O8	6h	mm2	0.1571	0.3142	$\frac{1}{4}$		trigonal prism Fe <sub>6</sub>
Ti9	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.03431		octahedron O <sub>6</sub>
Ti10	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.07814		octahedron O <sub>6</sub>
Ba11	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.13397		cuboctahedron O <sub>12</sub>
Fe12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.18553	0.5	
Ba13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.21016	0.5	
O14	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.2156	0.5	
Ba15	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.52209		cuboctahedron O <sub>12</sub>
Ba16	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.59143		cuboctahedron O <sub>12</sub>
Ti17	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.64763		octahedron O <sub>6</sub>
Ti18	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.69273		octahedron O <sub>6</sub>
Ba19	4e	3m.	0	0	0.05675		anticuboctahedron O <sub>12</sub>
Ti20	4e	3m.	0	0	0.11303		octahedron O <sub>6</sub>
Ba21	4e	3m.	0	0	0.17069		anticuboctahedron O <sub>12</sub>
Fe22	4e	3m.	0	0	0.22702		octahedron O <sub>6</sub>
O23	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		trigonal prism Fe <sub>6</sub>
Ti24	2a	-3m.	0	0	0		octahedron O <sub>6</sub>

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

Remarks: Partial disorder Fe/Ti ignored, the idealized site occupations reported here indicate preferential order. Short interatomic distances for partly occupied site(s).

References: [1] Siegrist T., Svensson C., Vanderah T.A., Roth R.S. (2000), Solid State Sci. 2, 539-544.

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hP150

$\text{H}_{2.6}\text{Na}_{4.3}(\text{Al}_{0.14}\text{Si}_{0.86})_{48}\text{O}_{96}$	<i>hP150</i>	(194) $P6_3/mmc - \text{I}^3\text{k}^4\text{jig}$
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**$\text{Na}_{4.3}\text{H}_{2.6}\text{Al}_{6.9}\text{Si}_{41.1}\text{O}_{96}$**  [1], zeolite AFX

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form an AFX-type zeolite framework (6-rings in ABBAACCA stacking) with channels delimited by 8-rings perpendicular to [001]; Na at the centers of 8-rings in the channels.

Lobo R.F. et al. (1996) [1]

$\text{Al}_{7.20}\text{Na}_{3.06}\text{O}_{96}\text{Si}_{40.80}$

$a = 1.36447$ ,  $c = 1.97293$  nm,  $c/a = 1.446$ ,  $V = 3.1810$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.0005	0.2296	0.0768		tetrahedron O <sub>4</sub>
O2	24l	1	0.0193	0.3313	0.1277		non-colinear Si <sub>2</sub>
M3	24l	1	0.1063	0.4404	0.1727		tetrahedron O <sub>4</sub>
O4	12k	.m.	0.0972	0.1944	0.0809		non-colinear Si <sub>2</sub>
O5	12k	.m.	0.1277	0.2554	0.5898		non-colinear Si <sub>2</sub>
O6	12k	.m.	0.2378	0.4757	0.1645		non-colinear Si <sub>2</sub>
O7	12k	.m.	0.5525	0.105	0.6445		non-colinear Si <sub>2</sub>
O8	12j	m..	0.0738	0.4018	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O9	12i	.2.	0.2647	0	0		non-colinear Si <sub>2</sub>
Na10	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0	0.51	coplanar square O <sub>4</sub>

M1 = 0.85Si + 0.15Al; M3 = 0.85Si + 0.15Al

Experimental: powder, diffractometer, X-rays, synchrotron,  $R_p = 0.079$ ,  $T = 298$  K

Remarks: Composition  $\text{Na}_{4.3}\text{H}_{2.7}[\text{Al}_{6.9}\text{Si}_{41.1}\text{O}_{96}]$  from chemical analysis. We adjusted the charge balance in the chemical formula given above by removing H. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lobo R.F., Zones S.I., Medrud R.C. (1996), Chem. Mater. 8, 2409-2411.

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hP152

$\text{Ba}_4(\text{Al}_{0.33}\text{Si}_{0.67})_{24}\text{O}_{48}[\text{H}_2\text{O}]_{19}$	<i>hP152</i>	(194) $P6_3/mmc - \text{Ik}^4\text{j}^4\text{ih}^2\text{fe}$
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**$\text{Ba}_4\text{Al}_8\text{Si}_{16}\text{O}_{48}\cdot 19\text{H}_2\text{O}$**  [1], zeolite GME-Ba hydrated

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; Ba near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings), H<sub>2</sub>O delocalized over seven sites.

Vigdorchik A.G., Malinovskii Y.A. (1986) [1]

$\text{Al}_{7.92}\text{Ba}_{3.44}\text{H}_{38.24}\text{O}_{67.12}\text{Si}_{16.08}$

$a = 1.3793$ ,  $c = 1.0021$  nm,  $c/a = 0.727$ ,  $V = 1.6510$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.4381	0.1044	0.0928		tetrahedron O <sub>4</sub>

Ba2	12k	.m.	0.0935	0.1871	0.0436	0.11	
(OH <sub>2</sub> )3	12k	.m.	0.1135	0.227	0.115	0.37	
O4	12k	.m.	0.2156	0.4312	0.5547		non-colinear Si <sub>2</sub>
O5	12k	.m.	0.5662	0.1324	0.0601		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )6	12j	m..	0.133	0.319	<sup>1</sup> / <sub>4</sub>	0.14	
(OH <sub>2</sub> )7	12j	m..	0.141	0.547	<sup>1</sup> / <sub>4</sub>	0.33	
(OH <sub>2</sub> )8	12j	m..	0.19	0.472	<sup>1</sup> / <sub>4</sub>	0.3	
O9	12j	m..	0.4079	0.0667	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle Si <sub>2</sub> (OH <sub>2</sub> )
O10	12i	.2.	0.345	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )11	6h	mm2	0.195	0.39	<sup>1</sup> / <sub>4</sub>	0.22	
(OH <sub>2</sub> )12	6h	mm2	0.911	0.822	<sup>1</sup> / <sub>4</sub>	0.42	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
Ba13	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.106	0.53	
(OH <sub>2</sub> )14	4e	3m.	0	0	0.1	0.4	

M1 = 0.67Si + 0.33Al

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

Remarks: Natural specimen of gmelinite-(K), ion-exchanged with Ba(NO<sub>3</sub>)<sub>2</sub> solution. Short interatomic distances: d(O9-(OH<sub>2</sub>)7) = 0.166 nm. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the z-coordinate of former W(2) is misprinted as <sup>3</sup>/<sub>4</sub> instead of <sup>1</sup>/<sub>4</sub> (from the description of the structure); in the title the chemical formula is misprinted as Ba<sub>4</sub>[Al<sub>3</sub>Si<sub>16</sub>O<sub>48</sub>]·nH<sub>2</sub>O instead of Ba<sub>4</sub>[Al<sub>8</sub>Si<sub>16</sub>O<sub>48</sub>]·nH<sub>2</sub>O.

References: [1] Vigdorchik A.G., Malinovskii Y.A. (1986), Sov. Phys. Crystallogr. 31, 519-521 (Kristallografiya 31, 879-882).

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hP154

Cu <sub>18</sub> [SO <sub>4</sub> ] <sub>0.18</sub> [NO <sub>3</sub> ] <sub>0.65</sub> Cl <sub>3.9</sub> [OH] <sub>31.1</sub> [H <sub>2</sub> O] <sub>2.6</sub>	hP154	(194) <i>P6<sub>3</sub>/mmc</i> – <i>I</i> <sup>2</sup> <i>k</i> <sup>2</sup> <i>j</i> <i>h</i> <sup>6</sup> <i>g</i> <sup>3</sup> <i>ca</i>
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**Cu<sub>36</sub>(NO<sub>3</sub>)<sub>1.3</sub>(SO<sub>4</sub>)<sub>0.35</sub>(OH)<sub>62.2</sub>Cl<sub>7.8</sub>·5.2H<sub>2</sub>O** [1], buttgenbachite

Structural features: Cu(OH)<sub>4</sub> squares share vertices to form a 3D-framework; NO<sub>3</sub> trigonal units, SO<sub>4</sub> tetrahedra and part of the H<sub>2</sub>O molecules and Cl atoms (disorder) in large channels parallel to [001].

Hibbs D.E. et al. (2003) [1]

Cl<sub>3.90</sub>Cu<sub>18</sub>H<sub>34.32</sub>N<sub>0.66</sub>O<sub>36.36</sub>S<sub>0.18</sub>

*a* = 1.5739, *c* = 0.9127 nm, *c/a* = 0.58, *V* = 1.9580 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH)1	24l	1	0.08	0.4503	0.0918		non-colinear Cu <sub>2</sub>
(OH)2	24l	1	0.3256	0.0708	0.1101		non-coplanar triangle Cu <sub>3</sub>
(OH)3	12k	.m.	0.0749	0.1498	0.5993		non-coplanar triangle Cu <sub>2</sub> Cl
O4	12k	.m.	0.2885	0.577	0.1	0.24	
Cu5	12j	m..	0.0172	0.3592	<sup>1</sup> / <sub>4</sub>		coplanar square (OH) <sub>4</sub>
Cu6	12i	.2.	0.2014	0	0		coplanar square (OH) <sub>4</sub>
Cl7	6h	mm2	0.1387	0.2774	<sup>1</sup> / <sub>4</sub>		trigonal prism Cu <sub>6</sub>
O8	6h	mm2	0.3774	0.7548	<sup>1</sup> / <sub>4</sub>	0.18	
O9	6h	mm2	0.3845	0.769	<sup>1</sup> / <sub>4</sub>	0.18	
(OH)10	6h	mm2	0.5563	0.1126	<sup>1</sup> / <sub>4</sub>		6-vertex polyhedron (OH <sub>2</sub> ) <sub>2</sub> Cu <sub>4</sub>
(OH <sub>2</sub> )11	6h	mm2	0.746	0.492	<sup>1</sup> / <sub>4</sub>	0.18	coplanar triangle Cu(OH) <sub>2</sub>
Cu12	6h	mm2	0.8323	0.6646	<sup>1</sup> / <sub>4</sub>		non-coplanar square (OH) <sub>4</sub>
Cu13	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		coplanar square (OH) <sub>4</sub>
O14	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.032	0.09	
M15	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1	0.3	

S16	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1955	0.09	
M17	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.48	
Cl18	2a	-3m.	0	0	0	0.6	octahedron (OH) <sub>6</sub>

M15 = 0.8N + 0.2OH<sub>2</sub>; M17 = 0.625Cl + 0.375N

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

Experimental: single crystal, diffractometer, X-rays, R = 0.054, T = 288 K

Remarks: Natural specimen from Likasi, Congo. Ambiguous data: the same cell parameters are reported for T = 100 and 288 K. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hibbs D.E., Leverett P., Williams P.A. (2003), Mineral. Mag. 67, 47-60.

194  
hP158

$K_{4.29}Na_{2.25}Ca_{0.73}(Al_{0.33}Si_{0.67})_{24}O_{48}[H_2O]_{26}$	hP158	(194) $P6_3/mmc - I^2K^4J^3ihfe$
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**K<sub>4.29</sub>Na<sub>2.25</sub>Ca<sub>0.73</sub>Al<sub>8</sub>Si<sub>16</sub>O<sub>48</sub>~26H<sub>2</sub>O** [1], gmelinite-(K), zeolite GME-K hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; (K,Na,Ca) near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and near 8-rings in the large channels, H<sub>2</sub>O delocalized over four sites. CHA-type stacking faults (AABBCC).

Malinovskii Y.A. (1984) [1]

Al<sub>8.59</sub>Ca<sub>0.54</sub>H<sub>17.88</sub>K<sub>3.21</sub>Na<sub>1.69</sub>O<sub>56.94</sub>Si<sub>17.21</sub>

$a = 1.3696$ ,  $c = 1.0203$  nm,  $c/a = 0.745$ ,  $V = 1.6575$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.003	0.231	0.094	0.05	
M2	24l	1	0.4355	0.1012	0.0947		tetrahedron O <sub>4</sub>
(OH <sub>2</sub> )3	12k	.m.	0.081	0.162	0.618	0.08	non-colinear Si <sub>2</sub>
M4	12k	.m.	0.121	0.242	0.079	0.12	
O5	12k	.m.	0.2129	0.4258	0.5669		non-colinear Si <sub>2</sub>
O6	12k	.m.	0.5664	0.1328	0.0693		non-colinear Si <sub>2</sub>
M7	12j	m..	0.105	0.435	$\frac{1}{4}$	0.05	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )8	12j	m..	0.168	0.552	$\frac{1}{4}$	0.33	
O9	12j	m..	0.3993	0.0584	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O10	12i	.2.	0.3458	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )11	6h	mm2	0.17	0.34	$\frac{1}{4}$	0.47	tetrahedron Si <sub>2</sub> K <sub>2</sub>
M12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0702		
(OH <sub>2</sub> )13	4e	3m.	0	0	0.058	0.3	single atom (OH <sub>2</sub> )

M1 = 0.667Si + 0.333Al; M2 = 0.667Si + 0.333Al; M4 = 0.59K + 0.31Na + 0.10Ca; M7 = 0.667Si + 0.333Al; M12 = 0.59K + 0.31Na + 0.10Ca

Experimental: single crystal, diffractometer, X-rays, R = 0.076

Remarks: Natural specimen from the Kola Peninsula. Composition K<sub>4.29</sub>Na<sub>2.25</sub>Ca<sub>0.73</sub>[Al<sub>8</sub>Si<sub>16</sub>O<sub>48</sub>]·xH<sub>2</sub>O from chemical analysis. The occupancies of sites M1 and M7 were refined considering f(O), occ(M1) = 0.13, occ(M7) = 0.44, however, the authors state that these positions probably correspond to (Si,Al) in chabazite-type stacking faults; we assigned arbitrary small values to the site occupancies considering (Si,Al). Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into

consideration for Pearson symbol, Wyckoff sequence and atomic environments. Ambiguous data: the authors state that the occupancies of the H<sub>2</sub>O sites correspond to 13 molecules per cell, however, the published values give 9 H<sub>2</sub>O per cell.

References: [1] Malinovskii Y.A. (1984), Sov. Phys. Crystallogr. 29, 256-258 (Kristallografiya 29, 426-430).

194  
hP160

$K_2Sr_2Ca_6(Al_{0.5}Si_{0.5})_{36}O_{72}[H_2O]_{30}$	<i>hP160</i>	(194) $P6_3/mmc - I^2k^5j^2h^2f^2eda$
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**(K,Ba,Sr)<sub>2</sub>Sr<sub>2</sub>Ca<sub>2</sub>(Ca,Na)<sub>4</sub>Al<sub>18</sub>Si<sub>18</sub>O<sub>72</sub>·30H<sub>2</sub>O** [1], bellbergite, zeolite EAB-Ca,Sr,K hydrated  
Structural features: (Al,Si)O<sub>4</sub> tetrahedra share vertices to form an EAB-type zeolite framework (6-rings in ABBACC stacking) with channels delimited by 8-rings perpendicular to [001]; K above the centers of 8-rings, Sr above the centers of 6-rings, Ca at the centers of 6-rings and in cages, H<sub>2</sub>O delocalized over five sites.

Rüdinger B. et al. (1993) [1]

Al<sub>18</sub>Ca<sub>6</sub>H<sub>60</sub>K<sub>2</sub>O<sub>102</sub>Si<sub>18</sub>Sr<sub>2</sub>

$a = 1.3244$ ,  $c = 1.5988$  nm,  $c/a = 1.207$ ,  $V = 2.4286$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.0	0.3182	0.0842		non-colinear Al <sub>2</sub>
M2	24l	1	0.4215	0.0902	0.1538		tetrahedron O <sub>4</sub>
O3	12k	.m.	0.1127	0.2254	0.003		non-colinear Al <sub>2</sub>
(OH <sub>2</sub> )4	12k	.m.	0.218	0.436	0.159		single atom Ca
O5	12k	.m.	0.2295	0.459	0.636		non-colinear Al <sub>2</sub>
O6	12k	.m.	0.541	0.082	0.138		non-colinear Al <sub>2</sub>
(OH <sub>2</sub> )7	12k	.m.	0.587	0.174	0.535	0.5	single atom Ca
O8	12j	m..	0.369	0.042	$\frac{1}{4}$		non-colinear Al <sub>2</sub>
M9	12i	.2.	0.2476	0	0		tetrahedron O <sub>4</sub>
K10	6h	mm2	0.105	0.21	$\frac{1}{4}$	0.333	octahedron (OH <sub>2</sub> ) <sub>4</sub> O <sub>2</sub>
(OH <sub>2</sub> )11	6h	mm2	0.413	0.826	$\frac{1}{4}$		6-vertex polyhedron Ca <sub>2</sub> (OH <sub>2</sub> ) <sub>4</sub>
Ca12	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.13		tricapped trigonal prism (OH <sub>2</sub> ) <sub>9</sub>
Sr13	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.5881	0.5	10-vertex polyhedron O <sub>6</sub> (OH <sub>2</sub> ) <sub>4</sub>
(OH <sub>2</sub> )14	4e	3m.	0	0	0.143		single atom Ca
(OH <sub>2</sub> )15	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		colinear Sr <sub>2</sub>
Ca16	2a	-3m.	0	0	0		8-vertex polyhedron (OH <sub>2</sub> ) <sub>2</sub> O <sub>6</sub>

M2 = 0.50Al + 0.50Si; M9 = 0.50Al + 0.50Si

Experimental: single crystal, diffractometer, X-rays, R = 0.122

Remarks: Natural specimen from the Bellberg volcano, Laacher See, Eifel, Germany. Composition Na<sub>0.72</sub>K<sub>1.33</sub>Ba<sub>0.26</sub>Sr<sub>2.36</sub>Ca<sub>5.32</sub>Al<sub>17.55</sub>Si<sub>18.36</sub>O<sub>72</sub>·30H<sub>2</sub>O from electron microprobe analysis. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Rüdinger B., Tillmanns E., Hentschel G. (1993), Mineral. Petrol. 48, 147-152.

194  
hP162

$Ag_5Ta_{14.6}O_{39}[H_2O]_5$	<i>hP162</i>	(194) $P6_3/mmc - k^{11}h^2f^3eb$
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**Ag<sub>10</sub>Ta<sub>29.2</sub>O<sub>78</sub>·10H<sub>2</sub>O** [1]



Structural features: TaO<sub>6</sub> octahedra share edges and vertices to form a 3D-framework with channels perpendicular to [001]. Two kinds of double HTB-type (Ta forms a Kagomé mesh) layer (common vertices in the former, common edges and vertices in the latter) interconnected via additional TaO<sub>6</sub> octahedra; additional Ta in trigonal prismatic and distorted octahedral voids.

Marini A. et al. (1979) [1]

Ag<sub>4.99</sub>H<sub>10</sub>O<sub>44</sub>Ta<sub>14.60</sub>

$a = 0.754$ ,  $c = 3.643$  nm,  $c/a = 4.832$ ,  $V = 1.7936$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>k</i>	. <i>m</i> .	0.115	0.23	0.705		non-colinear Ta <sub>2</sub>
O2	12 <i>k</i>	. <i>m</i> .	0.128	0.256	0.59		non-colinear Ta <sub>2</sub>
O3	12 <i>k</i>	. <i>m</i> .	0.131	0.262	0.148		non-colinear Ta <sub>2</sub>
O4	12 <i>k</i>	. <i>m</i> .	0.138	0.276	0.025		non-coplanar triangle Ta <sub>3</sub>
Ta5	12 <i>k</i>	. <i>m</i> .	0.1651	0.3302	0.5345		octahedron O <sub>6</sub>
Ta6	12 <i>k</i>	. <i>m</i> .	0.1732	0.3464	0.1955		octahedron O <sub>6</sub>
Ag7	12 <i>k</i>	. <i>m</i> .	0.301	0.602	0.0603	0.196	
Ag8	12 <i>k</i>	. <i>m</i> .	0.5	0.0	0.1158	0.397	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O9	12 <i>k</i>	. <i>m</i> .	0.548	0.096	0.684		non-colinear Ta <sub>2</sub>
O10	12 <i>k</i>	. <i>m</i> .	0.555	0.11	0.037		non-colinear Ta <sub>2</sub>
Ag11	12 <i>k</i>	. <i>m</i> .	0.7	0.4	0.2071	0.239	
O12	6 <i>h</i>	<i>mm</i> 2	0.168	0.336	<sup>1</sup> / <sub>4</sub>		non-colinear Ta <sub>2</sub>
(OH <sub>2</sub> )13	6 <i>h</i>	<i>mm</i> 2	0.572	0.144	<sup>1</sup> / <sub>4</sub>	0.333	
(OH <sub>2</sub> )14	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.122		
Ta15	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.231	0.15	
(OH <sub>2</sub> )16	4 <i>f</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.618		non-coplanar triangle Ag <sub>3</sub>
Ta17	4 <i>e</i>	3 <i>m</i> .	0	0	0.119		octahedron O <sub>6</sub>
Ta18	2 <i>b</i>	-6 <i>m</i> 2	0	0	<sup>1</sup> / <sub>4</sub>	0.3	tricapped trigonal prism O <sub>9</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays, R<sub>B</sub> = 0.070

Remarks: Cell parameters omitted, we derived approximate values in agreement with the cell volume estimated from fig. 1 in [1]. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table II of [1] the Wyckoff position of former Ta(IV) is misprinted as 4*e* instead of 2*b*.

References: [1] Marini A., Michel C., Raveau B. (1979), Rev. Chim. Miner. 16, 73-79.

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hP164

K <sub>2.7</sub> Na <sub>0.2</sub> Sr <sub>0.4</sub> Ca <sub>2</sub> (Al <sub>0.32</sub> Si <sub>0.68</sub> ) <sub>24</sub> O <sub>48</sub> [H <sub>2</sub> O] <sub>23.5</sub>	hP164	(194) <i>P</i> 6 <sub>3</sub> / <i>mmc</i> – lk <sup>6</sup> j <sup>3</sup> ih <sup>2</sup> fe
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**K<sub>2.7</sub>Na<sub>0.2</sub>Sr<sub>0.4</sub>Ca<sub>2</sub>Al<sub>7.75</sub>Si<sub>16.25</sub>O<sub>48</sub>·23.5H<sub>2</sub>O** [1], gmelinite-(K), zeolite GME-K,Ca hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form a GME-type zeolite framework (6-rings in BBCC stacking) with channels delimited by 12-rings parallel to [001] and by 8-rings perpendicular to [001]; non-framework cations near 6-rings in gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and near 8-rings in the large channels, H<sub>2</sub>O delocalized over eight sites.

Vezzalini G. et al. (1990) [1]

Al<sub>7.75</sub>Ca<sub>1.46</sub>H<sub>37.88</sub>K<sub>2.37</sub>Na<sub>0.19</sub>O<sub>66.94</sub>Si<sub>16.25</sub>Sr<sub>0.34</sub>

$a = 1.3621$ ,  $c = 1.0254$  nm,  $c/a = 0.753$ ,  $V = 1.6476$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.4339	0.0995	0.0989		tetrahedron O <sub>4</sub>
(OH <sub>2</sub> )2	12k	.m.	0.089	0.178	0.016	0.19	
(OH <sub>2</sub> )3	12k	.m.	0.103	0.206	0.11	0.34	
M4	12k	.m.	0.124	0.248	0.049	0.03	
(OH <sub>2</sub> )5	12k	.m.	0.164	0.328	0.211	0.33	
O6	12k	.m.	0.2144	0.4288	0.5703		non-colinear Si <sub>2</sub>
O7	12k	.m.	0.5641	0.1282	0.0696		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )8	12j	m..	0.169	0.558	<sup>1</sup> / <sub>4</sub>	0.24	
(OH <sub>2</sub> )9	12j	m..	0.185	0.505	<sup>1</sup> / <sub>4</sub>	0.12	
O10	12j	m..	0.3973	0.0544	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O11	12i	.2.	0.3433	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )12	6h	mm2	0.236	0.472	<sup>1</sup> / <sub>4</sub>	0.28	
(OH <sub>2</sub> )13	6h	mm2	0.918	0.836	<sup>1</sup> / <sub>4</sub>	0.21	8-vertex polyhedron (OH <sub>2</sub> ) <sub>8</sub>
M14	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0655		
(OH <sub>2</sub> )15	4e	3m.	0	0	0.049	0.34	single atom (OH <sub>2</sub> )

M1 = 0.677Si + 0.323Al; M4 = 0.544K + 0.334Ca + 0.078Sr + 0.044Na; M14 = 0.544K + 0.334Ca + 0.078Sr + 0.044Na

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

Remarks: Natural specimen from Fara Vicentina, Vicenza, Italy. Composition Na<sub>0.22</sub>K<sub>2.72</sub>Mg<sub>0.13</sub>Ca<sub>1.67</sub>Sr<sub>0.39</sub>Al<sub>7.79</sub>Si<sub>16.32</sub>O<sub>48</sub> from electron microprobe analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Vezzalini G., Quartieri S., Passaglia E. (1990), Neues Jahrb. Mineral., Monatsh. 1990, 504-516.

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hP168

K <sub>2.0</sub> Na <sub>0.9</sub> Ca <sub>2.4</sub> Mg <sub>0.7</sub> (Al <sub>0.25</sub> Si <sub>0.75</sub> ) <sub>36</sub> O <sub>72</sub>	hP168	(194) <i>P6<sub>3</sub>/mmc</i> – <i>l</i> <sup>3</sup> <i>k</i> <sup>2</sup> <i>j</i> <sup>2</sup> <i>ih</i> <sup>4</sup> <i>gdc</i> <i>b</i>
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**K<sub>2.0</sub>Na<sub>0.9</sub>Ca<sub>2.4</sub>Mg<sub>0.7</sub>Al<sub>9.1</sub>Si<sub>26.9</sub>O<sub>72</sub>** [1], erionite-(Ca), zeolite ERI-Ca,K

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; Ca at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), K at the centers of planar 8-rings, (Na,Mg) at the centers of planar 6-rings. OFF-type stacking faults.

Schlenker J.L. et al. (1977) [1]

Al<sub>9.11</sub>Ca<sub>2</sub>K<sub>1.60</sub>Mg<sub>0.88</sub>Na<sub>1.13</sub>O<sub>72</sub>Si<sub>26.89</sub>

*a* = 1.3252, *c* = 1.481 nm, *c/a* = 1.118, *V* = 2.2524 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.0	0.2304	0.1071		
O2	24l	1	0.0338	0.3501	0.1593	0.942	
O3	24l	1	0.3501	0.0338	0.1593	0.058	
O4	12k	.m.	0.093	0.186	0.1346		non-colinear Si <sub>2</sub>
O5	12k	.m.	0.1258	0.2516	0.641		non-colinear Si <sub>2</sub>
M6	12j	m..	0.0938	0.4256	<sup>1</sup> / <sub>4</sub>	0.942	tetrahedron O <sub>4</sub>
M7	12j	m..	0.4256	0.0938	<sup>1</sup> / <sub>4</sub>	0.058	tetrahedron O <sub>4</sub>
O8	12i	.2.	0.2523	0	0		non-colinear Si <sub>2</sub>
O9	6h	mm2	0.2363	0.4726	<sup>1</sup> / <sub>4</sub>	0.95	non-colinear Si <sub>2</sub>
O10	6h	mm2	0.4552	0.9104	<sup>1</sup> / <sub>4</sub>	0.95	non-colinear Si <sub>2</sub>

O11	6h	mm2	0.5448	0.0896	$\frac{1}{4}$	0.05	non-colinear Si <sub>2</sub>
O12	6h	mm2	0.7637	0.5274	$\frac{1}{4}$	0.05	non-colinear Si <sub>2</sub>
K13	6g	.2/m.	$\frac{1}{2}$	0	0	0.267	
M14	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$	0.05	coplanar triangle O <sub>3</sub>
M15	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.95	coplanar triangle O <sub>3</sub>
Ca16	2b	-6m2	0	0	$\frac{1}{4}$		trigonal prism O <sub>6</sub>

M1 = 0.747Si + 0.253Al; M6 = 0.747Si + 0.253Al; M7 = 0.747Si + 0.253Al; M14 = 0.5625Na + 0.4375Mg; M15 = 0.5625Na + 0.4375Mg

Experimental: single crystal, diffractometer, X-rays, wR = 0.061

Remarks: Natural specimen from Mazé, Niigata, Japan, dehydrated. Composition Na<sub>0.8-0.9</sub>Mg<sub>0.5-0.8</sub>K<sub>1.9-2.0</sub>Ca<sub>2.3-2.6</sub>Al<sub>9.5-9.8</sub>Si<sub>26.4-26.7</sub>O<sub>72</sub> from electron microprobe analysis; no Fe detected (experimental limit 0.2 wt.%). Short interatomic distances for partly occupied site(s).

References: [1] Schlenker J.L., Pluth J.J., Smith J.V. (1977), Acta Crystallogr. B 33, 3265-3268.

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hP186

K <sub>1.9</sub> Na <sub>0.2</sub> Ca <sub>2.5</sub> Mg <sub>0.9</sub> (Al <sub>0.25</sub> Si <sub>0.75</sub> ) <sub>36</sub> O <sub>72</sub> [H <sub>2</sub> O] <sub>29.8</sub>	hP186	(194) <i>P6<sub>3</sub>/mmc</i> – <i>1<sup>2</sup>k<sup>7</sup>jih<sup>2</sup>f<sup>4</sup>b</i>
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**K<sub>1.9</sub>Na<sub>0.2</sub>Ca<sub>2.5</sub>Mg<sub>0.9</sub>Al<sub>8.9</sub>Si<sub>27.1</sub>O<sub>72</sub>·29.8H<sub>2</sub>O** [1], erionite-(Ca), zeolite ERI-Ca,K hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; K at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Mg and Ca in large (erionite-type) cages, H<sub>2</sub>O delocalized over five sites.

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

Al<sub>9</sub>Ca<sub>2.72</sub>H<sub>63.12</sub>K<sub>1.74</sub>Mg<sub>0.80</sub>O<sub>103.56</sub>Si<sub>27</sub>

*a* = 1.3289, *c* = 1.5079 nm, *c/a* = 1.135, *V* = 2.3062 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.0005	0.2337	0.1015		tetrahedron O <sub>4</sub>
O2	24l	1	0.3305	0.0175	0.1752		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.0915	0.183	0.6176		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.1101	0.2202	0.1371		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )5	12k	.m.	0.245	0.49	0.606	0.33	non-colinear CaO
(OH <sub>2</sub> )6	12k	.m.	0.2658	0.5316	0.2009	0.86	non-colinear (OH <sub>2</sub> )Ca
(OH <sub>2</sub> )7	12k	.m.	0.531	0.062	0.073	0.3	non-coplanar triangle (OH <sub>2</sub> ) <sub>2</sub> O
(OH <sub>2</sub> )8	12k	.m.	0.559	0.118	0.711	0.24	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )9	12k	.m.	0.578	0.156	0.603	0.9	single atom (OH <sub>2</sub> )
M10	12j	.m.	0.4249	0.0897	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O11	12i	.2.	0.2693	0	0		non-colinear Si <sub>2</sub>
O12	6h	mm2	0.5182	0.0365	$\frac{1}{4}$		tetrahedron Si <sub>2</sub> (OH <sub>2</sub> ) <sub>2</sub>
O13	6h	mm2	0.7671	0.5342	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
Mg14	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.049	0.2	
Ca15	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0953	0.22	
Ca16	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.177	0.16	
Ca17	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6137	0.3	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
K18	2b	-6m2	0	0	$\frac{1}{4}$	0.87	hexagonal prism O <sub>12</sub>

M1 = 0.75Si + 0.25Al; M10 = 0.75Si + 0.25Al

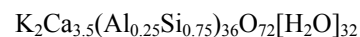
Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, wR<sub>p</sub> = 0.093

Remarks: Natural specimen from Agate Beach, Oregon. Composition  $\text{Na}_{0.18}\text{K}_{1.77}\text{Mg}_{0.82}\text{Ca}_{2.42}(\text{Al}_{8.92}\text{Si}_{27.18}\text{O}_{72})\cdot 29.82\text{H}_2\text{O}$  from electron microprobe analysis. No attempt was made to distinguish Ca and Na; partial substitution by Na on sites ( $\text{OH}_2$ ) could not be excluded. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3A of [1] the z-coordinate of former W3b is misprinted as -0.602 instead of -0.062 (agreement with the site multiplicity; checked on interatomic distances).

References: [1] Gualtieri A., Artioli G., Passaglia E., Bigi S., Viani A., Hanson J.C. (1998), Am. Mineral. 83, 590-606.

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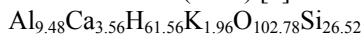
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(194)  $P6_3/mmc - I^2k^7j\bar{1}h^3\bar{1}b$ 

**$\text{K}_2\text{Ca}_{3.5}\text{Al}_9\text{Si}_{27}\text{O}_{72}\cdot 32\text{H}_2\text{O}$**  [1], erionite-(Ca), zeolite ERI-Ca,K hydrated

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; K at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Ca in large (erionite-type) cages,  $\text{H}_2\text{O}$  delocalized over six sites.

Alberti A. et al. (1997) [1]



$a = 1.3311$ ,  $c = 1.5095$  nm,  $c/a = 1.134$ ,  $V = 2.3162$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.2335	0.0001	0.1049		tetrahedron O <sub>4</sub>
O2	24l	1	0.3486	0.0265	0.1611		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.0975	0.195	0.6263		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.1259	0.2518	0.1349		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )5	12k	.m.	0.2522	0.5044	0.5203	0.7	non-colinear Ca <sub>2</sub>
(OH <sub>2</sub> )6	12k	.m.	0.2547	0.5094	0.1834	0.43	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )7	12k	.m.	0.5291	0.0582	0.018	0.28	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )8	12k	.m.	0.5523	0.1046	0.5706	0.44	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )9	12k	.m.	0.5785	0.157	0.64	0.56	single atom (OH <sub>2</sub> )
M10	12j	m..	0.425	0.0932	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O11	12i	.2.	0.2654	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )12	6h	mm2	0.2396	0.4792	$\frac{1}{4}$	0.31	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O13	6h	mm2	0.5416	0.0832	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O14	6h	mm2	0.7692	0.5384	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
Ca15	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0623	0.57	7-vertex polyhedron Ca(OH <sub>2</sub> ) <sub>6</sub>
Ca16	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1948	0.1	
Ca17	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6207	0.22	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
K18	2b	-6m2	0	0	$\frac{1}{4}$	0.98	trigonal prism O <sub>6</sub>

M1 = 0.76Si + 0.24Al; M10 = 0.69Si + 0.31Al

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.044

Remarks: Natural specimen from Nizhnyaya Tunguska, Siberia. Composition  $\text{Na}_{0.03}\text{K}_{1.70}\text{Mg}_{0.04}\text{Ca}_{3.52}\text{Ba}_{0.02}\text{Al}_{9.57}\text{Fe}_{0.03}\text{Si}_{26.59}\text{O}_{72}\cdot 31.6\text{H}_2\text{O}$  from electron microprobe analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Alberti A., Martucci A., Galli E., Vezzolini G. (1997), Zeolites 19, 349-352.

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$\text{K}_{2.5}\text{Na}_{0.3}\text{Ca}_{1.4}\text{Mg}_{2.1}(\text{Al}_{0.27}\text{Si}_{0.73})_{36}\text{O}_{72}[\text{H}_2\text{O}]_{28}$  *hP190* (194)  $P6_3/mmc - l^3k^2j^3ih^5gfec$

**$\text{K}_{2.5}\text{Na}_{0.3}\text{Ca}_{1.4}\text{Mg}_{2.1}\text{Al}_{9.8}\text{Si}_{26.2}\text{O}_{72} \cdot 28\text{H}_2\text{O}$**  [1], mazzite, zeolite MAZ-K,Mg,Ca hydrated

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form a MAZ-type zeolite framework with gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and channels delimited by 12-rings and 8-rings parallel to [001]; Mg at the centers of gmelinite-type cages, Ca at the centers of 12-rings, (K,Na,Ca) at the centers of 6-rings,  $\text{H}_2\text{O}$  delocalized over seven sites.

Galli E. (1975) [1]

$\text{Al}_{9.72}\text{Ca}_{1.06}\text{H}_{62.96}\text{K}_{2.52}\text{Mg}_2\text{Na}_{0.30}\text{O}_{103.48}\text{Si}_{26.28}$

$a = 1.8392$ ,  $c = 0.7646$  nm,  $c/a = 0.416$ ,  $V = 2.2399$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24 <i>l</i>	1	0.0933	0.3536	0.0444		tetrahedron $\text{O}_4$
(OH <sub>2</sub> )2	24 <i>l</i>	1	0.148	0.028	0.03	0.23	single atom (OH <sub>2</sub> )
O3	24 <i>l</i>	1	0.4352	0.1114	0.0721		non-colinear $\text{Si}_2$
O4	12 <i>k</i>	. <i>m</i> .	0.1614	0.3228	0.0016		non-colinear $\text{Si}_2$
(OH <sub>2</sub> )5	12 <i>k</i>	. <i>m</i> .	0.533	0.066	0.661	0.5	
O6	12 <i>j</i>	. <i>m</i> ..	0.1004	0.3822	$\frac{1}{4}$		non-colinear $\text{Si}_2$
(OH <sub>2</sub> )7	12 <i>j</i>	. <i>m</i> ..	0.211	0.566	$\frac{1}{4}$	0.44	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
M8	12 <i>j</i>	. <i>m</i> ..	0.4902	0.1584	$\frac{1}{4}$		tetrahedron $\text{O}_4$
O9	12 <i>i</i>	.2.	0.2741	0	0		non-colinear $\text{Si}_2$
(OH <sub>2</sub> )10	6 <i>h</i>	<i>mm</i> 2	0.076	0.152	$\frac{1}{4}$	0.45	coplanar square (OH <sub>2</sub> ) <sub>4</sub>
(OH <sub>2</sub> )11	6 <i>h</i>	<i>mm</i> 2	0.271	0.542	$\frac{1}{4}$	0.44	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O12	6 <i>h</i>	<i>mm</i> 2	0.5751	0.1502	$\frac{1}{4}$		non-colinear $\text{Si}_2$
O13	6 <i>h</i>	<i>mm</i> 2	0.7411	0.4822	$\frac{1}{4}$		non-colinear $\text{Si}_2$
(OH <sub>2</sub> )14	6 <i>h</i>	<i>mm</i> 2	0.912	0.824	$\frac{1}{4}$	0.89	coplanar square (OH <sub>2</sub> ) <sub>4</sub>
M15	6 <i>g</i>	.2/ <i>m</i> .	$\frac{1}{2}$	0	0	0.5	
(OH <sub>2</sub> )16	4 <i>f</i>	3. <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.516		single atom Mg
Ca17	4 <i>e</i>	3. <i>m</i> .	0	0	0.072	0.22	
Mg18	2 <i>c</i>	-6 <i>m</i> 2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		

M1 = 0.73Si + 0.27Al; M8 = 0.73Si + 0.27Al; M15 = 0.84K + 0.10Na + 0.06Ca

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

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: Natural specimen from Mont Semiol, Loire, France. Composition  $\text{Na}_{0.8}\text{K}_{2.5}\text{Ca}_{1.4}\text{Mg}_{2.1}[\text{Al}_{9.9}\text{Si}_{26.5}\text{O}_{72}] \cdot 28\text{H}_2\text{O}$  from chemical analysis We adjusted the chemical formula given above so that it contains 36 Al+Si atoms, and the charge balance by removing Na. Short interatomic distances for partly occupied site(s). Space groups (186)  $P6_3mc$  and (190)  $P-62c$  were tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Galli E. (1975), Rend. Soc. Ital. Mineral. Petrol. 31, 599-612.

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$\text{K}_2\text{Ca}_{3.8}(\text{Al}_{0.27}\text{Si}_{0.73})_{36}\text{O}_{72}[\text{H}_2\text{O}]_{31.6}$  *hP194* (194)  $P6_3/mmc - l^2k^7jih^3gf^3b$

**$\text{K}_2\text{Ca}_{3.8}\text{Al}_{9.6}\text{Si}_{26.4}\text{O}_{72} \cdot 31.6\text{H}_2\text{O}$**  [1], erionite-(Ca), zeolite ERI-Ca,K hydrated

Structural features: (Si,Al) $\text{O}_4$  tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; K at the centers of

cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Ca in large (erionite-type) cages and at the centers of planar 8-rings, H<sub>2</sub>O delocalized over six sites.

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

Al<sub>9.72</sub>Ca<sub>3.60</sub>H<sub>53.52</sub>K<sub>1.70</sub>O<sub>98.76</sub>Si<sub>26.28</sub>

$a = 1.3304$ ,  $c = 1.5078$  nm,  $c/a = 1.133$ ,  $V = 2.3112$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.003	0.2332	0.1057		tetrahedron O <sub>4</sub>
O2	24l	1	0.0223	0.3453	0.1616		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.0952	0.1904	0.1255		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.1259	0.2518	0.6383		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )5	12k	.m.	0.238	0.476	0.678	0.46	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )6	12k	.m.	0.2476	0.4952	0.02	0.39	non-colinear Ca <sub>2</sub>
(OH <sub>2</sub> )7	12k	.m.	0.534	0.068	0.004	0.33	
(OH <sub>2</sub> )8	12k	.m.	0.5663	0.1326	0.118	0.74	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )9	12k	.m.	0.579	0.158	0.211	0.19	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
M10	12j	m..	0.0945	0.4227	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O11	12i	.2.	0.2661	0	0		non-colinear Si <sub>2</sub>
O12	6h	mm2	0.2284	0.4568	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O13	6h	mm2	0.4639	0.9278	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )14	6h	mm2	0.758	0.516	<sup>1</sup> / <sub>4</sub>	0.24	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
Ca15	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0	0.04	
Ca16	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.113	0.16	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
Ca17	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5737	0.55	7-vertex polyhedron Ca(OH <sub>2</sub> ) <sub>6</sub>
Ca18	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.719	0.13	
K19	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>	0.85	trigonal prism O <sub>6</sub>

M1 = 0.73Si + 0.27Al; M10 = 0.73Si + 0.27Al

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.026

Remarks: Natural specimen from Nizhnyaya Tunguska, Russia. Composition Na<sub>0.06</sub>K<sub>1.69</sub>Mg<sub>0.07</sub>Ca<sub>3.77</sub>(Al<sub>9.60</sub>Si<sub>26.41</sub>O<sub>72</sub>)·31.63H<sub>2</sub>O from electron microprobe analysis. Small amounts of Na and Mg ignored; we adjusted the charge balance in the formula given above by adding K. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gualtieri A., Artioli G., Passaglia E., Bigi S., Viani A., Hanson J.C. (1998), Am. Mineral. 83, 590-606.

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K<sub>2</sub>Na<sub>0.1</sub>Ca<sub>1.7</sub>Mg<sub>2</sub>(Al<sub>0.26</sub>Si<sub>0.74</sub>)<sub>36</sub>O<sub>72</sub>[H<sub>2</sub>O]<sub>28</sub> *hP196* (194) *P6<sub>3</sub>/mmc* – 1<sup>3</sup>k<sup>3</sup>j<sup>3</sup>ih<sup>4</sup>gfed

**K<sub>2</sub>Na<sub>0.1</sub>Ca<sub>1.7</sub>Mg<sub>2</sub>Al<sub>9.5</sub>Si<sub>26.5</sub>O<sub>72</sub>·28H<sub>2</sub>O** [1], mazzite, zeolite MAZ-K,Mg,Ca hydrated

Structural features: (Si,Al)<sub>4</sub> tetrahedra share vertices to form a MAZ-type zeolite framework with gmelinite-type cages (14-face polyhedron formed by two hexagons, nine squares and three non-planar 8-rings) and channels delimited by 12-rings and 8-rings parallel to [001]; Mg at the centers of gmelinite-type cages, Ca at the centers of 12-rings, (K,Ca,Na) at the centers of 6-rings, H<sub>2</sub>O delocalized over seven sites.

Galli E. (1974) [1]

Al<sub>9.68</sub>Ca<sub>1.41</sub>H<sub>64.76</sub>K<sub>2.15</sub>Mg<sub>2</sub>Na<sub>0.03</sub>O<sub>104.38</sub>Si<sub>26.32</sub>

$a = 1.8392$ ,  $c = 0.7646$  nm,  $c/a = 0.416$ ,  $V = 2.2399$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH <sub>2</sub> )1	24l	1	0.022	0.145	0.048	0.25	single atom (OH <sub>2</sub> )
O2	24l	1	0.1116	0.4353	0.0723		non-colinear Si <sub>2</sub>
M3	24l	1	0.3536	0.0933	0.0444		tetrahedron O <sub>4</sub>
(OH <sub>2</sub> )4	12k	.m.	0.077	0.154	0.728	0.39	
O5	12k	.m.	0.1612	0.3224	0.5005		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )6	12k	.m.	0.533	0.066	0.158	0.57	non-colinear (OH <sub>2</sub> )K
M7	12j	m..	0.1583	0.4902	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O8	12j	m..	0.3821	0.1004	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )9	12j	m..	0.567	0.212	<sup>1</sup> / <sub>4</sub>	0.3	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O10	12i	.2.	0.274	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )11	6h	mm2	0.089	0.178	<sup>1</sup> / <sub>4</sub>	0.81	non-coplanar square (OH <sub>2</sub> ) <sub>4</sub>
O12	6h	mm2	0.2589	0.5178	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O13	6h	mm2	0.4248	0.8496	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )14	6h	mm2	0.729	0.458	<sup>1</sup> / <sub>4</sub>	0.4	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
M15	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0	0.46	
(OH <sub>2</sub> )16	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.016		single atom Mg
Ca17	4e	3m.	0	0	0.068	0.21	
Mg18	2d	-6m2	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>3</sup> / <sub>4</sub>		

M3 = 0.731Si + 0.269Al; M7 = 0.731Si + 0.269Al; M15 = 0.780K + 0.208Ca + 0.012Na

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Natural specimen from Mont Semiol, Loire, France. Composition K<sub>1.91</sub>Na<sub>0.03</sub>Ca<sub>1.35</sub>Mg<sub>1.99</sub>Al<sub>9.77</sub>Si<sub>26.53</sub>O<sub>72</sub>·28.06H<sub>2</sub>O probably from chemical analysis. We adjusted the chemical formula given above so that it contains 36 Al+Si atoms, and the charge balance by adding Ca. We assigned approximate values to the cation ratio of sites M based on the nominal composition. 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] Galli E. (1974), Cryst. Struct. Commun. 3, 339-344.

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hP204

K <sub>2.1</sub> Na <sub>0.2</sub> Ca <sub>2.5</sub> Mg <sub>0.6</sub> (Al <sub>0.24</sub> Si <sub>0.76</sub> ) <sub>36</sub> O <sub>72</sub> [H <sub>2</sub> O] <sub>28.9</sub>	hP204	(194) P6 <sub>3</sub> /mmc – I <sup>2</sup> k <sup>8</sup> jih <sup>2</sup> gf <sup>4</sup> b
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**K<sub>2.1</sub>Na<sub>0.2</sub>Ca<sub>2.5</sub>Mg<sub>0.6</sub>Al<sub>8.5</sub>Si<sub>27.5</sub>O<sub>72</sub>·28.9H<sub>2</sub>O** [1], erionite-(Ca), zeolite ERI-Ca,K hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; K at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Ca and Mg in large (erionite-type) cages, additional Ca at the centers of planar 8-rings, H<sub>2</sub>O delocalized over six sites.

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

Al<sub>8.64</sub>Ca<sub>2.44</sub>H<sub>43.20</sub>K<sub>2</sub>Mg<sub>0.52</sub>O<sub>93.60</sub>Si<sub>27.36</sub>

a = 1.3264, c = 1.5067 nm, c/a = 1.136, V = 2.2957 nm<sup>3</sup>, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.2329	0.0006	0.1052		tetrahedron O <sub>4</sub>
O2	24l	1	0.3473	0.0251	0.1609		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.0973	0.1946	0.6261		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.1263	0.2526	0.132		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )5	12k	.m.	0.235	0.47	0.218	0.36	

(OH <sub>2</sub> ) <sub>6</sub>	12k	.m.	0.261	0.522	0.194	0.18	
(OH <sub>2</sub> ) <sub>7</sub>	12k	.m.	0.266	0.532	0.508	0.29	non-colinear MgCa
(OH <sub>2</sub> ) <sub>8</sub>	12k	.m.	0.535	0.07	0.721	0.14	
(OH <sub>2</sub> ) <sub>9</sub>	12k	.m.	0.537	0.074	0.029	0.22	
(OH <sub>2</sub> ) <sub>10</sub>	12k	.m.	0.569	0.138	0.597	0.61	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
M11	12j	m..	0.4226	0.0926	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O12	12i	.2.	0.268	0	0		non-colinear Si <sub>2</sub>
O13	6h	mm2	0.5485	0.097	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O14	6h	mm2	0.769	0.538	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
Ca15	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0	0.14	
Mg16	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.073	0.13	
Ca17	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.113	0.12	
Ca18	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.201	0.13	
Ca19	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.604	0.15	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
K20	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>

M1 = 0.76Si + 0.24Al; M11 = 0.76Si + 0.24Al

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.028

Remarks: Natural specimen from Shourdo, Russia. Composition Na<sub>0.15</sub>K<sub>2.02</sub>Mg<sub>0.53</sub>Ca<sub>2.42</sub>(Al<sub>8.51</sub>Si<sub>27.59</sub>O<sub>72</sub>)·28.86H<sub>2</sub>O from electron microprobe analysis. No attempt was made to distinguish Ca and Na; partial substitution of Na for H<sub>2</sub>O could not be excluded. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3A of [1] the site multiplicities of former Ca3 and Ca4 are misprinted as 6 and 4 instead of 4 and 6.

References: [1] Gualtieri A., Artioli G., Passaglia E., Bigi S., Viani A., Hanson J.C. (1998), Am. Mineral. 83, 590-606.

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hP206

K<sub>2.2</sub>Na<sub>0.2</sub>Ca<sub>4.3</sub>(Al<sub>0.31</sub>Si<sub>0.69</sub>)<sub>36</sub>O<sub>72</sub>[H<sub>2</sub>O]<sub>36.4</sub>

hP206

(194) *P*6<sub>3</sub>/*mmc* – l<sup>2</sup>k<sup>8</sup>j<sup>3</sup>gh<sup>3</sup>b

**K<sub>2.2</sub>Na<sub>0.2</sub>Ca<sub>4.3</sub>Al<sub>11</sub>Si<sub>25</sub>O<sub>72</sub>·36.4H<sub>2</sub>O** [1], erionite-(Ca), zeolite ERI-Ca,K hydrated

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an ERI-type zeolite framework (6-rings in AABAAC stacking) with channels delimited by 8-rings perpendicular to [001]; K at the centers of cancrinite-type cages (11-face polyhedra formed by six 4-rings, two planar and three non-planar 6-rings), Ca in large (erionite-type) cages and at the centers of planar 8-rings, H<sub>2</sub>O delocalized over seven sites.

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

Al<sub>11.16</sub>Ca<sub>4</sub>H<sub>59.40</sub>K<sub>2</sub>O<sub>101.70</sub>Si<sub>24.84</sub>

*a* = 1.3339, *c* = 1.5112 nm, *c/a* = 1.133, *V* = 2.3286 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.2308	0.0012	0.1058		tetrahedron O <sub>4</sub>
O2	24l	1	0.3443	0.0295	0.1584		non-colinear Si <sub>2</sub>
O3	12k	.m.	0.0991	0.1982	0.6285		non-colinear Si <sub>2</sub>
O4	12k	.m.	0.1266	0.2532	0.1284		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> ) <sub>5</sub>	12k	.m.	0.2439	0.4878	0.5154	0.46	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> ) <sub>6</sub>	12k	.m.	0.254	0.508	0.191	0.29	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> ) <sub>7</sub>	12k	.m.	0.2705	0.541	0.06	0.39	non-colinear (OH <sub>2</sub> )Ca
(OH <sub>2</sub> ) <sub>8</sub>	12k	.m.	0.53	0.06	0.027	0.38	
(OH <sub>2</sub> ) <sub>9</sub>	12k	.m.	0.5586	0.1172	0.5859	0.62	single atom (OH <sub>2</sub> )



(OH <sub>2</sub> ) <sub>10</sub>	12k	.m.	0.5795	0.159	0.6586	0.18	single atom (OH <sub>2</sub> )
M11	12j	m..	0.419	0.0871	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O12	12i	.2.	0.2645	0	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> ) <sub>13</sub>	6h	mm2	0.205	0.41	<sup>1</sup> / <sub>4</sub>	0.31	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O14	6h	mm2	0.5552	0.1105	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
O15	6h	mm2	0.7686	0.5372	<sup>1</sup> / <sub>4</sub>		non-colinear Si <sub>2</sub>
Ca16	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0	0.04	
Ca17	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.058	0.47	
Ca18	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.221	0.07	
Ca19	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.618	0.4	4-vertex polyhedron (OH <sub>2</sub> ) <sub>3</sub> Ca
K20	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>		trigonal prism O <sub>6</sub>

M1 = 0.69Si + 0.31Al; M11 = 0.69Si + 0.31Al

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.032

Remarks: Natural specimen from Lady Hill Quarry, Northern Ireland. Composition Na<sub>0.21</sub>K<sub>2.24</sub>Mg<sub>0.03</sub>Ca<sub>4.25</sub>(Al<sub>11.03</sub>Si<sub>24.97</sub>O<sub>72</sub>)·36.36H<sub>2</sub>O from electron microprobe analysis. Small amounts of Mg ignored; no attempt was made to distinguish Ca and Na; partial substitution of Na for H<sub>2</sub>O could not be excluded. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gualtieri A., Artioli G., Passaglia E., Bigi S., Viani A., Hanson J.C. (1998), Am. Mineral. 83, 590-606.

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hP232

Li <sub>18.8</sub> Ni <sub>5.1</sub> Si <sub>32.4</sub>	hP232	(194) P6 <sub>3</sub> /mmc – 1 <sup>3</sup> k <sup>9</sup> j <sup>2</sup> h <sup>2</sup> t <sup>3</sup> e
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**Li<sub>77-x</sub>Ni<sub>20</sub>Si<sub>135-y</sub>** [1]

Structural features: 3D-framework with Ni and Si mainly in icosahedral (or 11-vertex) coordination.

Pavlyuk V.V. et al. (1991) [1]

Li<sub>18.75</sub>Ni<sub>5.07</sub>Si<sub>32.42</sub>

*a* = 1.287, *c* = 2.1446 nm, *c/a* = 1.666, *V* = 3.0763 nm<sup>3</sup>, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	24l	1	0.017	0.3477	0.1937		11-vertex polyhedron Si <sub>5</sub> NiLi <sub>5</sub>
Li2	24l	1	0.042	0.333	0.064		16-vertex Frank-Kasper Si <sub>9</sub> Li <sub>6</sub> Ni
Si3	24l	1	0.4825	0.1474	0.1341		icosahedron Si <sub>4</sub> Li <sub>8</sub>
M4	12k	.m.	0.06065	0.1213	0.0765		11-vertex polyhedron Si <sub>6</sub> Li <sub>5</sub>
M5	12k	.m.	0.10685	0.2137	0.5216		11-vertex polyhedron Si <sub>6</sub> Li <sub>5</sub>
Si6	12k	.m.	0.12435	0.2487	0.1616		11-vertex polyhedron Si <sub>5</sub> NiLi <sub>5</sub>
Li7	12k	.m.	0.129	0.258	0.643		16-vertex Frank-Kasper Si <sub>12</sub> Li <sub>4</sub>
M8	12k	.m.	0.21155	0.4231	0.5427		icosahedron Si <sub>4</sub> Li <sub>8</sub>
M9	12k	.m.	0.2291	0.4582	0.1528		11-vertex polyhedron Si <sub>7</sub> Li <sub>4</sub>
Si10	12k	.m.	0.2679	0.5358	0.0501		icosahedron Si <sub>4</sub> NiLi <sub>7</sub>
Li11	12k	.m.	0.545	0.09	0.624		16-vertex Frank-Kasper Ni <sub>2</sub> Si <sub>9</sub> Li <sub>5</sub>
M12	12k	.m.	0.5557	0.1114	0.0231		14-vertex Frank-Kasper Si <sub>6</sub> Li <sub>8</sub>
Si13	12j	m..	0.1721	0.5001	<sup>1</sup> / <sub>4</sub>	0.58	pentagonal pyramid Si <sub>4</sub> Ni <sub>2</sub>
M14	12j	m..	0.1843	0.0016	<sup>1</sup> / <sub>4</sub>		11-vertex polyhedron Si <sub>6</sub> Li <sub>5</sub>
Li15	6h	mm2	0.546	0.092	<sup>1</sup> / <sub>4</sub>		16-vertex Frank-Kasper Si <sub>10</sub> Li <sub>6</sub>
Li16	6h	mm2	0.796	0.592	<sup>1</sup> / <sub>4</sub>		16-vertex Frank-Kasper Si <sub>10</sub> Li <sub>6</sub>
Si17	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1581		15-vertex polyhedron Ni <sub>3</sub> Si <sub>9</sub> Li <sub>3</sub>
Li18	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.568	0.5	16-vertex Frank-Kasper Li <sub>4</sub> Si <sub>12</sub>

M19	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6866	14-vertex Frank-Kasper $\text{Li}_8\text{Si}_6$
Li20	4e	3m.	0	0	0.183	16-vertex Frank-Kasper $\text{Si}_{12}\text{Li}_4$

M4 = 0.83Si + 0.17Ni; M5 = 0.87Si + 0.13Ni; M8 = 0.61Si + 0.39Ni; M9 = 0.68Ni + 0.32Si; M12 = 0.57Li + 0.43Si; M14 = 0.68Si + 0.32Ni; M19 = 0.54Li + 0.46Si

Experimental: single crystal, diffractometer, X-rays, R = 0.049

References: [1] Pavlyuk V.V., Bodak O.I., Sobolev A.N. (1991), Sov. Phys. Crystallogr. 36, 494-496 (Kristallografiya 36, 883-886).

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hP234

$\text{H}_2\text{Rb}_4\text{W}_{21}\text{As}_2\text{O}_{69}[\text{H}_2\text{O}]_{35}$	hP234	(194) $P6_3/mmc - I^{4k^7}jh^6fd$
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# **$\text{Rb}_4\text{H}_2[\text{As}_2\text{W}_{21}\text{O}_{69}(\text{H}_2\text{O})]\cdot 34\text{H}_2\text{O}$ [1]**

Structural features:  $\text{As}_2\text{W}_{21}\text{O}_{69}(\text{H}_2\text{O})$  units (two partial Keggin units consisting of nine edge- and vertex-linked  $\text{WO}_6$  octahedra sharing vertices with an  $\text{AsO}_3$   $\psi$ -tetrahedron are interconnected via common vertices with two  $\text{WO}_5$  square pyramids and one  $\text{W}[\text{O}_5(\text{OH}_2)]$  octahedron in statistical disorder) in a Mg-type (h.c.p.) arrangement; Rb,  $\text{H}_3\text{O}$  and additional  $\text{H}_2\text{O}$  between the units.

Jeannin Y., Martin Frère J. (1981) [1]

$\text{As}_2\text{H}_{35}\text{O}_{86}\text{Rb}_3\text{W}_{21}$

$a = 1.6926$ ,  $c = 1.8767$  nm,  $c/a = 1.109$ ,  $V = 4.6562$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.034	0.358	0.09		single atom W
W2	24l	1	0.1213	0.4618	0.083		octahedron $\text{O}_6$
O3	24l	1	0.168	0.49	0.178		
O4	24l	1	0.479	0.115	0.017		non-collinear $\text{W}_2$
$(\text{OH}_2)_5$	12k	.m.	0.173	0.346	0.591		non-coplanar square $\text{O}_4$
O6	12k	.m.	0.219	0.438	0.063		non-collinear $\text{W}_2$
O7	12k	.m.	0.532	0.064	0.602		non-collinear $\text{W}_2$
O8	12k	.m.	0.571	0.142	0.154		single atom W
W9	12k	.m.	0.5941	0.1882	0.0627		octahedron $\text{O}_6$
O10	12k	.m.	0.613	0.226	0.564		single atom As
O11	12k	.m.	0.719	0.438	0.07		non-collinear $\text{W}_2$
$(\text{OH}_2)_{12}$	12j	m..	0.364	0.052	$\frac{1}{4}$		non-collinear $\text{Rb}(\text{OH}_2)$
O13	6h	mm2	0.176	0.352	$\frac{1}{4}$		single atom W
W14	6h	mm2	0.23	0.46	$\frac{1}{4}$	0.667	
W15	6h	mm2	0.2489	0.4978	$\frac{1}{4}$	0.333	
$(\text{OH}_2)_{16}$	6h	mm2	0.304	0.608	$\frac{1}{4}$	0.333	coplanar triangle $(\text{OH}_2)_2\text{W}$
Rb17	6h	mm2	0.497	0.994	$\frac{1}{4}$		bicapped square prism $\text{O}_8(\text{OH}_2)_2$
$(\text{OH}_2)_{18}$	6h	mm2	0.753	0.506	$\frac{1}{4}$		single atom $(\text{OH}_3)$
As19	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1064		non-coplanar triangle $\text{O}_3$
$(\text{OH}_3)_{20}$	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		coplanar triangle $(\text{OH}_2)_3$

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

Remarks: Part of Rb and  $\text{H}_2\text{O}$  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. In table III of [1] the z-coordinate of former O(12) is misprinted as 0.017 instead of -0.017 (checked on interatomic distances).

References: [1] Jeannin Y., Martin Frère J. (1981), J. Am. Chem. Soc. 103, 1664-1667.

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hP246

$\text{Fe}_{23}\text{Al}_{81}\text{Si}_{15}$	<i>hP246</i>	(194) $P6_3/mmc - I^2K^{12}Ih^6fc$
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**(AlFeSi)  $\alpha$  [1]**Structural features:  $\text{Fe}(\text{Al},\text{Si})_n$  polyhedra ( $n = 9-12$ ) share atoms to form a dense 3D-framework.

Corby R.N., Black P.J. (1977) [1]

 $\text{Al}_{81.02}\text{Fe}_{23}\text{Si}_{15}$  $a = 1.2404$ ,  $c = 2.6234$  nm,  $c/a = 2.115$ ,  $V = 3.4956$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Al1	24l	1	0.011	0.3425	0.198		
Al2	24l	1	0.3467	0.0561	0.1027		pseudo Frank-Kasper $\text{Fe}_3\text{Al}_8\text{Si}_2$
Si3	12k	.m.	0.0693	0.1386	0.0766		11-vertex polyhedron $\text{FeSi}_2\text{Al}_8$
Al4	12k	.m.	0.0835	0.167	0.6681		tricapped pentagonal prism $\text{Fe}_2\text{Si}_3\text{Al}_8$
Al5	12k	.m.	0.1105	0.221	0.5176		11-vertex polyhedron $\text{FeAl}_7\text{Si}_3$
Fe6	12k	.m.	0.1305	0.261	0.1503		pseudo Frank-Kasper $\text{SiAl}_9\text{Fe}$
Al7	12k	.m.	0.2025	0.405	0.0683		14-vertex Frank-Kasper $\text{Fe}_3\text{Al}_{10}\text{Si}$
Fe8	12k	.m.	0.216	0.432	0.5307		10-vertex polyhedron $\text{Al}_8\text{Si}_2$
Al9	12k	.m.	0.2513	0.5026	0.6737		tricapped pentagonal prism $\text{Fe}_2\text{Al}_8\text{Si}_3$
Al10	12k	.m.	0.2521	0.5042	0.1652		
Fe11	12k	.m.	0.5406	0.0812	0.1601		tricapped trigonal prism $\text{Al}_8\text{Si}$
Al12	12k	.m.	0.5467	0.0934	0.6063		14-vertex Frank-Kasper $\text{Fe}_2\text{Al}_{11}\text{Si}$
Al13	12k	.m.	0.5959	0.1918	0.5169		pseudo Frank-Kasper $\text{Fe}_3\text{Al}_7\text{Si}$
Si14	12k	.m.	0.5968	0.1936	0.0814		pseudo Frank-Kasper $\text{Fe}_3\text{Al}_8\text{Si}_2$
Al15	12i	.2.	0.3726	0	0		15-vertex Frank-Kasper $\text{Fe}_2\text{Al}_{11}\text{Si}_2$
Al16	6h	mm2	0.0921	0.1842	$\frac{1}{4}$	0.93	15-vertex Frank-Kasper $\text{Fe}_3\text{Al}_{10}\text{Si}_2$
Fe17	6h	mm2	0.2084	0.4168	$\frac{1}{4}$		
Al18	6h	mm2	0.4195	0.839	$\frac{1}{4}$	0.32	
Al19	6h	mm2	0.4423	0.8846	$\frac{1}{4}$	0.66	
Al20	6h	mm2	0.573	0.146	$\frac{1}{4}$		
Si21	6h	mm2	0.8384	0.6768	$\frac{1}{4}$		icosahedron $\text{Al}_{12}$
Fe22	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0995		icosahedron $\text{Al}_{12}$
Al23	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.29	coplanar triangle $\text{Al}_3$

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

Remarks: Composition  $\text{Fe}_{44.9}\text{Al}_{167.8}\text{Si}_{23.9}$  from chemical analysis. Refinement using scattering factors for Fe and Al; the authors conclude that sites with  $\text{occ}(\text{Al}) > 1$  are occupied by Si. We ignored partial vacancies smaller than 4 %. Short interatomic distances for partly occupied site(s). Preliminary data in [2]. In table 1 of [1] the  $y$ -coordinate of former Al(13) is misprinted as 0.1976 instead of 0.1936 (checked on interatomic distances) and the Wyckoff position of former Al(22) as 5h instead of 6h.

References: [1] Corby R.N., Black P.J. (1977), Acta Crystallogr. B 33, 3468-3475. [2] Robinson K., Black P.J. (1953), Philos. Mag. 44, 1392-1397.

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hP248

$\text{Mg}_{30}\text{Zn}_{81}\text{Sm}_{13}$	<i>hP248</i>	(194) $P6_3/mmc - I^2K^6J^6Ih^4fda$
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 **$\text{Mg}_{30}\text{Zn}_{81}\text{Sm}_{13}$  [1]**

Structural features: Two kinds of Laves-type column parallel to [001].

Abe E. et al. (1999) [1]

 $\text{Mg}_{30}\text{Sm}_{13}\text{Zn}_{81}$  $a = 2.35$ ,  $c = 0.86$  nm,  $c/a = 0.366$ ,  $V = 4.1131$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	24l	1	0.1703	0.4729	0.1055		4-vertex polyhedron $\text{Zn}_2\text{SmMg}$
Zn2	24l	1	0.3384	0.0734	0.1019		icosahedron $\text{Zn}_7\text{Mg}_2\text{Sm}_3$
Mg3	12k	.m.	0.0749	0.1498	0.5697		16-vertex Frank-Kasper $\text{Mg}_4\text{Zn}_{12}$
Mg4	12k	.m.	0.1387	0.2774	0.0463		14-vertex Frank-Kasper $\text{Zn}_9\text{Mg}_2\text{Sm}_3$
Zn5	12k	.m.	0.201	0.402	0.1066		tetrahedron $\text{Mg}_3\text{Zn}$
Zn6	12k	.m.	0.265	0.53	0.5856		icosahedron $\text{Zn}_7\text{Mg}_2\text{Sm}_3$
Mg7	12k	.m.	0.538	0.076	0.0657		16-vertex Frank-Kasper $\text{Zn}_{12}\text{Mg}_4$
Zn8	12k	.m.	0.6067	0.2134	0.0		icosahedron $\text{Zn}_6\text{Mg}_3\text{Sm}_3$
Zn9	12j	m..	0.0317	0.1794	$\frac{1}{4}$		icosahedron $\text{Zn}_5\text{Mg}_6\text{Sm}$
Zn10	12j	m..	0.0439	0.4565	$\frac{1}{4}$		icosahedron $\text{Zn}_5\text{SmMg}_6$
Sm11	12j	m..	0.0556	0.3343	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Zn}_{14}\text{Mg}_4$
Zn12	12j	m..	0.248	0.074	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn13	12j	m..	0.431	0.074	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn14	12j	m..	0.54	0.181	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn15	12i	.2.	0.2158	0	0		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn16	12i	.2.	0.39	0	0		icosahedron $\text{Zn}_6\text{Mg}_4\text{Sm}_2$
Zn17	6h	mm2	0.035	0.07	$\frac{1}{4}$		icosahedron $\text{Zn}_6\text{Mg}_6$
Sm18	6h	mm2	0.265	0.53	$\frac{1}{4}$		non-coplanar square $\text{Mg}_4$
Zn19	6h	mm2	0.43	0.86	$\frac{1}{4}$		icosahedron $\text{Zn}_4\text{Mg}_6\text{Sm}_2$
Sm20	6h	mm2	0.8	0.6	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Zn}_{14}\text{Mg}_6$
Zn21	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1019		pseudo Frank-Kasper $\text{Zn}_7\text{Sm}_4$
Sm22	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		pseudo Frank-Kasper $\text{Zn}_{20}$
Zn23	2a	-3m.	0	0	0		icosahedron $\text{Zn}_6\text{Mg}_6$

Experimental: polycrystalline sample, electron diffraction

Remarks: Short interatomic distances:  $d(\text{Mg1-Sm18}) = 0.230$  nm.

References: [1] Abe E., Takakura H., Singh A., Tsai A.P. (1999), J. Alloys Compd. 283, 169-172.

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hP260 $\text{H}_2\text{K}_4\text{W}_{21}\text{P}_2\text{O}_{71}[\text{H}_2\text{O}]_{31}$ 

hP260

(194)  $P6_3/mmc - 1^5k^7jh^6f^2$  $\text{K}_4\text{H}_2[\text{P}_2\text{W}_{21}\text{O}_{71}(\text{OH}_2)_3] \cdot 28\text{H}_2\text{O}$  [1]

Structural features:  $\text{P}_2\text{W}_{21}\text{O}_{72}(\text{OH}_2)_2$  units (two partial Keggin units consisting of nine edge- and vertex-linked  $\text{WO}_6$  octahedra sharing vertices with a  $\text{PO}_4$  tetrahedron are interconnected via an additional  $\text{WO}_6$  octahedron and two  $\text{W}[\text{O}_5(\text{OH}_2)]$  octahedra in statistical disorder) in a Mg-type (h.c.p.) arrangement; K,  $\text{H}_3\text{O}$  and additional  $\text{H}_2\text{O}$  between the units.

Tourné C.M. et al. (1986) [1]

 $\text{H}_{48}\text{K}_3\text{O}_{95}\text{P}_2\text{W}_{21}$  $a = 1.6295$ ,  $c = 1.9771$  nm,  $c/a = 1.213$ ,  $V = 4.5464$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.0106	0.3561	0.0777		single atom W
W2	24l	1	0.12095	0.44774	0.08845		octahedron $\text{O}_6$
O3	24l	1	0.1349	0.4326	0.1824		
(OH <sub>2</sub> )4	24l	1	0.4021	0.0903	0.1899		single atom (OH <sub>2</sub> )

O5	24l	1	0.4963	0.1501	0.0014	non-colinear W <sub>2</sub>
(OH <sub>2</sub> )6	12k	.m.	0.1679	0.3358	0.5886	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O7	12k	.m.	0.1927	0.3854	0.0701	non-colinear W <sub>2</sub>
O8	12k	.m.	0.2821	0.5642	0.1068	single atom P
O9	12k	.m.	0.5501	0.1002	0.6101	non-colinear W <sub>2</sub>
O10	12k	.m.	0.5561	0.1122	0.1302	single atom W
W11	12k	.m.	0.59707	0.19414	0.06507	octahedron O <sub>6</sub>
O12	12k	.m.	0.721	0.442	0.1042	non-colinear W <sub>2</sub>
O13	12j	m..	0.2636	0.5728	<sup>1</sup> / <sub>4</sub>	0.333
M14	6h	mm2	0.1448	0.2896	<sup>1</sup> / <sub>4</sub>	single atom W
W15	6h	mm2	0.20012	0.40024	<sup>1</sup> / <sub>4</sub>	0.333
W16	6h	mm2	0.22139	0.44278	<sup>1</sup> / <sub>4</sub>	0.667
(OH <sub>2</sub> )17	6h	mm2	0.2847	0.5694	<sup>1</sup> / <sub>4</sub>	0.333
K18	6h	mm2	0.4941	0.9881	<sup>1</sup> / <sub>4</sub>	hexagonal prism O <sub>8</sub> (OH <sub>2</sub> ) <sub>4</sub>
(OH <sub>2</sub> )19	6h	mm2	0.7265	0.453	<sup>1</sup> / <sub>4</sub>	8-vertex polyhedron O <sub>2</sub> (OH <sub>2</sub> ) <sub>6</sub>
O20	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0031	single atom P
P21	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0813	tetrahedron O <sub>4</sub>

M14 = 0.667OH<sub>2</sub> + 0.333O

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

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

Remarks: Part of K and H<sub>2</sub>O not located. [P<sub>2</sub>W<sub>21</sub>O<sub>71</sub>(OH<sub>2</sub>)<sub>3</sub>] units are considered in the chemical formula given above, however, [P<sub>2</sub>W<sub>21</sub>O<sub>72</sub>(OH<sub>2</sub>)<sub>2</sub>] units were found from the structure refinement and nuclear magnetic resonance. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the site labels O31i and O32i are interchanged (with respect to the list of interatomic distances and the description of the structure).

References: [1] Tourné C.M., Tourné G.F., Weakley T.J.R. (1986), J. Chem. Soc., Dalton Trans. 1986, 2237-2242.

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hP278

Li<sub>36.6</sub>Mg<sub>16.4</sub>Cu<sub>7.8</sub>Al<sub>75.2</sub>

hP278

(194) *P6<sub>3</sub>/mmc* – *I*<sup>3</sup>*k*<sup>12</sup>*j*<sup>1</sup>*h*<sup>3</sup>*f*<sup>3</sup>*e*<sup>2</sup>

**Li<sub>26</sub>Mg<sub>10</sub>Cu<sub>5</sub>Al<sub>59</sub>** [1]

Structural features: Half Samson polyhedra (Samson polyhedron: an icosahedron surrounded by a rhombic triacontahedron and a truncated icosahedron) are interconnected to form a dense 3D-framework.

Le Bail A. et al. (1991) [1]

Al<sub>75.25</sub>Cu<sub>7.75</sub>Li<sub>36.62</sub>Mg<sub>16.38</sub>

*a* = 1.4116, *c* = 2.8235 nm, *c/a* = 2.000, *V* = 4.8724 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24l	1	0.0008	0.3812	0.0963		16-vertex Frank-Kasper Li <sub>4</sub> Al <sub>10</sub> Mg <sub>2</sub>
M2	24l	1	0.02106	0.35629	0.20282		11-vertex polyhedron Al <sub>5</sub> Li <sub>5</sub> Mg
M3	24l	1	0.18824	0.00008	0.15467		icosahedron Al <sub>5</sub> MgLi <sub>6</sub>
M4	12k	.m.	0.0624	0.1248	0.50066	0.5	
Al5	12k	.m.	0.1204	0.2408	0.07231		
Al6	12k	.m.	0.1212	0.2424	0.57386		
M7	12k	.m.	0.2081	0.4162	0.6577		16-vertex Frank-Kasper Al <sub>12</sub> Li <sub>4</sub>
Li8	12k	.m.	0.211	0.422	0.1448		15-vertex Frank-Kasper Al <sub>11</sub> Li <sub>3</sub> Mg
M9	12k	.m.	0.22388	0.44776	0.04302		icosahedron Al <sub>4</sub> Li <sub>6</sub> Mg <sub>2</sub>
M10	12k	.m.	0.22499	0.44998	0.55005		icosahedron Al <sub>4</sub> Li <sub>6</sub> Mg <sub>2</sub>

M11	12k	.m.	0.54526	0.09052	0.17416	11-vertex polyhedron Al <sub>6</sub> Li <sub>5</sub>
Mg12	12k	.m.	0.5546	0.1092	0.00478	14-vertex Frank-Kasper MgLi <sub>7</sub> Al <sub>6</sub>
M13	12k	.m.	0.56143	0.12286	0.67286	11-vertex polyhedron Al <sub>3</sub> Li <sub>4</sub> Mg <sub>2</sub>
M14	12k	.m.	0.60147	0.20294	0.58816	icosahedron Al <sub>6</sub> MgLi <sub>5</sub>
M15	12k	.m.	0.60206	0.20412	0.09704	icosahedron Al <sub>5</sub> MgLi <sub>6</sub>
M16	12j	.m.	0.4844	0.15325	<sup>1</sup> / <sub>4</sub>	11-vertex polyhedron Al <sub>6</sub> Li <sub>5</sub>
M17	12i	.2.	0.2976	0	0	14-vertex polyhedron Li <sub>2</sub> Al <sub>10</sub> Mg <sub>2</sub>
Li18	6h	mm2	0.1204	0.2408	<sup>1</sup> / <sub>4</sub>	15-vertex Frank-Kasper Al <sub>8</sub> Li <sub>4</sub> Mg <sub>3</sub>
Mg19	6h	mm2	0.2521	0.5042	<sup>1</sup> / <sub>4</sub>	15-vertex polyhedron Al <sub>10</sub> Li <sub>3</sub> Mg <sub>2</sub>
Li20	6h	mm2	0.8697	0.7394	<sup>1</sup> / <sub>4</sub>	16-vertex Frank-Kasper Al <sub>10</sub> Li <sub>4</sub> Mg <sub>2</sub>
M21	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.17146	icosahedron Al <sub>6</sub> Mg <sub>3</sub> Li <sub>3</sub>
Li22	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5021	15-vertex Frank-Kasper Mg <sub>3</sub> Al <sub>12</sub>
M23	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6923	16-vertex Frank-Kasper Al <sub>12</sub> Li <sub>4</sub>
Li24	4e	3m.	0	0	0.0961	
Mg25	4e	3m.	0	0	0.2009	14-vertex Frank-Kasper MgLi <sub>7</sub> Al <sub>6</sub>

M1 = 0.66Li + 0.34Mg; M2 = 0.975Al + 0.025Cu; M3 = 0.975Al + 0.025Cu; M4 = 0.856Al + 0.144Cu; M7 = 0.93Li + 0.07Mg; M9 = 0.975Al + 0.025Cu; M10 = 0.975Al + 0.025Cu; M11 = 0.664Al + 0.336Cu; M13 = 0.761Al + 0.239Cu; M14 = 0.975Al + 0.025Cu; M15 = 0.877Al + 0.123Cu; M16 = 0.800Al + 0.200Cu; M17 = 0.91Li + 0.09Mg; M21 = 0.561Al + 0.439Cu; M23 = 0.83Li + 0.17Mg  
Experimental: single crystal, diffractometer, X-rays, R = 0.042

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

References: [1] Le Bail A., Leblanc M., Audier M. (1991), Acta Crystallogr. B 47, 451-457.

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hP300

K<sub>6.6</sub>Na<sub>5.4</sub>V<sub>3</sub>W<sub>18</sub>As<sub>2</sub>O<sub>69</sub>[H<sub>2</sub>O]<sub>29</sub> *hP300* (194) *P6<sub>3</sub>/mmc* – I<sup>4</sup>k<sup>12</sup>j<sup>13</sup>gf<sup>2</sup>ba

#### K<sub>6.6</sub>Na<sub>5.4</sub>[(VO)<sub>3</sub>(AsW<sub>9</sub>O<sub>33</sub>)<sub>2</sub>]·29H<sub>2</sub>O [1]

Structural features: As<sub>2</sub>V<sub>3</sub>W<sub>18</sub>O<sub>69</sub> units (two partial Keggin units consisting of nine edge- and vertex-linked WO<sub>6</sub> octahedra sharing vertices with an :AsO<sub>3</sub> ψ-tetrahedron are interconnected via common vertices with three VO<sub>5</sub> square pyramids) in a Mg-type (h.c.p.) arrangement; K, Na and H<sub>2</sub>O between the units.

Drewes D. et al. (2004) [1]

As<sub>2</sub>H<sub>58</sub>K<sub>6.60</sub>Na<sub>5.40</sub>O<sub>98</sub>V<sub>3</sub>W<sub>18</sub>

*a* = 1.5124, *c* = 2.4209 nm, *c/a* = 1.601, *V* = 4.7956 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
W1	24l	1	0.10514	0.43155	0.12472		octahedron O <sub>6</sub>
O2	24l	1	0.1217	0.421	0.0432		non-colinear W <sub>2</sub>
O3	24l	1	0.1369	0.4805	0.1953		non-colinear WV
O4	24l	1	0.3472	0.0158	0.1303		single atom W
(OH <sub>2</sub> )5	12k	.m.	0.0735	0.147	0.1166		non-colinear Na <sub>2</sub>
Na6	12k	.m.	0.0735	0.147	0.5586	0.4	
K7	12k	.m.	0.1226	0.2452	0.5911	0.6	
(OH <sub>2</sub> )8	12k	.m.	0.132	0.264	0.64	0.5	
O9	12k	.m.	0.1798	0.3596	0.1338		non-colinear W <sub>2</sub>
O10	12k	.m.	0.2253	0.4506	0.5548		single atom W
(OH <sub>2</sub> )11	12k	.m.	0.231	0.462	0.648	0.333	single atom O
W12	12k	.m.	0.25122	0.50244	0.00994		octahedron O <sub>6</sub>
O13	12k	.m.	0.274	0.548	0.1028		single atom As
O14	12k	.m.	0.5393	0.0786	0.6064		non-colinear W <sub>2</sub>

(OH <sub>2</sub> )15	12k	.m.	0.5849	0.1698	0.14	0.5	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
O16	12k	.m.	0.6085	0.217	0.5013		non-coplanar W <sub>2</sub>
(OH <sub>2</sub> )17	12j	m..	0.012	0.251	<sup>1</sup> / <sub>4</sub>		single atom Na
(OH <sub>2</sub> )18	12i	.2.	0.2212	0	0		non-coplanar Na <sub>2</sub>
Na19	6h	mm2	0.1879	0.3758	<sup>1</sup> / <sub>4</sub>		trigonal prism (OH <sub>2</sub> ) <sub>2</sub> O <sub>4</sub>
V20	6h	mm2	0.45227	0.90454	<sup>1</sup> / <sub>4</sub>		square pyramid O <sub>5</sub>
O21	6h	mm2	0.5132	0.0264	<sup>1</sup> / <sub>4</sub>		single atom V
K22	6g	.2/m.	<sup>1</sup> / <sub>2</sub>	0	0		square prism (cube) O <sub>8</sub>
As23	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1402		non-coplanar triangle O <sub>3</sub>
(OH <sub>2</sub> )24	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.612	0.5	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
(OH <sub>2</sub> )25	2b	-6m2	0	0	<sup>1</sup> / <sub>4</sub>		anticuboctahedron (OH <sub>2</sub> ) <sub>12</sub>
(OH <sub>2</sub> )26	2a	-3m.	0	0	0		octahedron Na <sub>6</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.063, T = 213 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Drewes D., Limanski E.M., Piepenbrink M., Krebs B. (2004), Z. Anorg. Allg. Chem. 630, 58-62.

194  
hP316

Na <sub>20</sub> (Al <sub>0.21</sub> Si <sub>0.79</sub> ) <sub>96</sub> O <sub>192</sub>	hP316	(194) P6 <sub>3</sub> /mmc – 1 <sup>8</sup> k <sup>8</sup> jif
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**Na<sub>20</sub>Al<sub>20</sub>Si<sub>76</sub>O<sub>192</sub>** [1], zeolite EMT-Na

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an EMT-type zeolite framework with puckered layers of β cages (14-face truncated octahedra) interconnected via double 6-rings (AB stacking) and channels delimited by 12-rings parallel and perpendicular to [001]; Na near the centers of 6-rings.

Yonkeu A.L. et al. (2001) [1]

Al<sub>20.16</sub>Na<sub>18</sub>O<sub>192</sub>Si<sub>75.84</sub>

*a* = 1.74426, *c* = 2.8446 nm, *c/a* = 1.631, *V* = 7.4950 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24l	1	0.069	0.43	0.108		non-coplanar Si <sub>2</sub>
O2	24l	1	0.126	0.456	0.018		non-coplanar Si <sub>2</sub>
M3	24l	1	0.151	0.484	0.072		tetrahedron O <sub>4</sub>
M4	24l	1	0.374	0.096	0.019		tetrahedron O <sub>4</sub>
O5	24l	1	0.405	0.093	0.071		non-coplanar Si <sub>2</sub>
M6	24l	1	0.428	0.039	0.109		tetrahedron O <sub>4</sub>
O7	24l	1	0.428	0.071	0.162		non-coplanar Si <sub>2</sub>
M8	24l	1	0.488	0.154	0.196		tetrahedron O <sub>4</sub>
O9	12k	.m.	0.17	0.34	0.516		non-coplanar Si <sub>2</sub>
Na10	12k	.m.	0.203	0.406	0.617	0.7	non-coplanar triangle O <sub>3</sub>
O11	12k	.m.	0.237	0.474	0.679		non-coplanar Si <sub>2</sub>
O12	12k	.m.	0.238	0.476	0.089		non-coplanar Si <sub>2</sub>
O13	12k	.m.	0.53	0.06	0.097		non-coplanar Si <sub>2</sub>
Na14	12k	.m.	0.555	0.11	0.014	0.6	non-coplanar O <sub>2</sub>
O15	12k	.m.	0.591	0.182	0.576		non-coplanar Si <sub>2</sub>
O16	12k	.m.	0.592	0.184	0.193		non-coplanar Si <sub>2</sub>
O17	12j	m..	0.453	0.127	<sup>1</sup> / <sub>4</sub>		non-coplanar Si <sub>2</sub>
O18	12i	.2.	0.293	0	0		non-coplanar Si <sub>2</sub>

Na19    4f   3m.     $\frac{1}{3}$      $\frac{2}{3}$     0.103    0.6    non-coplanar triangle O<sub>3</sub>

M3 = 0.79Si + 0.21Al; M4 = 0.79Si + 0.21Al; M6 = 0.79Si + 0.21Al; M8 = 0.79Si + 0.21Al

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.022

References: [1] Yonkeu A.L., Buschmann V., Mieh G., Fuess H., Goossens A.M., Martens J.A. (2001), Cryst. Eng. 4, 253-267.

194  
hP320

Na<sub>20</sub>(Al<sub>0.21</sub>Si<sub>0.79</sub>)<sub>96</sub>O<sub>192</sub>

hP320

(194) P6<sub>3</sub>/mmc – 1<sup>8</sup>k<sup>8</sup>jif<sup>2</sup>

Na<sub>20</sub>Al<sub>20</sub>Si<sub>76</sub>O<sub>192</sub> [1], zeolite EMT-Na

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an EMT-type zeolite framework with puckered layers of β cages (14-face truncated octahedra) interconnected via double 6-rings (AB stacking) and channels delimited by 12-rings parallel and perpendicular to [001]; Na near the centers of β cages and near the centers of 6-rings.

Yonkeu A.L. et al. (2001) [1]

Al<sub>20.16</sub>Na<sub>20.24</sub>O<sub>192</sub>Si<sub>75.84</sub>

a = 1.745, c = 2.8453 nm, c/a = 1.631, V = 7.5032 nm<sup>3</sup>, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.039	0.427	0.105		tetrahedron O <sub>4</sub>
O2	24l	1	0.07	0.417	0.159		non-colinear Si <sub>2</sub>
O3	24l	1	0.098	0.4	0.072		non-colinear Si <sub>2</sub>
M4	24l	1	0.102	0.384	0.017		tetrahedron O <sub>4</sub>
M5	24l	1	0.15	0.482	0.1953		tetrahedron O <sub>4</sub>
O6	24l	1	0.433	0.073	0.104		non-colinear Si <sub>2</sub>
O7	24l	1	0.471	0.134	0.018		non-colinear Si <sub>2</sub>
M8	24l	1	0.496	0.162	0.073		tetrahedron O <sub>4</sub>
O9	12k	.m.	0.175	0.35	0.008		non-colinear Si <sub>2</sub>
Na10	12k	.m.	0.191	0.382	0.121	0.62	non-coplanar triangle O <sub>3</sub>
O11	12k	.m.	0.235	0.47	0.594		non-colinear Si <sub>2</sub>
O12	12k	.m.	0.245	0.49	0.179		non-colinear Si <sub>2</sub>
O13	12k	.m.	0.534	0.068	0.597		non-colinear Si <sub>2</sub>
O14	12k	.m.	0.579	0.158	0.688		non-colinear Si <sub>2</sub>
Na15	12k	.m.	0.584	0.168	0.529	0.85	non-coplanar triangle O <sub>3</sub>
O16	12k	.m.	0.605	0.21	0.078		non-colinear Si <sub>2</sub>
O17	12j	m..	0.127	0.452	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O18	12i	.2.	0.306	0	0		non-colinear Si <sub>2</sub>
Na19	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.077	0.32	tetrahedron Na <sub>4</sub>
Na20	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.179	0.33	7-vertex polyhedron O <sub>6</sub> Na

M1 = 0.79Si + 0.21Al; M4 = 0.79Si + 0.21Al; M5 = 0.79Si + 0.21Al; M8 = 0.79Si + 0.21Al

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

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.048

References: [1] Yonkeu A.L., Buschmann V., Mieh G., Fuess H., Goossens A.M., Martens J.A. (2001), Cryst. Eng. 4, 253-267.

194  
hP326

Na<sub>22</sub>(Al<sub>0.23</sub>Si<sub>0.77</sub>)<sub>96</sub>O<sub>192</sub>

hP326

(194) P6<sub>3</sub>/mmc – 1<sup>8</sup>k<sup>8</sup>jigf<sup>2</sup>



**Na<sub>22</sub>Al<sub>22</sub>Si<sub>74</sub>O<sub>192</sub>** [1], zeolite EMT-Na

Structural features: (Si,Al)O<sub>4</sub> tetrahedra share vertices to form an EMT-type zeolite framework with puckered layers of  $\beta$  cages (14-face truncated octahedra) interconnected via double 6-rings (AB stacking) and channels delimited by 12-rings parallel and perpendicular to [001]; Na between double 6-rings and near the centers of 6-rings.

Lievens J.L. et al. (1992) [1]

Al<sub>22.08</sub>Na<sub>18.76</sub>O<sub>192</sub>Si<sub>73.92</sub>

$a = 1.74489$  nm,  $c/a = 1.631$ ,  $V = 7.5029$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	24l	1	0.033	0.429	0.106		tetrahedron O <sub>4</sub>
O2	24l	1	0.078	0.426	0.161		non-colinear Si <sub>2</sub>
O3	24l	1	0.093	0.404	0.073		non-colinear Si <sub>2</sub>
M4	24l	1	0.097	0.372	0.016		tetrahedron O <sub>4</sub>
M5	24l	1	0.156	0.49	0.194		tetrahedron O <sub>4</sub>
O6	24l	1	0.429	0.074	0.102		non-colinear Si <sub>2</sub>
O7	24l	1	0.463	0.128	0.015		non-colinear Si <sub>2</sub>
M8	24l	1	0.492	0.157	0.072		tetrahedron O <sub>4</sub>
O9	12k	.m.	0.165	0.33	0.02		non-colinear Si <sub>2</sub>
Na10	12k	.m.	0.183	0.366	0.122	0.5	non-coplanar triangle O <sub>3</sub>
O11	12k	.m.	0.237	0.474	0.583		non-colinear Si <sub>2</sub>
O12	12k	.m.	0.246	0.492	0.18		non-colinear Si <sub>2</sub>
O13	12k	.m.	0.525	0.05	0.599		non-colinear Si <sub>2</sub>
O14	12k	.m.	0.589	0.178	0.692		non-colinear Si <sub>2</sub>
O15	12k	.m.	0.605	0.21	0.076		non-coplanar triangle Si <sub>2</sub> Na
Na16	12k	.m.	0.611	0.222	0.531	0.37	non-colinear O <sub>2</sub>
O17	12j	m..	0.115	0.451	$\frac{1}{4}$		non-colinear Si <sub>2</sub>
O18	12i	.2.	0.276	0	0		non-colinear Si <sub>2</sub>
Na19	6g	.2/m.	$\frac{1}{2}$	0	0	0.24	octahedron O <sub>6</sub>
Na20	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.164		non-coplanar triangle O <sub>3</sub>
Na21	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6	0.72	non-coplanar triangle O <sub>3</sub>

M1 = 0.77Si + 0.23Al; M4 = 0.77Si + 0.23Al; M5 = 0.77Si + 0.23Al; M8 = 0.77Si + 0.23Al

Experimental: powder, diffractometer, X-rays,  $R_B = 0.049$ ,  $T = 723$  K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. In table 1b of [1] the  $z$ -coordinate of former M1'b is misprinted as -0.164 instead of 0.164 (checked on interatomic distances).

References: [1] Lievens J.L., Verduijn J.P., Bons A.J., Mortier W.J. (1992), Zeolites 12, 698-705.

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hP456

Na <sub>96</sub> Ni <sub>2</sub> In <sub>97</sub>	hP456	(194) $P6_3/mmc - 1^7k^{19}jh^3f^4e^2dca$
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**Na<sub>96</sub>In<sub>97</sub>Ni<sub>2</sub>** [1]; Na<sub>96</sub>In<sub>97</sub>Pd<sub>2</sub> [1]

Structural features: NiIn<sub>84</sub>Na<sub>39</sub> units (a central Ni atom surrounded by an In<sub>10</sub> polyhedron in partial disorder, a Na<sub>39</sub> polyhedron and an In<sub>74</sub> cage with 12 pentagonal and 24 hexagonal faces) and NiIn<sub>58</sub>Na<sub>44</sub> units (a central Ni atom surrounded by an In<sub>10</sub> polyhedron, a Na<sub>32</sub> polyhedron and an In<sub>48</sub>Na<sub>12</sub> fullerene-like cage) in a NiAs-type arrangement (common atoms).

Sevov S.C., Corbett J.D. (1993) [1]

In<sub>97.04</sub>Na<sub>96</sub>Ni<sub>2</sub>

$a = 1.5969$  nm,  $c/a = 2.968$ ,  $V = 10.4658$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	24l	1	0.008	0.388	0.1859		
In2	24l	1	0.1424	0.4765	0.07721		icosahedron In <sub>4</sub> Na <sub>8</sub>
In3	24l	1	0.175	0.0331	0.0151	0.478	non-colinear In <sub>2</sub>
In4	24l	1	0.1916	0.0013	0.14958		icosahedron In <sub>4</sub> Na <sub>8</sub>
Na5	24l	1	0.3383	0.0485	0.0418		single atom In
In6	24l	1	0.3555	0.0244	0.11507		icosahedron In <sub>4</sub> Na <sub>8</sub>
In7	24l	1	0.558	0.1646	0.2198	0.363	
In8	12k	.m.	0.034	0.068	0.5511	0.195	
In9	12k	.m.	0.0634	0.1268	0.0438	0.546	
Na10	12k	.m.	0.1108	0.2216	0.5897		single atom In
Na11	12k	.m.	0.1156	0.2312	0.7107		
In12	12k	.m.	0.12711	0.25422	0.20015		icosahedron In <sub>4</sub> Na <sub>8</sub>
Na13	12k	.m.	0.133	0.266	0.0888		single atom In
Na14	12k	.m.	0.1902	0.3804	0.0214		
Na15	12k	.m.	0.2033	0.4066	0.6625		
Na16	12k	.m.	0.2104	0.4208	0.1441		16-vertex Frank-Kasper Na <sub>4</sub> In <sub>12</sub>
In17	12k	.m.	0.22703	0.45406	0.59284		icosahedron In <sub>4</sub> Na <sub>8</sub>
In18	12k	.m.	0.22792	0.45584	0.21841		icosahedron In <sub>4</sub> Na <sub>8</sub>
In19	12k	.m.	0.2318	0.4636	0.7394	0.455	
In20	12k	.m.	0.26845	0.5369	0.53139		icosahedron In <sub>4</sub> Na <sub>8</sub>
In21	12k	.m.	0.3982	0.7964	0.18408		icosahedron In <sub>5</sub> Na <sub>7</sub>
In22	12k	.m.	0.54067	0.08134	0.6317		icosahedron In <sub>5</sub> Na <sub>7</sub>
Na23	12k	.m.	0.5426	0.0852	0.0708		15-vertex Frank-Kasper Na <sub>5</sub> In <sub>10</sub>
Na24	12k	.m.	0.5582	0.1164	0.5131		14-vertex Frank-Kasper Na <sub>10</sub> In <sub>4</sub>
Na25	12k	.m.	0.5855	0.171	0.1403		
In26	12k	.m.	0.6119	0.2238	0.2036	0.278	
Na27	12j	m..	0.015	0.309	$\frac{1}{4}$		
In28	6h	mm2	0.0637	0.1275	$\frac{1}{4}$		icosahedron In <sub>4</sub> Na <sub>8</sub>
Na29	6h	mm2	0.4541	0.9082	$\frac{1}{4}$		
In30	6h	mm2	0.562	0.124	$\frac{1}{4}$	0.08	
Na31	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0437		16-vertex Frank-Kasper Na <sub>7</sub> In <sub>9</sub>
Na32	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.1183		16-vertex Frank-Kasper Na <sub>4</sub> In <sub>12</sub>
In33	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.58673		icosahedron In <sub>6</sub> Na <sub>6</sub>
In34	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6923	0.43	
Na35	4e	3m.	0	0	0.1156		
Na36	4e	3m.	0	0	0.187		16-vertex Frank-Kasper Na <sub>4</sub> In <sub>12</sub>
Ni37	2d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{4}$		
Na38	2c	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		15-vertex Frank-Kasper In <sub>12</sub> Na <sub>3</sub>
Ni39	2a	-3m.	0	0	0		

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

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Slightly different partly occupied sites are reported for Na<sub>96</sub>In<sub>97</sub>Pd<sub>2</sub>. In the data deposited for Na<sub>96</sub>In<sub>97</sub>Pd<sub>2</sub> the Wyckoff position of Na(4) is misprinted as 12k instead of 24l.

References: [1] Sevov S.C., Corbett J.D. (1993), Science (Washington D.C.) 262, 880-883.

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hP480

Mg<sub>58.0</sub>Zn<sub>155.4</sub>Sm<sub>26.6</sub>

hP480

(194)  $P6_3/mmc - I^6k^9j^{12}i^3h^7fa$

**Mg<sub>24.2</sub>Zn<sub>64.7</sub>Sm<sub>11.1</sub>** [1]

Structural features: Columns of Zn-centered icosahedra are intergrown to form a dense 3D-framework.

Sugiyama K. et al. (1999) [1]

Mg<sub>58.01</sub>Sm<sub>26.61</sub>Zn<sub>155.38</sub> $a = 3.3565$ ,  $c = 0.8873$  nm,  $c/a = 0.264$ ,  $V = 8.6571$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Mg1	24l	1	0.0989	0.4803	0.0432		14-vertex Frank-Kasper Zn <sub>9</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Mg2	24l	1	0.0997	0.337	0.0437		14-vertex Frank-Kasper Zn <sub>9</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Zn3	24l	1	0.1543	0.436	0.0009		icosahedron Zn <sub>6</sub> Mg <sub>3</sub> Sm <sub>3</sub>
Zn4	24l	1	0.24488	0.05372	0.0847		icosahedron Zn <sub>7</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Mg5	24l	1	0.3821	0.0477	0.0699		16-vertex Frank-Kasper Mg <sub>4</sub> Zn <sub>12</sub>
Zn6	24l	1	0.52535	0.1921	0.0861		icosahedron Zn <sub>7</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Mg7	12k	.m.	0.0511	0.1022	0.5656		16-vertex Frank-Kasper Mg <sub>4</sub> Zn <sub>12</sub>
Mg8	12k	.m.	0.0977	0.1954	0.0463		bicapped square prism Zn <sub>9</sub> Mg
Zn9	12k	.m.	0.14507	0.29014	0.1055		pseudo Frank-Kasper Zn <sub>4</sub> Mg <sub>3</sub> Sm <sub>4</sub>
Zn10	12k	.m.	0.19184	0.38368	0.5656		icosahedron Zn <sub>7</sub> Sm <sub>3</sub> Mg <sub>2</sub>
Zn11	12k	.m.	0.23954	0.47908	0.0875		pseudo Frank-Kasper Zn <sub>7</sub> Sm <sub>4</sub>
Zn12	12k	.m.	0.28192	0.56384	0.002		icosahedron Zn <sub>6</sub> Mg <sub>3</sub> Sm <sub>3</sub>
Zn13	12k	.m.	0.52651	0.05302	0.0848		icosahedron Zn <sub>7</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Zn14	12k	.m.	0.5721	0.1442	0.6046		pseudo Frank-Kasper Zn <sub>4</sub> Mg <sub>3</sub> Sm <sub>4</sub>
Mg15	12k	.m.	0.6181	0.2362	0.5409		14-vertex Frank-Kasper Zn <sub>9</sub> Mg <sub>2</sub> Sm <sub>3</sub>
Zn16	12j	m..	0.02838	0.13408	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>5</sub> Mg <sub>6</sub> Sm
Zn17	12j	m..	0.0293	0.3334	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>5</sub> Mg <sub>6</sub> Sm
Zn18	12j	m..	0.0293	0.414	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>5</sub> Mg <sub>6</sub> Sm
Sm19	12j	m..	0.04039	0.23856	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>14</sub> Mg <sub>4</sub>
Zn20	12j	m..	0.1091	0.4134	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>4</sub> Mg <sub>6</sub> Sm <sub>2</sub>
Zn21	12j	m..	0.17899	0.05184	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Sm22	12j	m..	0.1949	0.52297	<sup>1</sup> / <sub>4</sub>		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
Zn23	12j	m..	0.30811	0.05111	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn24	12j	m..	0.38397	0.12697	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn25	12j	m..	0.46096	0.05117	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn26	12j	m..	0.46101	0.12708	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn27	12j	m..	0.59013	0.25643	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn28	12i	.2.	0.15562	0	0		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn29	12i	.2.	0.2806	0	0		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
Zn30	12i	.2.	0.43716	0	0		icosahedron Zn <sub>6</sub> Mg <sub>4</sub> Sm <sub>2</sub>
M31	6h	mm2	0.02707	0.05414	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>
Sm32	6h	mm2	0.19535	0.3907	<sup>1</sup> / <sub>4</sub>		16-vertex Frank-Kasper Zn <sub>12</sub> Mg <sub>4</sub>
M33	6h	mm2	0.30547	0.61094	<sup>1</sup> / <sub>4</sub>		icosahedron Zn <sub>4</sub> Mg <sub>6</sub> Sm <sub>2</sub>
Sm34	6h	mm2	0.47939	0.95878	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>14</sub> Mg <sub>4</sub>
Sm35	6h	mm2	0.57302	0.14604	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>14</sub> Mg <sub>6</sub>
Sm36	6h	mm2	0.76108	0.52216	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>20</sub>
M37	6h	mm2	0.85425	0.7085	<sup>1</sup> / <sub>4</sub>		pseudo Frank-Kasper Zn <sub>14</sub> Mg <sub>6</sub>
Mg38	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5691		16-vertex Frank-Kasper Mg <sub>4</sub> Zn <sub>12</sub>
Zn39	2a	-3m.	0	0	0		icosahedron Zn <sub>6</sub> Mg <sub>6</sub>

M31 = 0.75Zn + 0.25Mg; M33 = 0.71Zn + 0.29Mg; M37 = 0.87Sm + 0.13Mg

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

Remarks: Phase referred to as  $\mu_7$ -(MgSmZn).

References: [1] Sugiyama K., Yasuda K., Horikawa Y., Ohsuna T., Hiraga K. (1999), J. Alloys Compd. 285, 172-178.

194  
hP574

Mn <sub>55</sub> Al <sub>226.58</sub>	hP574	(194) $P6_3/mmc - 1^{11}k^{16}j^5ih^5gfeb$
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### MnAl<sub>4</sub> μ [2]

Structural features: Mn<sub>3</sub> trigonal and Mn<sub>4</sub> tetrahedral clusters. 108 of 110 Mn atoms have icosahedral coordination.

Brink Shoemaker C. et al. (1989) [1]

Al<sub>226.58</sub>Mn<sub>55</sub>

$a = 1.998$ ,  $c = 2.4673$  nm,  $c/a = 1.235$ ,  $V = 8.5299$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24l	1	0.00056	0.23676	0.05749		tricapped pentagonal prism Al <sub>10</sub> Mn <sub>3</sub>
Al2	24l	1	0.00201	0.38667	0.05667		tricapped pentagonal prism Al <sub>10</sub> Mn <sub>3</sub>
Al3	24l	1	0.02443	0.20495	0.15939		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al4	24l	1	0.02882	0.44214	0.15923		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al5	24l	1	0.10759	0.36195	0.19247		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al6	24l	1	0.10969	0.36518	0.00420		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al7	24l	1	0.15748	0.46151	0.09740		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al8	24l	1	0.33588	0.05052	0.15640		pseudo Frank-Kasper Al <sub>10</sub> Mn <sub>3</sub>
Al9	24l	1	0.45985	0.15706	0.08948		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al10	24l	1	0.49104	0.13061	0.19239		pseudo Frank-Kasper Al <sub>10</sub> Mn <sub>3</sub>
Mn11	24l	1	0.49545	0.12642	0.00205		icosahedron Al <sub>10</sub> Mn <sub>2</sub>
Al12	12k	.m.	0.04315	0.08630	0.17336	0.672	
Al13	12k	.m.	0.07818	0.15636	0.59580		14-vertex Frank-Kasper Mn <sub>3</sub> Al <sub>11</sub>
Mn14	12k	.m.	0.07909	0.15818	0.08775		icosahedron Al <sub>11</sub> Mn
Mn15	12k	.m.	0.12702	0.25404	0.50160		icosahedron Al <sub>11</sub> Mn
Al16	12k	.m.	0.13151	0.26302	0.69343		
Al17	12k	.m.	0.15687	0.31374	0.09720		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al18	12k	.m.	0.15800	0.31601	0.59064		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Mn19	12k	.m.	0.20769	0.41538	0.66213		icosahedron Al <sub>11</sub> Mn
Al20	12k	.m.	0.25446	0.50892	0.00456		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al21	12k	.m.	0.25491	0.50982	0.19219		12-vertex polyhedron Al <sub>10</sub> Mn <sub>2</sub>
Al22	12k	.m.	0.38427	0.76854	0.05694		icosahedron Mn <sub>3</sub> Al <sub>9</sub>
Al23	12k	.m.	0.53926	0.07852	0.09319		tricapped pentagonal prism Al <sub>10</sub> Mn <sub>3</sub>
Mn24	12k	.m.	0.54024	0.08048	0.58714		icosahedron Al <sub>10</sub> Mn <sub>2</sub>
Al25	12k	.m.	0.58834	0.17668	0.65976		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al26	12k	.m.	0.61805	0.23610	0.05753		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al27	12k	.m.	0.71456	0.42912	0.15312		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Mn28	12j	m..	0.00123	0.37949	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>11</sub> Mn
Al29	12j	m..	0.12891	0.49139	<sup>1</sup> / <sub>4</sub>		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al30	12j	m..	0.13345	0.04238	<sup>1</sup> / <sub>4</sub>	0.424	
Mn31	12j	m..	0.24315	0.00231	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>11</sub> Mn
Al32	12j	m..	0.37677	0.12434	<sup>1</sup> / <sub>4</sub>		icosahedron Mn <sub>5</sub> Al <sub>7</sub>
Al33	12i	.2.	0.12651	0	0		icosahedron Al <sub>8</sub> Mn <sub>4</sub>
Al34	6h	mm2	0.12167	0.24334	<sup>1</sup> / <sub>4</sub>		14-vertex polyhedron Mn <sub>2</sub> Al <sub>12</sub>
Mn35	6h	mm2	0.37919	0.75838	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>10</sub> Mn <sub>2</sub>
Al36	6h	mm2	0.51015	0.02030	<sup>1</sup> / <sub>4</sub>		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Al37	6h	mm2	0.61909	0.23818	<sup>1</sup> / <sub>4</sub>		12-vertex polyhedron Mn <sub>2</sub> Al <sub>10</sub>
Mn38	6h	mm2	0.74685	0.49370	<sup>1</sup> / <sub>4</sub>		icosahedron Al <sub>10</sub> Mn <sub>2</sub>

Al39	6g	.2/m.	$\frac{1}{2}$	0	0	icosahedron Mn <sub>6</sub> Al <sub>6</sub>
Al40	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.16029	icosahedron Al <sub>9</sub> Mn <sub>3</sub>
Al41	4e	3m.	0	0	0.06624	16-vertex Frank-Kasper Mn <sub>3</sub> Al <sub>13</sub>
Mn42	2b	-6m2	0	0	$\frac{1}{4}$	

Experimental: single crystal, diffractometer, X-rays, R = 0.053, T = 296 K

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

References: [1] Brink Shoemaker C., Keszler D.A., Shoemaker D.P. (1989), Acta Crystallogr. B 45, 13-20. [2] Brink Shoemaker C. (1988), Phys. Rev. B: Condens. Matter 38, 8511-8514.

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hP632

Zn <sub>10</sub> Fe	hP632	(194) $P6_3/mmc - I^9k^{28}j^{37}f^2e^2a$
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### FeZn<sub>10</sub> [1]

Structural features: 3D-framework with mainly icosahedral coordination, including icosahedra in partial rotational disorder around axes parallel to [001].

Belin C.H.E., Belin R.C.H. (2000) [1]

Fe<sub>1.04</sub>Zn<sub>10.08</sub>

$a = 1.2787$ ,  $c = 5.7222$  nm,  $c/a = 4.475$ ,  $V = 8.1027$  nm<sup>3</sup>,  $Z = 50$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.0247	0.3547	0.1382		
M2	24l	1	0.0614	0.3609	0.2264		tricapped pentagonal prism Zn <sub>13</sub>
M3	24l	1	0.1293	0.468	0.0655		pseudo Frank-Kasper Zn <sub>13</sub>
M4	24l	1	0.3142	0.0427	0.0452		tricapped pentagonal prism Zn <sub>13</sub>
M5	24l	1	0.3177	0.0392	0.0927		
M6	24l	1	0.3245	0.0256	0.1832		
Fe7	24l	1	0.4786	0.1783	0.1159	0.333	
Fe8	24l	1	0.5255	0.1497	0.1656	0.333	
M9	24l	1	0.5342	0.1268	0.1222	0.333	
M10	12k	.m.	0.0704	0.1408	0.0347		12-vertex polyhedron Zn <sub>12</sub>
M11	12k	.m.	0.0711	0.1422	0.6801		icosahedron Zn <sub>12</sub>
M12	12k	.m.	0.0733	0.1466	0.5726		12-vertex polyhedron Zn <sub>12</sub>
M13	12k	.m.	0.083	0.1661	0.1091		14-vertex polyhedron Zn <sub>14</sub>
M14	12k	.m.	0.1123	0.2246	0.204		icosahedron Zn <sub>12</sub>
M15	12k	.m.	0.1129	0.2258	0.5086		12-vertex polyhedron Zn <sub>12</sub>
M16	12k	.m.	0.1148	0.2296	0.1569		icosahedron Zn <sub>12</sub>
M17	12k	.m.	0.1166	0.2332	0.7245		14-vertex Frank-Kasper Zn <sub>14</sub>
M18	12k	.m.	0.1193	0.2387	0.6339		
M19	12k	.m.	0.1357	0.2714	0.0692		icosahedron Zn <sub>12</sub>
M20	12k	.m.	0.1947	0.3894	0.0279		12-vertex polyhedron Zn <sub>12</sub>
M21	12k	.m.	0.2036	0.4073	0.1046		icosahedron Zn <sub>12</sub>
M22	12k	.m.	0.2177	0.4354	0.1851		12-vertex polyhedron Zn <sub>12</sub>
M23	12k	.m.	0.2209	0.4418	0.5165		icosahedron Zn <sub>12</sub>
Fe24	12k	.m.	0.2254	0.4508	0.6578	0.667	non-coplanar triangle Fe <sub>2</sub> Zn
M25	12k	.m.	0.2261	0.4522	0.7068		
M26	12k	.m.	0.2274	0.4548	0.6241	0.333	
M27	12k	.m.	0.2513	0.5026	0.562		15-vertex Frank-Kasper Fe <sub>3</sub> Zn <sub>12</sub>
M28	12k	.m.	0.2635	0.527	0.1415		pseudo Frank-Kasper Zn <sub>13</sub>
M29	12k	.m.	0.4062	0.8125	0.2115		12-vertex polyhedron Zn <sub>12</sub>
M30	12k	.m.	0.5306	0.0612	0.2094		

M31	12k	.m.	0.5397	0.0794	0.0781	
M32	12k	.m.	0.5456	0.0912	0.0316	14-vertex Frank-Kasper Zn <sub>14</sub>
M33	12k	.m.	0.5485	0.097	0.6678	
M34	12k	.m.	0.5492	0.0984	0.6107	
Fe35	12k	.m.	0.5547	0.1094	0.1558	0.333
M36	12k	.m.	0.5894	0.1788	0.5135	14-vertex Frank-Kasper Zn <sub>14</sub>
M37	12k	.m.	0.6494	0.2989	0.1851	0.333
M38	12j	m..	0.46	0.1324	<sup>1</sup> / <sub>4</sub>	pseudo Frank-Kasper Zn <sub>13</sub>
M39	12i	.2.	0.3643	0	0	12-vertex polyhedron Zn <sub>12</sub>
M40	6h	mm2	0.094	0.188	<sup>1</sup> / <sub>4</sub>	12-vertex polyhedron Zn <sub>12</sub>
M41	6h	mm2	0.2612	0.5224	<sup>1</sup> / <sub>4</sub>	12-vertex polyhedron Zn <sub>12</sub>
M42	6h	mm2	0.4662	0.9325	<sup>1</sup> / <sub>4</sub>	icosahedron Zn <sub>12</sub>
M43	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0486	pseudo Frank-Kasper Zn <sub>13</sub>
M44	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0952	16-vertex Frank-Kasper Zn <sub>16</sub>
M45	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1763	icosahedron Zn <sub>12</sub>
M46	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5246	icosahedron Zn <sub>12</sub>
Fe47	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5944	
M48	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6399	
M49	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.7283	
M50	4e	3m.	0	0	0.1403	icosahedron Zn <sub>12</sub>
M51	4e	3m.	0	0	0.2195	icosahedron Zn <sub>12</sub>
M52	2a	-3m.	0	0	0	icosahedron Zn <sub>12</sub>

M1-M52 = 0.962Zn + 0.038Fe

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

Remarks: Phase referred to as δ-(FeZn). Homogeneity range Fe<sub>100-x</sub>Zn<sub>x</sub>, 86.5 < x < 92. We assigned an approximate value to the Fe/Zn ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s). We assume that in table 4 of [1] the y-coordinate of former Zn(7) is misprinted as 2x instead of x/2, the Wyckoff position of former Zn(24) as 12k instead of 24l, and the z-coordinate of former Zn(36) as <sup>1</sup>/<sub>4</sub> instead of <sup>3</sup>/<sub>4</sub> (better agreement with expected interatomic distances).

References: [1] Belin C.H.E., Belin R.C.H. (2000), J. Solid State Chem. 151, 85-95.

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hP730

[NH <sub>4</sub> ] <sub>15</sub> V <sub>12</sub> Mo <sub>57</sub> [NO] <sub>6</sub> O <sub>192</sub> [OH] <sub>3</sub> [H <sub>2</sub> O] <sub>74</sub>	hP730	(194) <i>P6<sub>3</sub>/mmc</i> – 1 <sup>17</sup> k <sup>19</sup> j <sup>5</sup> h <sup>5</sup> f
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(NH<sub>4</sub>)<sub>15</sub>[H<sub>3</sub>Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>189</sub>(H<sub>2</sub>O)<sub>12</sub>(VO)<sub>6</sub>]·~60H<sub>2</sub>O [1]

Structural features: Keggin-related Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>186</sub>(OH)<sub>3</sub>(H<sub>2</sub>O)<sub>12</sub>(VO)<sub>6</sub> units (MoO<sub>6</sub>, Mo[O<sub>5</sub>(OH)] and Mo[O<sub>5</sub>(OH<sub>2</sub>)] octahedra, Mo[O<sub>6</sub>(NO)] pentagonal bipyramids, VO<sub>5</sub> square pyramids and VO<sub>4</sub> tetrahedra sharing edges and vertices) in a Mg-type (h.c.p.) arrangement; NH<sub>4</sub> and additional H<sub>2</sub>O between the units.

Yang W. et al. (2000) [1]

H<sub>151</sub>Mo<sub>57</sub>N<sub>6</sub>O<sub>275</sub>V<sub>12</sub>

a = 2.3612, c = 2.6859 nm, c/a = 1.138, V = 12.9684 nm<sup>3</sup>, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.0202	0.1975	0.1489		single atom Mo
Mo2	24l	1	0.04284	0.25925	0.18984		octahedron O <sub>6</sub>
O3	24l	1	0.0446	0.3702	0.0574		single atom Mo
Mo4	24l	1	0.07202	0.40711	0.11314		octahedron O <sub>6</sub>
O5	24l	1	0.0847	0.3371	0.1465		non-coplanar triangle Mo <sub>3</sub>
O6	24l	1	0.0935	0.4888	0.1012		non-colinear MoV
O7	24l	1	0.1052	0.4527	0.1992		single atom Mo

O8	24l	1	0.1655	0.4321	0.1045		non-coplanar triangle Mo <sub>3</sub>
O9	24l	1	0.2168	0.5512	0.0635		non-colinear MoV
O10	24l	1	0.2953	0.0263	0.1957		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )11	24l	1	0.3462	0.1039	0.0478		single atom (OH <sub>2</sub> )
O12	24l	1	0.382	0.0058	0.1464		non-colinear Mo <sub>2</sub>
O13	24l	1	0.3974	0.131	0.149		single atom Mo
Mo14	24l	1	0.40204	0.07908	0.18904		octahedron O <sub>6</sub>
(OH <sub>2</sub> )15	24l	1	0.4526	0.1044	0.0463		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O16	24l	1	0.4901	0.1083	0.1868		non-colinear MoV
(OH <sub>2</sub> )17	24l	1	0.542	0.209	0.074	0.5	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
(OH <sub>2</sub> )18	12k	.m.	0.0446	0.0892	0.2244	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )19	12k	.m.	0.0715	0.143	0.732	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )20	12k	.m.	0.1341	0.2682	0.6297		monocapped trigonal prism O <sub>4</sub> (OH <sub>2</sub> ) <sub>3</sub>
O21	12k	.m.	0.1369	0.2738	0.0416		single atom N
O22	12k	.m.	0.1439	0.2878	0.1864		non-coplanar triangle Mo <sub>3</sub>
N23	12k	.m.	0.1553	0.3106	0.076		single atom O
Mo24	12k	.m.	0.17895	0.3579	0.13005		7-vertex polyhedron NO <sub>6</sub>
O25	12k	.m.	0.2086	0.4172	0.1989		single atom Mo
O26	12k	.m.	0.2294	0.4588	0.0116		single atom Mo
Mo27	12k	.m.	0.2485	0.497	0.06789		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )28	12k	.m.	0.263	0.526	0.6203		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )29	12k	.m.	0.2689	0.5378	0.1544		single atom Mo
O30	12k	.m.	0.5079	0.0158	0.7015		single atom V
O31	12k	.m.	0.5242	0.0485	0.1013		single atom V
V32	12k	.m.	0.53049	0.06099	0.16758		tetrahedron O <sub>4</sub>
O33	12k	.m.	0.5599	0.1199	0.5165		single atom V
V34	12k	.m.	0.57459	0.14918	0.57174		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )35	12k	.m.	0.5968	0.1936	0.6549		single atom V
(OH <sub>2</sub> )36	12k	.m.	0.613	0.226	0.061	0.5	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O37	12j	m..	0.0317	0.2113	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
Mo38	12j	m..	0.06943	0.46478	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>5</sub> (OH)
O39	12j	m..	0.0943	0.3335	<sup>1</sup> / <sub>4</sub>		single atom Mo
O40	12j	m..	0.3993	0.1186	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
O41	12j	m..	0.4007	0.0123	<sup>1</sup> / <sub>4</sub>		single atom Mo
Mo42	6h	mm2	0.18295	0.3659	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
(OH)43	6h	mm2	0.4402	0.8803	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )44	6h	mm2	0.6063	0.213	<sup>1</sup> / <sub>4</sub>		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )45	6h	mm2	0.7381	0.4762	<sup>1</sup> / <sub>4</sub>		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )46	6h	mm2	0.855	0.71	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>2</sub> (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )47	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0145		9-vertex polyhedron (OH <sub>2</sub> ) <sub>3</sub> O <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.055, T = 293 K

Remarks: NH<sub>4</sub> 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] Yang W., Lin X., Lu C., Zhuang H., Huang J. (2000), Inorg. Chem. 39, 2706-2707.

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hP774

[NH <sub>4</sub> ] <sub>21</sub> V <sub>6</sub> Mo <sub>57</sub> [NO] <sub>6</sub> O <sub>180</sub> [OH] <sub>3</sub> [H <sub>2</sub> O] <sub>71</sub>	hP774	(194) P6 <sub>3</sub> /mmc – 1 <sup>17</sup> k <sup>21</sup> ; <sup>5</sup> ; <sup>2</sup> j <sup>1</sup> i <sup>3</sup> h <sup>3</sup> t <sup>2</sup> e
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(NH<sub>4</sub>)<sub>21</sub>[H<sub>3</sub>Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>183</sub>(H<sub>2</sub>O)<sub>18</sub>]·53H<sub>2</sub>O [1]

Structural features: Keggin-related  $\text{Mo}_{57}\text{V}_6(\text{NO})_6\text{O}_{180}(\text{OH})_3(\text{H}_2\text{O})_{18}$  units ( $\text{MoO}_6$ ,  $\text{Mo}[\text{O}_5(\text{OH}_2)]$  and  $\text{Mo}[\text{O}_3(\text{OH})(\text{OH}_2)_2]$  octahedra,  $\text{Mo}[\text{O}_6(\text{NO})]$  pentagonal bipyramids and  $\text{V}[\text{O}_5(\text{OH}_2)]$  octahedra sharing edges and vertices) in a Mg-type (h.c.p.) arrangement;  $\text{NH}_4$  and additional  $\text{H}_2\text{O}$  between the units. See Fig. III.53.

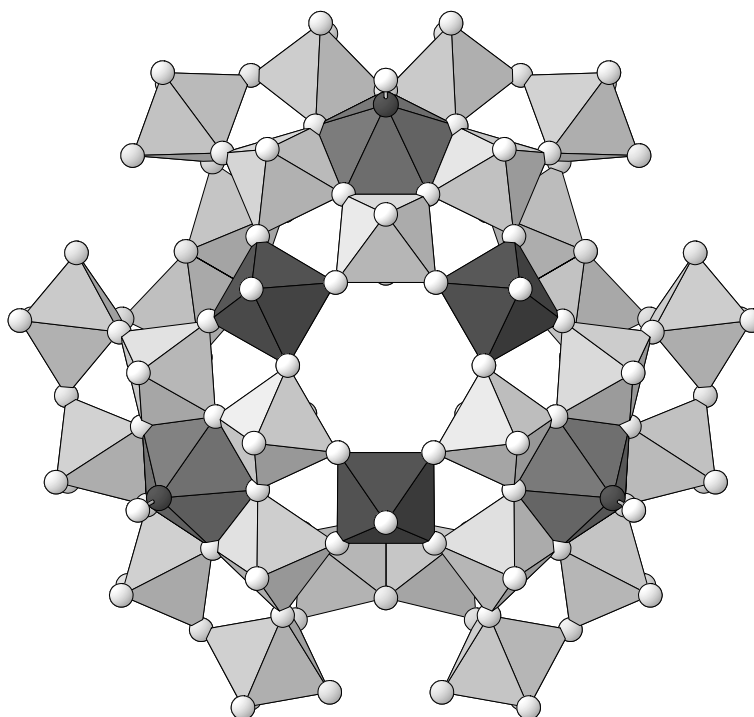


Fig. III.53.  $(\text{NH}_4)_{21}[\text{H}_3\text{Mo}_{57}\text{V}_6(\text{NO})_6\text{O}_{183}(\text{H}_2\text{O})_{18}] \cdot 53\text{H}_2\text{O}$

Units formed by  $\text{VO}_6$  (dark) and  $\text{MoO}_6$  (light) octahedra,  $\text{Mo}[\text{O}_6(\text{NO})]$  pentagonal bipyramids (medium; N atoms dark, O atoms light) viewed along  $[001]$  (H atoms ignored).

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

$\text{H}_{201}\text{Mo}_{57}\text{N}_{27}\text{O}_{260}\text{V}_6$

$a = 2.35637$ ,  $c = 2.69055$  nm,  $c/a = 1.142$ ,  $V = 12.9377$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	24f	1	0.0205	0.196	0.1479		single atom Mo
Mo2	24f	1	0.0413	0.2579	0.19		octahedron $\text{O}_6$
O3	24f	1	0.0435	0.3687	0.0573		single atom Mo
Mo4	24f	1	0.0714	0.4068	0.1143		octahedron $\text{O}_6$
O5	24f	1	0.0847	0.3364	0.1469		non-coplanar triangle $\text{Mo}_3$
O6	24f	1	0.0917	0.488	0.1017		non-colinear MoV
O7	24f	1	0.1061	0.4529	0.1978		single atom Mo
O8	24f	1	0.1651	0.4304	0.1048		non-coplanar triangle $\text{Mo}_3$
O9	24f	1	0.2159	0.5511	0.0637		non-colinear MoV
O10	24f	1	0.294	0.0266	0.1956		single atom Mo
O11	24f	1	0.3532	0.1119	0.0413	0.5	single atom N
O12	24f	1	0.381	0.0072	0.147		non-colinear $\text{Mo}_2$



O13	24l	1	0.3969	0.1332	0.1487		single atom Mo
Mo14	24l	1	0.4065	0.0824	0.1888		octahedron O <sub>6</sub>
N15	24l	1	0.4514	0.1014	0.0446	0.5	non-colinear O <sub>2</sub>
O16	24l	1	0.4895	0.1123	0.1874		single atom Mo
O17	24l	1	0.5688	0.2218	0.0557	0.5	single atom O
O18	12k	.m.	0.0427	0.0854	0.6491		non-colinear O <sub>2</sub>
O19	12k	.m.	0.0473	0.0947	0.2335	0.5	
N20	12k	.m.	0.0633	0.1267	0.0784	0.5	non-coplanar square O <sub>4</sub>
O21	12k	.m.	0.0825	0.165	0.7239	0.5	single atom O
O22	12k	.m.	0.1363	0.2726	0.6311		non-coplanar triangle NO <sub>2</sub>
O23	12k	.m.	0.1369	0.2739	0.0414		single atom N
O24	12k	.m.	0.144	0.288	0.1872		non-coplanar triangle Mo <sub>3</sub>
N25	12k	.m.	0.1487	0.2974	0.7347	0.5	
N26	12k	.m.	0.1537	0.3073	0.0772		non-colinear OMo
Mo27	12k	.m.	0.1779	0.3559	0.1302		7-vertex polyhedron NO <sub>6</sub>
O28	12k	.m.	0.2087	0.4174	0.1981		single atom Mo
O29	12k	.m.	0.2289	0.4578	0.012		single atom Mo
Mo30	12k	.m.	0.2481	0.4962	0.0678		octahedron O <sub>6</sub>
O31	12k	.m.	0.2535	0.507	0.6101		non-colinear O <sub>2</sub>
O32	12k	.m.	0.2692	0.5384	0.1535		single atom Mo
O33	12k	.m.	0.5084	0.0169	0.6993		non-colinear Mo <sub>2</sub>
N34	12k	.m.	0.5233	0.0467	0.1034		single atom O
O35	12k	.m.	0.5601	0.1202	0.5163		single atom V
V36	12k	.m.	0.574	0.1481	0.571		octahedron O <sub>6</sub>
O37	12k	.m.	0.5961	0.1922	0.6543		single atom V
O38	12k	.m.	0.7404	0.4808	0.2267	0.5	single atom O
O39	12j	m..	0.034	0.2104	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
Mo40	12j	m..	0.067	0.4622	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
O41	12j	m..	0.092	0.3318	<sup>1</sup> / <sub>4</sub>		single atom Mo
O42	12j	m..	0.3991	0.0129	<sup>1</sup> / <sub>4</sub>		single atom Mo
O43	12j	m..	0.3991	0.1206	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
O44	12i	.2.	0.254	0	0		4-vertex polyhedron O <sub>4</sub>
O45	12i	.2.	0.442	0	0	0.5	non-colinear N <sub>2</sub>
Mo46	6h	mm2	0.1827	0.3653	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
O47	6h	mm2	0.4357	0.8714	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
N48	6h	mm2	0.603	0.206	<sup>1</sup> / <sub>4</sub>		square prism (cube) O <sub>8</sub>
O49	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0056		hexagonal prism O <sub>12</sub>
O50	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.675		non-coplanar hexagon N <sub>3</sub> O <sub>3</sub>
O51	4e	3m.	0	0	0.212	0.5	4-vertex polyhedron O <sub>4</sub>
H52	24l	1	0.0516	0.15	0.094	0.5	
H53	24l	1	0.0982	0.011	0.138		
H54	24l	1	0.1461	0.0351	0.233	0.25	
H55	24l	1	0.2211	0.5766	0.1565	0.5	
H56	24l	1	0.2406	0.5583	0.1581	0.5	
H57	24l	1	0.271	0.018	0.002		
H58	24l	1	0.2901	0.113	0.1096	0.5	
H59	24l	1	0.378	0.0907	0.054	0.5	
H60	24l	1	0.389	0.15	0.023	0.5	
H61	24l	1	0.419	0.068	0.024	0.5	
H62	24l	1	0.425	0.031	0.002	0.5	
H63	24l	1	0.432	0.118	0.066	0.5	
H64	24l	1	0.474	0.084	0.063	0.5	
H65	24l	1	0.482	0.136	0.024	0.5	

H66	24l	1	0.4935	0.056	0.0891	
H67	24l	1	0.527	0.235	0.087	0.5
H68	12k	.m.	0.041	0.082	0.038	0.5
H69	12k	.m.	0.1377	0.2754	0.6674	
H70	12k	.m.	0.2315	0.463	0.626	
H71	12k	.m.	0.2492	0.4984	0.1749	
H72	12k	.m.	0.352	0.704	0.029	0.667
H73	12k	.m.	0.5022	0.0044	0.116	
H74	12k	.m.	0.5118	0.024	0.658	
H75	12k	.m.	0.5138	0.028	0.202	
H76	12k	.m.	0.5373	0.075	0.1312	
H77	12k	.m.	0.5735	0.147	0.72	0.5
H78	12k	.m.	0.5831	0.1662	0.6853	
H79	12k	.m.	0.5866	0.1733	0.2253	
H80	12j	m..	0.0607	0.1377	$\frac{1}{4}$	0.5
H81	12j	m..	0.3187	0.1329	$\frac{1}{4}$	
H82	12j	m..	0.5334	0.236	$\frac{1}{4}$	0.5
H83	12j	m..	0.5748	0.223	$\frac{1}{4}$	
H84	6h	mm2	0.7594	0.5188	$\frac{1}{4}$	
H85	6h	mm2	0.8999	0.7998	$\frac{1}{4}$	
H86	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.664	

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

Experimental: single crystal, diffractometer, neutrons, R = 0.130, T = 20 K

Remarks: Part of H not located. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances: d(O50-H86) = 0.030 nm and d(O44-H57) = 0.042 nm. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. A slightly different model was reported in [2]. In table 2 of [1] the Wyckoff position of former V(1) is misprinted as 24l instead of 12k (difference on the fourth decimal of the atom coordinates).

References: [1] Lutz H.D., Nagel R., Mason S.A., Müller A., Bögge H., Krickemeyer E. (2002), J. Solid State Chem. 165, 199-205. [2] Müller A., Krickemeyer E., Dillinger S., Bögge H., Plass W., Proust A., Dloczik L., Menke C., Meyer J., Rohlfing R. (1994), Z. Anorg. Allg. Chem. 620, 599-619.

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[NH <sub>4</sub> ] <sub>21</sub> V <sub>6</sub> Mo <sub>57</sub> [NO] <sub>6</sub> O <sub>180</sub> [OH] <sub>3</sub> [H <sub>2</sub> O] <sub>83</sub>	hP774	(194) <i>P6<sub>3</sub>/mmc</i> – $1^{17}k^{21}j^{55}i^{55}e$
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(NH<sub>4</sub>)<sub>21</sub>[H<sub>3</sub>Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>183</sub>(H<sub>2</sub>O)<sub>18</sub>]·65H<sub>2</sub>O [1]

Structural features: Keggin-related Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>180</sub>(OH)<sub>3</sub>(H<sub>2</sub>O)<sub>18</sub> units (MoO<sub>6</sub>, Mo[O<sub>5</sub>(OH<sub>2</sub>)]) and Mo[O<sub>3</sub>(OH)(OH<sub>2</sub>)<sub>2</sub>] octahedra, Mo[O<sub>6</sub>(NO)] pentagonal bipyramids and VO<sub>5</sub> square pyramids sharing edges and vertices; partial disorder for V, part of H<sub>2</sub>O replaced by VO) in a Mg-type (h.c.p.) arrangement; NH<sub>4</sub> and additional H<sub>2</sub>O between the units.

Müller A. et al. (1994) [1]

H<sub>251</sub>Mo<sub>57</sub>N<sub>27</sub>O<sub>272</sub>V<sub>7</sub>

*a* = 2.3696, *c* = 2.7095 nm, *c/a* = 1.143, *V* = 13.1756 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24l	1	0.0211	0.1976	0.1492		single atom Mo
Mo2	24l	1	0.0423	0.2589	0.1904		octahedron O <sub>6</sub>
O3	24l	1	0.0444	0.3689	0.0579		single atom Mo
Mo4	24l	1	0.0718	0.4068	0.1145		octahedron O <sub>6</sub>

O5	24l	1	0.0845	0.3372	0.1473		non-coplanar triangle Mo <sub>3</sub>
O6	24l	1	0.0928	0.4889	0.1026		
O7	24l	1	0.1069	0.4531	0.1986		single atom Mo
O8	24l	1	0.1658	0.4318	0.1052		non-coplanar triangle Mo <sub>3</sub>
O9	24l	1	0.2166	0.5511	0.0651		
O10	24l	1	0.2944	0.0258	0.1959		single atom Mo
(OH <sub>2</sub> )11	24l	1	0.3391	0.101	0.0472		single atom (NH <sub>4</sub> )
O12	24l	1	0.3798	0.0055	0.1477		non-collinear Mo <sub>2</sub>
O13	24l	1	0.3959	0.1319	0.1496		single atom Mo
Mo14	24l	1	0.4065	0.0817	0.1891		octahedron O <sub>6</sub>
M15	24l	1	0.4511	0.1004	0.0459		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
O16	24l	1	0.4895	0.111	0.1871		non-collinear MoV
(OH <sub>2</sub> )17	24l	1	0.5743	0.2229	0.0559	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )18	12k	.m.	0.0481	0.0962	0.6447		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
M19	12k	.m.	0.0607	0.1214	0.078		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )20	12k	.m.	0.083	0.166	0.7325	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )21	12k	.m.	0.1341	0.2682	0.633		non-collinear O <sub>2</sub>
O22	12k	.m.	0.1369	0.2738	0.041		single atom N
O23	12k	.m.	0.1439	0.2878	0.1867		non-coplanar triangle Mo <sub>3</sub>
N24	12k	.m.	0.1547	0.3094	0.0769		single atom O
Mo25	12k	.m.	0.1788	0.3576	0.1306		7-vertex polyhedron NO <sub>6</sub>
O26	12k	.m.	0.2091	0.4182	0.1993		single atom Mo
O27	12k	.m.	0.2291	0.4582	0.0136		single atom Mo
Mo28	12k	.m.	0.2484	0.4968	0.0687		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )29	12k	.m.	0.2548	0.5096	0.615		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )30	12k	.m.	0.2693	0.5386	0.1549		single atom Mo
(OH <sub>2</sub> )31	12k	.m.	0.5089	0.0178	0.7014		single atom V
M32	12k	.m.	0.5236	0.0473	0.0985		single atom V
V33	12k	.m.	0.5306	0.0613	0.1679	0.167	tetrahedron (OH <sub>2</sub> ) <sub>2</sub> O <sub>2</sub>
O34	12k	.m.	0.5604	0.1208	0.517		single atom V
V35	12k	.m.	0.5744	0.1488	0.5728	0.9	
V36	12k	.m.	0.5807	0.1614	0.5936	0.1	
(OH <sub>2</sub> )37	12k	.m.	0.5969	0.1938	0.6557		single atom V
(OH <sub>2</sub> )38	12k	.m.	0.7383	0.4766	0.2317	0.5	single atom (OH <sub>2</sub> )
O39	12j	m..	0.0321	0.21	<sup>1</sup> / <sub>4</sub>		non-collinear Mo <sub>2</sub>
Mo40	12j	m..	0.0682	0.4634	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>3</sub> (OH)(OH <sub>2</sub> ) <sub>2</sub>
O41	12j	m..	0.0937	0.3349	<sup>1</sup> / <sub>4</sub>		single atom Mo
O42	12j	m..	0.3987	0.1187	<sup>1</sup> / <sub>4</sub>		non-collinear Mo <sub>2</sub>
O43	12j	m..	0.399	0.0112	<sup>1</sup> / <sub>4</sub>		single atom Mo
(OH <sub>2</sub> )44	12i	.2.	0.4392	0	0		non-collinear (NH <sub>4</sub> ) <sub>2</sub>
(OH <sub>2</sub> )45	6h	mm2	0.0492	0.0984	<sup>1</sup> / <sub>4</sub>		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
Mo46	6h	mm2	0.1829	0.3658	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
(OH)47	6h	mm2	0.437	0.8741	<sup>1</sup> / <sub>4</sub>		non-collinear Mo <sub>2</sub>
M48	6h	mm2	0.6045	0.209	<sup>1</sup> / <sub>4</sub>		non-coplanar square (OH <sub>2</sub> ) <sub>4</sub>
M49	6h	mm2	0.8541	0.7082	<sup>1</sup> / <sub>4</sub>		
(OH <sub>2</sub> )50	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.5059		hexagonal prism (OH <sub>2</sub> ) <sub>6</sub> O <sub>6</sub>
(OH <sub>2</sub> )51	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6856		non-coplanar triangle (NH <sub>4</sub> ) <sub>3</sub>
(OH <sub>2</sub> )52	4e	3m.	0	0	0.2096	0.5	7-vertex polyhedron (OH <sub>2</sub> ) <sub>7</sub>

M15 = 0.875NH<sub>4</sub> + 0.125OH<sub>2</sub>; M19 = 0.875NH<sub>4</sub> + 0.125OH<sub>2</sub>; M32 = 0.833OH<sub>2</sub> + 0.167O; M48 = 0.875NH<sub>4</sub> + 0.125OH<sub>2</sub>; M49 = 0.875NH<sub>4</sub> + 0.125OH<sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.062, T = 193 K

Remarks: We assigned an approximate value to the  $\text{NH}_4/\text{OH}_2$  ratio of sites M15, M19, M48 and M49 based on the nominal composition. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The authors state that no electron density was detected in site V33 for other crystals; composition  $(\text{NH}_4)_{21}[\text{H}_3\text{Mo}_{57}\text{V}_6(\text{NO})_6(\text{VO})_x\text{O}_{183}(\text{H}_2\text{O})_{18-x}]\cdot 65\text{H}_2\text{O}$  considering this site.

References: [1] Müller A., Krickemeyer E., Dillinger S., Bögge H., Plass W., Proust A., Dłoczik L., Menke C., Meyer J., Rohlffing R. (1994), *Z. Anorg. Allg. Chem.* 620, 599-619.

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hP776

$[\text{NH}_4]_{15}\text{Mo}_{57}\text{Fe}_6[\text{NO}]_6\text{O}_{174}[\text{OH}]_3[\text{H}_2\text{O}]_{97}$	<i>hP776</i>	(194) $P6_3/mmc - 1^{19}k^{18:5}1^6f^2$
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**$(\text{NH}_4)_{15}[\text{H}_3\text{Mo}_{57}\text{Fe}_6(\text{NO})_6\text{O}_{177}(\text{H}_2\text{O})_{24}]\cdot 73\text{H}_2\text{O}$  [1]**

Structural features: Keggin-related  $\text{Mo}_{57}\text{Fe}_6(\text{NO})_6\text{O}_{174}(\text{OH})_3(\text{H}_2\text{O})_{24}$  units ( $\text{MoO}_6$ ,  $\text{Mo}[\text{O}_3(\text{OH})(\text{OH}_2)_2]$ ,  $\text{Mo}[\text{O}_5(\text{OH}_2)]$  and  $\text{Mo}[\text{O}_4(\text{OH}_2)_2]$  octahedra,  $\text{Mo}[\text{O}_6(\text{NO})]$  pentagonal bipyramids and  $\text{Fe}[\text{O}_4(\text{OH}_2)_2]$  octahedra sharing edges and vertices) in a Mg-type (h.c.p.) arrangement;  $\text{NH}_4$  and additional  $\text{H}_2\text{O}$  between the units.

Müller A. et al. (1994) [1]

$\text{Fe}_6\text{H}_{251}\text{Mo}_{57}\text{N}_{21}\text{O}_{277}$

$a = 2.373$ ,  $c = 2.7312$  nm,  $c/a = 1.151$ ,  $V = 13.3192$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24/	1	0.0217	0.1988	0.1498		single atom Mo
Mo2	24/	1	0.0426	0.2591	0.1911		octahedron O <sub>6</sub>
O3	24/	1	0.0463	0.3683	0.0611		single atom Mo
Mo4	24/	1	0.0724	0.4065	0.1163		octahedron O <sub>6</sub>
O5	24/	1	0.084	0.3365	0.1496		coplanar triangle Mo <sub>3</sub>
O6	24/	1	0.0913	0.4876	0.1043		non-collinear MoFe
O7	24/	1	0.1059	0.4551	0.1979		single atom Mo
O8	24/	1	0.1641	0.4321	0.1073		non-coplanar triangle Mo <sub>3</sub>
O9	24/	1	0.2177	0.5517	0.0696		non-collinear MoFe
(OH <sub>2</sub> )10	24/	1	0.2652	0.0448	0.0548		single atom (OH <sub>2</sub> )
O11	24/	1	0.2945	0.0257	0.1963		single atom Mo
(OH <sub>2</sub> )12	24/	1	0.378	0.1155	0.0393		single atom (OH <sub>2</sub> )
O13	24/	1	0.3784	0.006	0.1492		non-collinear Mo <sub>2</sub>
O14	24/	1	0.3954	0.1311	0.15		single atom Mo
Mo15	24/	1	0.4068	0.081	0.1901		octahedron O <sub>6</sub>
(OH <sub>2</sub> )16	24/	1	0.45	0.0597	0.0303		octahedron (OH <sub>2</sub> ) <sub>3</sub> O <sub>2</sub> (NH <sub>4</sub> )
O17	24/	1	0.4866	0.1102	0.1875		single atom Mo
(OH <sub>2</sub> )18	24/	1	0.5759	0.2197	0.1349	0.25	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )19	24/	1	0.5799	0.2249	0.0516	0.25	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )20	12k	.m.	0.0507	0.1014	0.6444	0.25	non-coplanar triangle O(NH <sub>4</sub> ) <sub>2</sub>
M21	12k	.m.	0.0606	0.1212	0.0881		non-coplanar square O <sub>4</sub>
(OH <sub>2</sub> )22	12k	.m.	0.0881	0.1762	0.72	0.25	single atom O
(OH <sub>2</sub> )23	12k	.m.	0.1325	0.265	0.6361		pseudo Frank-Kasper (OH <sub>2</sub> ) <sub>2</sub> O <sub>8</sub> (NH <sub>4</sub> )
O24	12k	.m.	0.1392	0.2784	0.0426		single atom N
O25	12k	.m.	0.1453	0.2906	0.1873		tetrahedron Mo <sub>4</sub>
N26	12k	.m.	0.1545	0.309	0.0802		non-collinear OMo
Mo27	12k	.m.	0.179	0.358	0.1327		7-vertex polyhedron NO <sub>6</sub>
O28	12k	.m.	0.2077	0.4154	0.1983		non-collinear Mo <sub>2</sub>
O29	12k	.m.	0.23	0.46	0.0161		single atom Mo

M30	12k	.m.	0.244	0.488	0.5949	monocapped square prism (OH <sub>2</sub> ) <sub>6</sub> O <sub>3</sub>
Mo31	12k	.m.	0.2485	0.497	0.0724	octahedron (OH <sub>2</sub> )O <sub>5</sub>
(OH <sub>2</sub> )32	12k	.m.	0.2688	0.5376	0.1601	single atom Mo
(OH <sub>2</sub> )33	12k	.m.	0.5083	0.0166	0.701	non-colinear Mo <sub>2</sub>
M34	12k	.m.	0.5242	0.0484	0.103	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )35	12k	.m.	0.5602	0.1204	0.5154	single atom Fe
Fe36	12k	.m.	0.577	0.154	0.5862	octahedron O <sub>4</sub> (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )37	12k	.m.	0.5956	0.1912	0.6594	single atom Fe
O38	12j	m..	0.0328	0.2108	<sup>1</sup> / <sub>4</sub>	non-colinear Mo <sub>2</sub>
Mo39	12j	m..	0.0688	0.4645	<sup>1</sup> / <sub>4</sub>	octahedron O <sub>3</sub> (OH)(OH <sub>2</sub> ) <sub>2</sub>
O40	12j	m..	0.0935	0.3345	<sup>1</sup> / <sub>4</sub>	single atom Mo
O41	12j	m..	0.3972	0.1177	<sup>1</sup> / <sub>4</sub>	non-colinear Mo <sub>2</sub>
O42	12j	m..	0.3977	0.0123	<sup>1</sup> / <sub>4</sub>	single atom Mo
(OH <sub>2</sub> )43	6h	mm2	0.0476	0.0952	<sup>1</sup> / <sub>4</sub>	non-colinear O <sub>2</sub>
Mo44	6h	mm2	0.1827	0.3654	<sup>1</sup> / <sub>4</sub>	octahedron O <sub>6</sub>
(OH <sub>2</sub> )45	6h	mm2	0.4383	0.8766	<sup>1</sup> / <sub>4</sub>	non-colinear Mo <sub>2</sub>
M46	6h	mm2	0.6027	0.2054	<sup>1</sup> / <sub>4</sub>	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )47	6h	mm2	0.7391	0.4782	<sup>1</sup> / <sub>4</sub>	non-colinear (NH <sub>4</sub> ) <sub>2</sub>
M48	6h	mm2	0.8541	0.7082	<sup>1</sup> / <sub>4</sub>	non-colinear O <sub>2</sub>
M49	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0002	hexagonal prism (OH <sub>2</sub> ) <sub>6</sub> O <sub>6</sub>
(OH <sub>2</sub> )50	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6816	non-coplanar hexagon (OH <sub>2</sub> ) <sub>6</sub>

M21 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>; M30 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>; M34 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>; M46 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>; M48 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>; M49 = 0.577NH<sub>4</sub> + 0.423OH<sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.104, T = 188 K

Remarks: Part of H<sub>2</sub>O (NH<sub>4</sub>) not located; we assigned an approximate value to the NH<sub>4</sub>/OH<sub>2</sub> ratio of sites M based on the number of NH<sub>4</sub> in the nominal composition. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Müller A., Bögge H., Krickemeyer E., Dillinger S. (1994), Bull. Pol. Acad. Sci. Chem. 42, 291-298.

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hP794

[NH <sub>4</sub> ] <sub>21</sub> V <sub>6</sub> Mo <sub>57</sub> [NO] <sub>6</sub> O <sub>180</sub> [OH] <sub>3</sub> [H <sub>2</sub> O] <sub>73</sub>	hP794	(194) <i>P6<sub>3</sub>/mmc</i> – <i>l</i> <sup>18</sup> <i>k</i> <sup>22</sup> <i>j</i> <sup>5</sup> <i>ih</i> <sup>3</sup> <i>f</i> <sup>2</sup>
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(NH<sub>4</sub>)<sub>21</sub>[H<sub>3</sub>Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>183</sub>(H<sub>2</sub>O)<sub>18</sub>]·55H<sub>2</sub>O [1]

Structural features: Keggin-related Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>180</sub>(OH)<sub>3</sub>(H<sub>2</sub>O)<sub>18</sub> units (MoO<sub>6</sub>, Mo[O<sub>5</sub>(OH<sub>2</sub>)] and Mo[O<sub>3</sub>(OH)(OH<sub>2</sub>)<sub>2</sub>] octahedra, Mo[O<sub>6</sub>(NO)] pentagonal bipyramids and VO<sub>5</sub> square pyramids sharing edges and vertices; partial disorder for V in a Mg-type (h.c.p.) arrangement; NH<sub>4</sub> and additional H<sub>2</sub>O between the units.

Müller A. et al. (1998) [1]

H<sub>233</sub>Mo<sub>57</sub>N<sub>27</sub>O<sub>262</sub>V<sub>6</sub>

*a* = 2.3496, *c* = 2.6811 nm, *c/a* = 1.141, *V* = 12.8183 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24l	1	0.0178	0.1941	0.148		single atom Mo
Mo2	24l	1	0.04009	0.25593	0.1898		octahedron O <sub>6</sub>
O3	24l	1	0.0426	0.368	0.0561		single atom Mo
Mo4	24l	1	0.06977	0.40469	0.11253		octahedron O <sub>6</sub>
O5	24l	1	0.0829	0.3345	0.1465		non-coplanar triangle Mo <sub>3</sub>

O6	24l	1	0.091	0.4873	0.1009		
O7	24l	1	0.1042	0.4517	0.198		single atom Mo
O8	24l	1	0.164	0.43	0.104		non-coplanar triangle Mo <sub>3</sub>
O9	24l	1	0.2156	0.5499	0.0626		
(OH <sub>2</sub> )10	24l	1	0.2887	0.0579	0.0477	0.5	single atom (OH <sub>2</sub> )
O11	24l	1	0.2936	0.0282	0.1955		single atom Mo
(OH <sub>2</sub> )12	24l	1	0.341	0.1043	0.0441	0.5	single atom (OH <sub>2</sub> )
O13	24l	1	0.381	0.0083	0.1469		non-collinear Mo <sub>2</sub>
O14	24l	1	0.3975	0.1346	0.148		single atom Mo
Mo15	24l	1	0.40791	0.08476	0.18863		octahedron O <sub>6</sub>
(OH <sub>2</sub> )16	24l	1	0.4533	0.1074	0.0484		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
O17	24l	1	0.4905	0.1136	0.1866		single atom Mo
(NH <sub>4</sub> )18	24l	1	0.5855	0.2235	0.0577	0.5	single atom (NH <sub>4</sub> )
(OH <sub>2</sub> )19	12k	.m.	0.0461	0.0922	0.2242	0.5	single atom (OH <sub>2</sub> )
(NH <sub>4</sub> )20	12k	.m.	0.0575	0.115	0.0784		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )21	12k	.m.	0.0685	0.137	0.5941	0.25	non-collinear (NH <sub>4</sub> ) <sub>2</sub>
(OH <sub>2</sub> )22	12k	.m.	0.0708	0.1416	0.7315	0.5	
(OH <sub>2</sub> )23	12k	.m.	0.1356	0.2712	0.6299		non-collinear (OH <sub>2</sub> )(NH <sub>4</sub> )
O24	12k	.m.	0.1359	0.2718	0.0392		single atom N
(NH <sub>4</sub> )25	12k	.m.	0.1421	0.2842	0.7397	0.5	
O26	12k	.m.	0.1424	0.2849	0.1866		non-coplanar triangle Mo <sub>3</sub>
N27	12k	.m.	0.1531	0.3061	0.076		non-collinear OMo
Mo28	12k	.m.	0.17768	0.35536	0.12943		7-vertex polyhedron NO <sub>6</sub>
O29	12k	.m.	0.2081	0.4163	0.1984		non-collinear Mo <sub>2</sub>
O30	12k	.m.	0.2285	0.457	0.0105		single atom Mo
Mo31	12k	.m.	0.24768	0.49536	0.06657		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )32	12k	.m.	0.2558	0.5116	0.6101		non-collinear (NH <sub>4</sub> ) <sub>2</sub>
(OH <sub>2</sub> )33	12k	.m.	0.2686	0.5371	0.1537		single atom Mo
(OH <sub>2</sub> )34	12k	.m.	0.509	0.018	0.6997		non-collinear Mo <sub>2</sub>
(NH <sub>4</sub> )35	12k	.m.	0.5252	0.0504	0.0987		non-collinear (OH <sub>2</sub> ) <sub>2</sub>
O36	12k	.m.	0.5588	0.1176	0.5155		single atom V
V37	12k	.m.	0.57393	0.14786	0.5711	0.87	
V38	12k	.m.	0.5794	0.1588	0.594	0.13	
(OH <sub>2</sub> )39	12k	.m.	0.5963	0.1926	0.6535		single atom V
(OH <sub>2</sub> )40	12k	.m.	0.7409	0.4818	0.2233	0.5	single atom (OH <sub>2</sub> )
O41	12j	m..	0.0309	0.2072	$\frac{1}{4}$		non-collinear Mo <sub>2</sub>
Mo42	12j	m..	0.06676	0.46189	$\frac{1}{4}$		octahedron O <sub>3</sub> (OH)(OH <sub>2</sub> ) <sub>2</sub>
O43	12j	m..	0.0915	0.3299	$\frac{1}{4}$		single atom Mo
O44	12j	m..	0.3987	0.0136	$\frac{1}{4}$		single atom Mo
O45	12j	m..	0.3989	0.1221	$\frac{1}{4}$		non-collinear Mo <sub>2</sub>
(OH <sub>2</sub> )46	12i	.2.	0.4429	0	0	0.25	single atom (OH <sub>2</sub> )
Mo47	6h	mm2	0.18175	0.3635	$\frac{1}{4}$		octahedron O <sub>6</sub>
(OH)48	6h	mm2	0.4379	0.8758	$\frac{1}{4}$		non-collinear Mo <sub>2</sub>
(OH <sub>2</sub> )49	6h	mm2	0.6063	0.2127	$\frac{1}{4}$		non-coplanar square (OH <sub>2</sub> ) <sub>4</sub>
(OH <sub>2</sub> )50	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.0058		non-coplanar hexagon (NH <sub>4</sub> ) <sub>6</sub>
(OH <sub>2</sub> )51	4f	3m.	$\frac{1}{3}$	$\frac{2}{3}$	0.6679		non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.049, T = 183 K

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

References: [1] Müller A., Meyer J., Krickemeyer E., Beugholt C., Bögge H., Peters F., Schmidtman M., Kögerler P., Koop M.J. (1998), Chem. Eur. J. 4, 1000-1006.

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$\text{Na}_3[\text{NH}_4]_{12}\text{Mo}_{57}\text{Fe}_6[\text{NO}]_6\text{O}_{174}[\text{OH}]_3[\text{H}_2\text{O}]_{100}$	hP804	(194) $P6_3/mmc - 1^{19}\text{k}^{20};^5\text{h}^6\text{f}^2\text{e}$
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**(NH<sub>4</sub>)<sub>12</sub>Na<sub>3</sub>[H<sub>3</sub>Mo<sub>57</sub>Fe<sub>6</sub>(NO)<sub>6</sub>O<sub>177</sub>(H<sub>2</sub>O)<sub>24</sub>].76H<sub>2</sub>O [1]**

Structural features: Keggin-related Mo<sub>57</sub>Fe<sub>6</sub>(NO)<sub>6</sub>O<sub>174</sub>(OH)<sub>3</sub>(H<sub>2</sub>O)<sub>24</sub> units (MoO<sub>6</sub>, Mo[O<sub>5</sub>(OH)<sub>2</sub>] and Mo[O<sub>3</sub>(OH)(OH)<sub>2</sub>] octahedra, Mo[O<sub>6</sub>(NO)] pentagonal bipyramids and Fe[O<sub>4</sub>(OH)<sub>2</sub>] octahedra sharing edges and vertices) in a Mg-type (h.c.p.) arrangement; Na, NH<sub>4</sub> and additional H<sub>2</sub>O between the units.

Müller A. et al. (1994) [1]

Fe<sub>6</sub>H<sub>239.02</sub>Mo<sub>57</sub>N<sub>18.01</sub>Na<sub>3</sub>O<sub>277</sub>

$a = 2.3806$ ,  $c = 2.7634$  nm,  $c/a = 1.161$ ,  $V = 13.5627$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.022	0.1994	0.1512		single atom Mo
Mo2	24l	1	0.0429	0.2599	0.1918		octahedron O <sub>6</sub>
O3	24l	1	0.0469	0.37	0.0629		single atom Mo
Mo4	24l	1	0.0726	0.4067	0.1171		octahedron O <sub>6</sub>
O5	24l	1	0.0851	0.3377	0.1501		coplanar triangle Mo <sub>3</sub>
O6	24l	1	0.0914	0.4877	0.1049		non-collinear MoFe
O7	24l	1	0.1047	0.4534	0.1995		single atom Mo
O8	24l	1	0.1664	0.433	0.1098		non-coplanar triangle Mo <sub>3</sub>
O9	24l	1	0.2172	0.5513	0.0713		non-collinear MoFe
(OH <sub>2</sub> )10	24l	1	0.2477	0.0289	0.048		non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>
O11	24l	1	0.2939	0.0243	0.1973		single atom Mo
(OH <sub>2</sub> )12	24l	1	0.3798	0.1177	0.0396		single atom Na
O13	24l	1	0.3801	0.005	0.1494		non-collinear Mo <sub>2</sub>
O14	24l	1	0.3958	0.1298	0.152		single atom Mo
Mo15	24l	1	0.4074	0.08	0.1907		octahedron O <sub>6</sub>
(OH <sub>2</sub> )16	24l	1	0.4512	0.0557	0.0268		octahedron (OH <sub>2</sub> ) <sub>3</sub> (NH <sub>4</sub> )O <sub>2</sub>
O17	24l	1	0.4889	0.1086	0.1876		single atom Mo
(OH <sub>2</sub> )18	24l	1	0.5715	0.2099	0.1248	0.25	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )19	24l	1	0.5793	0.2225	0.0475	0.25	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )20	12k	.m.	0.0564	0.1128	0.6473	0.5	non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(NH <sub>4</sub> )21	12k	.m.	0.0661	0.1323	0.0747	0.667	8-vertex polyhedron O <sub>3</sub> (OH <sub>2</sub> ) <sub>5</sub>
(OH <sub>2</sub> )22	12k	.m.	0.0863	0.1727	0.544	0.5	non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )23	12k	.m.	0.0873	0.1746	0.7271	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )24	12k	.m.	0.1339	0.2678	0.6386		single atom Na
O25	12k	.m.	0.1404	0.2808	0.0432		single atom N
O26	12k	.m.	0.1444	0.2888	0.188		non-coplanar triangle Mo <sub>3</sub>
N27	12k	.m.	0.157	0.314	0.0816		non-collinear OMo
Mo28	12k	.m.	0.1794	0.3588	0.1338		7-vertex polyhedron NO <sub>6</sub>
Na29	12k	.m.	0.1895	0.379	0.5969	0.5	octahedron (OH <sub>2</sub> ) <sub>4</sub> O <sub>2</sub>
O30	12k	.m.	0.2087	0.4174	0.2002		non-collinear Mo <sub>2</sub>
O31	12k	.m.	0.2302	0.4604	0.019		single atom Mo
(OH <sub>2</sub> )32	12k	.m.	0.2414	0.4828	0.5903	0.5	single atom Na
Mo33	12k	.m.	0.2486	0.4972	0.074		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )34	12k	.m.	0.269	0.538	0.1607		single atom Mo
(OH <sub>2</sub> )35	12k	.m.	0.5093	0.0186	0.7025		non-collinear Mo <sub>2</sub>
(NH <sub>4</sub> )36	12k	.m.	0.525	0.05	0.1029	0.667	non-collinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )37	12k	.m.	0.5615	0.123	0.5175		single atom Fe

Fe38	12k	.m.	0.577	0.154	0.5876		octahedron O <sub>4</sub> (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )39	12k	.m.	0.596	0.192	0.6611		single atom Fe
O40	12j	m..	0.0344	0.2116	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
Mo41	12j	m..	0.0692	0.4652	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>3</sub> (OH)(OH <sub>2</sub> ) <sub>2</sub>
O42	12j	m..	0.0941	0.3328	<sup>1</sup> / <sub>4</sub>		single atom Mo
O43	12j	m..	0.3988	0.1171	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
O44	12j	m..	0.3992	0.0112	<sup>1</sup> / <sub>4</sub>		single atom Mo
(OH <sub>2</sub> )45	6h	mm2	0.0491	0.0983	<sup>1</sup> / <sub>4</sub>		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
Mo46	6h	mm2	0.1828	0.3657	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
(OH)47	6h	mm2	0.4381	0.8763	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
(NH <sub>4</sub> )48	6h	mm2	0.6045	0.209	<sup>1</sup> / <sub>4</sub>	0.667	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )49	6h	mm2	0.7396	0.4792	<sup>1</sup> / <sub>4</sub>		non-colinear (NH <sub>4</sub> ) <sub>2</sub>
(NH <sub>4</sub> )50	6h	mm2	0.8523	0.7046	<sup>1</sup> / <sub>4</sub>	0.667	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )51	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0004	0.5	non-coplanar hexagon (OH <sub>2</sub> ) <sub>6</sub>
(OH <sub>2</sub> )52	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6747		non-coplanar hexagon (OH <sub>2</sub> ) <sub>6</sub>
(OH <sub>2</sub> )53	4e	3m.	0	0	0.201	0.5	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.063, T = 193 K

Remarks: Part of non-framework H<sub>2</sub>O not located. We assigned an approximate value to the occupancy of sites (NH<sub>4</sub>) based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The structure determination reported in [1] is discussed in [2].

References: [1] Müller A., Plass W., Krickemeyer E., Dillinger S., Bögge H., Armatage A., Beugholt C., Bergmann U. (1994), Monatsh. Chem. 125, 525-533. [2] Müller A., Plass W., Krickemeyer E., Dillinger S., Bögge H., Armatage A., Proust A., Beugholt C., Bergmann U. (1994), Angew. Chem. Int. Ed. Engl. 33, 849-851.

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Na <sub>3</sub> [NH <sub>4</sub> ] <sub>18</sub> V <sub>6</sub> Mo <sub>63</sub> [NO] <sub>6</sub> O <sub>192</sub> [OH] <sub>3</sub> [H <sub>2</sub> O] <sub>53</sub>	hP806	(194) <i>P6<sub>3</sub>/mmc</i> – 1 <sup>19</sup> k <sup>21</sup> ; <sup>5</sup> ; <sup>3</sup> f <sup>2</sup>
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**(NH<sub>4</sub>)<sub>18</sub>Na<sub>3</sub>[H<sub>3</sub>Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>189</sub>(H<sub>2</sub>O)<sub>12</sub>(MoO)<sub>6</sub>]·41H<sub>2</sub>O [1]**

Structural features: Keggin-related Mo<sub>57</sub>V<sub>6</sub>(NO)<sub>6</sub>O<sub>186</sub>(OH)<sub>3</sub>(H<sub>2</sub>O)<sub>12</sub>(MoO)<sub>6</sub> units (MoO<sub>6</sub>, Mo[O<sub>5</sub>(OH<sub>2</sub>)] and Mo[O<sub>5</sub>(OH)] octahedra, Mo[O<sub>6</sub>(NO)] pentagonal bipyramids, MoO<sub>4</sub> tetrahedra and V[O<sub>5</sub>(OH<sub>2</sub>)] octahedra sharing edges and vertices) in a Mg-type (h.c.p.) arrangement; Na, NH<sub>4</sub> and additional H<sub>2</sub>O between the units.

Müller A. et al. (1998) [1]

H<sub>181</sub>Mo<sub>63</sub>N<sub>24</sub>Na<sub>3</sub>O<sub>254</sub>V<sub>6</sub>

*a* = 2.3587, *c* = 2.6542 nm, *c/a* = 1.125, *V* = 12.7882 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24f	1	0.0191	0.1961	0.1468		single atom Mo
Mo2	24f	1	0.04218	0.25718	0.18852		octahedron O <sub>6</sub>
O3	24f	1	0.0442	0.3686	0.054		
Mo4	24f	1	0.0688	0.4064	0.11	0.8	
Mo5	24f	1	0.0797	0.4101	0.1239	0.2	
O6	24f	1	0.0835	0.3353	0.1445		
O7	24f	1	0.0927	0.4877	0.0982		
O8	24f	1	0.1056	0.4521	0.1975		single atom Mo
O9	24f	1	0.1652	0.4309	0.1025		
O10	24f	1	0.2169	0.5509	0.0609		non-colinear MoV



(OH <sub>2</sub> )11	24l	1	0.2431	0.0343	0.0439	0.5	single atom (OH <sub>2</sub> )
O12	24l	1	0.2961	0.0294	0.1942		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )13	24l	1	0.3209	0.0891	0.0428	0.5	single atom (OH <sub>2</sub> )
O14	24l	1	0.3833	0.0069	0.1434		
Mo15	24l	1	0.39441	0.07861	0.18858		octahedron O <sub>6</sub>
O16	24l	1	0.4006	0.1353	0.1468		single atom Mo
(NH <sub>4</sub> )17	24l	1	0.4522	0.1122	0.0471		single atom (OH <sub>2</sub> )
O18	24l	1	0.4914	0.1083	0.1864		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )19	24l	1	0.5829	0.2207	0.0729	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )20	12k	.m.	0.036	0.072	0.6512	0.5	single atom (OH <sub>2</sub> )
Na21	12k	.m.	0.0439	0.0878	0.227	0.5	
(NH <sub>4</sub> )22	12k	.m.	0.06	0.12	0.073	0.5	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )23	12k	.m.	0.0678	0.1356	0.7207	0.5	single atom (OH <sub>2</sub> )
(OH <sub>2</sub> )24	12k	.m.	0.1355	0.271	0.6212		non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O25	12k	.m.	0.1377	0.2754	0.0363		single atom N
(NH <sub>4</sub> )26	12k	.m.	0.1421	0.2842	0.7349	0.5	
O27	12k	.m.	0.1433	0.2866	0.1864		non-coplanar triangle Mo <sub>3</sub>
N28	12k	.m.	0.1541	0.3082	0.074		non-colinear OMo
Mo29	12k	.m.	0.17844	0.35688	0.12773		7-vertex polyhedron NO <sub>6</sub>
O30	12k	.m.	0.2084	0.4168	0.1985		single atom Mo
O31	12k	.m.	0.2282	0.4564	0.0073		single atom Mo
Mo32	12k	.m.	0.24785	0.4957	0.0648		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )33	12k	.m.	0.2611	0.5222	0.6071	0.5	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )34	12k	.m.	0.2685	0.537	0.152		single atom Mo
O35	12k	.m.	0.5062	0.0124	0.6996		single atom Mo
O36	12k	.m.	0.5258	0.0516	0.1025		single atom Mo
Mo37	12k	.m.	0.53119	0.06238	0.16662		tetrahedron O <sub>4</sub>
O38	12k	.m.	0.5593	0.1186	0.5118		single atom V
V39	12k	.m.	0.57408	0.14816	0.5688		octahedron O <sub>5</sub> (OH <sub>2</sub> )
(OH <sub>2</sub> )40	12k	.m.	0.5966	0.1932	0.653		single atom V
O41	12j	m..	0.0266	0.2082	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
Mo42	12j	m..	0.06848	0.4633	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>5</sub> (OH)
O43	12j	m..	0.0925	0.3307	<sup>1</sup> / <sub>4</sub>		single atom Mo
O44	12j	m..	0.3992	0.0127	<sup>1</sup> / <sub>4</sub>		single atom Mo
O45	12j	m..	0.4022	0.1228	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )46	12i	.2.	0.4397	0	0	0.5	7-vertex polyhedron O <sub>4</sub> (NH <sub>4</sub> ) <sub>2</sub> (OH <sub>2</sub> )
Mo47	6h	mm2	0.18222	0.36444	<sup>1</sup> / <sub>4</sub>		octahedron O <sub>6</sub>
(OH)48	6h	mm2	0.4395	0.879	<sup>1</sup> / <sub>4</sub>		non-colinear Mo <sub>2</sub>
(OH <sub>2</sub> )49	6h	mm2	0.6103	0.2206	<sup>1</sup> / <sub>4</sub>	0.667	trigonal prism (OH <sub>2</sub> ) <sub>2</sub> O <sub>4</sub>
(OH <sub>2</sub> )50	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0063		hexagonal prism O <sub>6</sub> (OH <sub>2</sub> ) <sub>6</sub>
(OH <sub>2</sub> )51	4f	3m.	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.6881	0.5	non-coplanar triangle (OH <sub>2</sub> ) <sub>3</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.067, T = 203 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Müller A., Meyer J., Krickemeyer E., Beugholt C., Bögge H., Peters F., Schmidtman M., Kögerler P., Koop M.J. (1998), Chem. Eur. J. 4, 1000-1006.