

Space group (193) $P6_3/mcm$ 193
hP8

Cs_3O	hP8	(193) $P6_3/mcm$ – gb
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Cs₃O [1]

Structural features: Distorted close-packed Cs layers in h stacking; O in octahedral voids. OCs_6 octahedra share faces to Landolt-Börnstein form infinite columns.

Tsai K.R. et al. (1956) [1]

 Cs_3O $a = 0.878$, $c = 0.752$ nm, $c/a = 0.856$, $V = 0.5020$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cs1	6g	$m2m$	0.250	0	$\frac{1}{4}$		non-colinear O_2
O2	2b	$-3.m$	0	0	0		octahedron Cs_6

Transformation from published data ($P6_3/mcm$ *): origin shift 0 0 $\frac{1}{4}$

Experimental: powder, film, X-rays

Remarks: Transformed from a non-conventional setting with the origin shifted by 0 0 $\frac{1}{4}$ with respect to the International Tables for Crystallography.

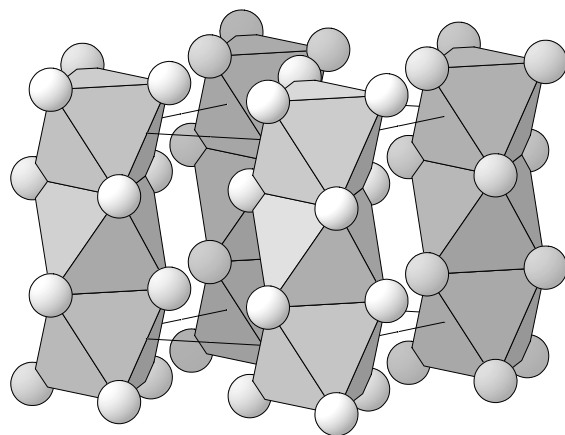
References: [1] Tsai K.R., Harris P.M., Lassetre E.N. (1956), J. Phys. Chem. 60, 345-347.

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hP8

TiCl_3	hP8	(193) $P6_3/mcm$ – gb
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TiCl₃ β [1]; TiBr_3 β (see remark); ZrI_3 [3]

Structural features: Close-packed Cl layers in h stacking; Ti in octahedral voids. TiCl_6 octahedra share faces to form infinite columns (infinite linear -Ti- chains). See Fig. III.54.

Fig. III.54. **TiCl₃ β**Arrangement of TiCl_6 octahedra.

Natta G. et al. (1958) [1]

 Cl_3Ti $a = 0.627$, $c = 0.582$ nm, $c/a = 0.928$, $V = 0.1982$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	6g	<i>m2m</i>	0.315	0	$\frac{1}{4}$		non-colinear Ti ₂
Ti2	2b	<i>-3.m</i>	0	0	0		octahedron Cl ₆

Experimental: powder, film, X-rays

Remarks: Additional reflections observed for TiI₃ and NbI₃ in [4] could be indexed with a 4-fold supercell (new axes 2a,2b,c). The same data are quoted in [2]. Referred to as TiBr₃ type in [1] (communication by W. Klemm, 1957).

References: [1] Natta G., Corradini P., Bassi W., Porri L. (1958), Atti Accad. Naz. Lincei, Cl. Sci. Fis., Mat. Nat., Rend. 24, 121-131. [2] Natta G., Corradini P., Allegra G. (1961), J. Polymer Sci. 51, 399-410. [3] Dahl L.F., Chiang T.I., Seabough P.W., Larsen E.M. (1964), Inorg. Chem. 3, 1236-1242. [4] Von Schnering H.G. (1966), Naturwissenschaften 53, 359-360.

193
hP12

Li ₂ [CO ₃]	hP12	(193) <i>P6₃/mcm</i> – gda
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Li₂CO₃ hp [1]

Structural features: 3D-framework of fused Li₁₂ hexagonal prisms, centered by CO₃ trigonal units; CO₃ units in consecutive layers are rotated by 60°.

Grzechnik A. et al. (2003) [1]

CLi₂O₃

a = 0.44568, *c* = 0.51254 nm, *c/a* = 1.150, *V* = 0.0882 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6g	<i>m2m</i>	0.2911	0	$\frac{1}{4}$		single atom C
Li2	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
C3	2a	<i>-62m</i>	0	0	$\frac{1}{4}$		coplanar triangle O ₃

Experimental: powder, diffractometer, X-rays, synchrotron, R_p = 0.014, p = 10 GPa

Remarks: Non-quenchable high-pressure phase.

References: [1] Grzechnik A., Bouvier P., Farina L. (2003), J. Solid State Chem. 173, 13-19.

193
hP14

Li ₂ PS ₃	hP14	(193) <i>P6₃/mcm</i> – ged
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Li₄P₂S₆ [1]

Structural features: Close-packed S layers in h stacking; Li atoms and P₂ dumbbells in octahedral voids (disorder for the latter). Single S₃P-PS₃ units.

Mercier R. et al. (1982) [1]

Li₂PS₃

a = 0.607, *c* = 0.6577 nm, *c/a* = 1.084, *V* = 0.2099 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	6g	<i>m2m</i>	0.3237	0	$\frac{1}{4}$		trigonal prism P ₂ Li ₄
P2	4e	3. <i>m</i>	0	0	0.1715	0.5	
Li3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron S ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.047$, $T = 293\text{ K}$

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

References: [1] Mercier R., Malugani J.P., Fahys B., Douglade J., Robert G. (1982), J. Solid State Chem. 43, 151-162.

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hP16

Mn_5Si_3

hP16

(193) $P6_3/mcm - g^2d$

Mn_5Si_3 [2], Strukturbericht notation $D8_8$

Structural features: SiMn_8Mn monocapped square antiprisms (SiMn_6Mn_3 tricapped trigonal prisms) share atoms to form a 3D-framework with infinite columns of face-linked Mn_6 octahedra along $0\ 0\ z$ and infinite linear $-\text{Mn}-$ chains along $\frac{1}{3}\ \frac{2}{3}\ z$. See Fig. III.55.

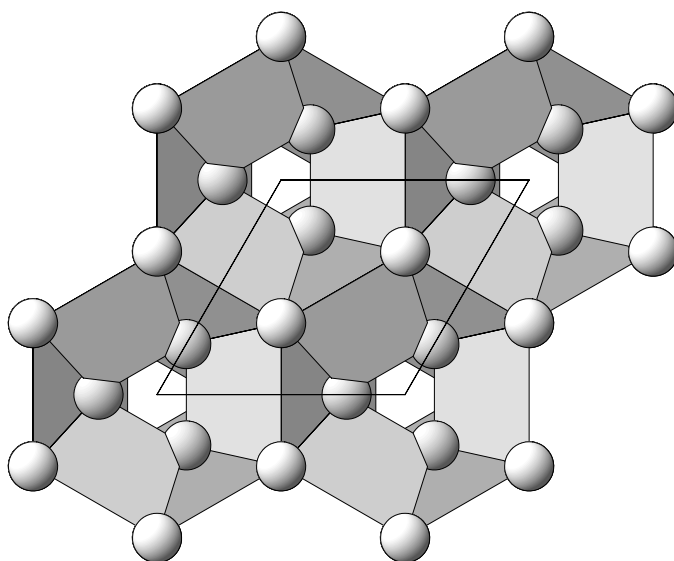


Fig. III.55. **Mn_5Si_3**

Arrangement of SiMn_6 trigonal prisms viewed along $[001]$.

Lander G.H., Brown P.J. (1967) [1]

Mn_5Si_3

$a = 0.6912$, $c = 0.4812\text{ nm}$, $c/a = 0.696$, $V = 0.1991\text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	6g	$m2m$	0.236	0	$\frac{1}{4}$		15-vertex polyhedron $\text{Si}_5\text{Mn}_{10}$
Si2	6g	$m2m$	0.5991	0	$\frac{1}{4}$		pseudo Frank-Kasper Mn_9Si_2
Mn3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex Frank-Kasper Mn_8Si_6

Experimental: single crystal, diffractometer, X-rays, $R = 0.056$

Remarks: Cell parameters from [2]. Electron density study. A refinement on neutron powder diffraction data is reported in [3].

References: [1] Lander G.H., Brown P.J. (1967), Philos. Mag. 16, 521-542. [2] Bmark K., Borén B., Westgren A. (1936), Metallwirtsch. Metallwiss. Metalltech. 15, 835-836. [3] Binczycka H., Dimitrijevic Z., Gajic B., Szytula A. (1973), Phys. Status Solidi A 19, K13-K17.

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hP16

$\text{Zr}_3\text{Ti}_2\text{Ga}_3$	<i>hP16</i>	(193) $P6_3/mcm - g^2d$
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(Zr,Ti)₅Ga₃ [1]

Structural features: $\text{Ga}(\text{Zr}_4\text{Ti}_4)\text{Zr}$ monocapped square antiprisms ($\text{Ga}(\text{Zr}_2\text{Ti}_4)\text{Zr}_3$ tricapped trigonal prisms) share atoms to form a 3D-framework with infinite columns of face-linked Zr_6 octahedra along $00z$ and infinite linear -Ti- chains along $\frac{1}{3}\frac{2}{3}z$. Ordering variant of Mn_5Si_3 .

Belyavina N.N. et al. (1982) [1]

 $\text{Ga}_3\text{Ti}_2\text{Zr}_3$ $a = 0.7954$, $c = 0.5532$ nm, $c/a = 0.695$, $V = 0.3031$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zr1	6g	<i>m2m</i>	0.239	0	$\frac{1}{4}$		15-vertex polyhedron $\text{Ga}_5\text{Zr}_6\text{Ti}_4$
Ga2	6g	<i>m2m</i>	0.61	0	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Zr}_5\text{Ti}_4\text{Ga}_2$
Ti3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex Frank-Kasper $\text{Ti}_2\text{Ga}_6\text{Zr}_6$

Experimental: powder, diffractometer, X-rays, $R = 0.076$

References: [1] Belyavina N.N., Suprunenko P.A., Markiv V.Y., Shevchenko I.P. (1982), Phys. Met. (Transl. of Metallofizika) 4, 179-184.

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hP16

ErCo_3Ge_2	<i>hP16</i>	(193) $P6_3/mcm - gedb$
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Er_{6-x}Co₆Ge₄ [1]

Structural features: Deformation derivative of CeCo_3B_2 with part of the Er atoms displaced out of the hexagon-mesh Ge layers (disorder).

Bodak O.I. et al. (1990) [1]

 $\text{Co}_3\text{Er}_{1.03}\text{Ge}_2$ $a = 0.5091$, $c = 0.7861$ nm, $c/a = 1.544$, $V = 0.1764$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	6g	<i>m2m</i>	0.4813	0	$\frac{1}{4}$		trigonal prism Co_6
Er2	4e	3. <i>m</i>	0	0	0.1533	0.274	
Ge3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		
Er4	2b	-3. <i>m</i>	0	0	0	0.48	

Transformation from published data: origin shift $00\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.036$

Remarks: Short interatomic distances: $d(\text{Er1-Er1}) = 0.241$ nm; the authors did not consider possible occupation of site 4e by Co or Ge (replacement of R atoms by M_2 dumbbells). Short interatomic distances for partly occupied site(s).

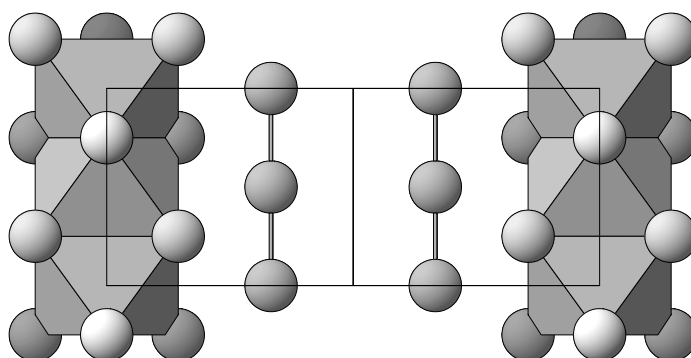
References: [1] Bodak O.I., Oleksin O.Y., Pecharskii V.K., Belsky V.K., Zhukov S.G. (1990), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1990(2), 30-34.

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hP18

Ti_5Ga_4	<i>hP18</i>	(193) $P6_3/mcm - g^2db$
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Ti₅Ga₄ [1]

Structural features: Infinite columns of face-sharing GaTi₆ octahedra share atoms with GaTi₈Ti monocapped square antiprisms (GaTi₆Ti₃ tricapped trigonal prisms) to form a 3D-framework with infinite linear -Ti- chains along $\frac{1}{3} \frac{2}{3} z$. See Fig. III.56.

Fig. III.56. **Ti₅Ga₄**

Arrangement of GaTi₆ octahedra and infinite linear -Ti- chains in (110).

Pötzschke M., Schubert K. (1962) [1]

Ga₄Ti₅

$a = 0.7861$, $c = 0.5452$ nm, $c/a = 0.694$, $V = 0.2918$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	6g	$m2m$	0.29	0	$\frac{1}{4}$		pentacapped trigonal prism Ga ₇ Ti ₄
Ga2	6g	$m2m$	0.62	0	$\frac{1}{4}$		pseudo Frank-Kasper Ti ₉ Ga ₄
Ti3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex Frank-Kasper Ti ₈ Ga ₆
Ga4	2b	$-3.m$	0	0	0		14-vertex Frank-Kasper Ti ₆ Ga ₈

Experimental: powder, film, X-rays, $R = 0.121$

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

References: [1] Pötzschke M., Schubert K. (1962), Z. Metallkd. 53, 474-488. [2] Schubert K., Meissner H.G., Pötzschke M., Rossteutscher W., Stolz E. (1962), Naturwissenschaften 49, 57.

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hP18

CuHf₅Sn₃

hP18

(193) $P6_3/mcm - g^2db$

Hf₅Sn₃Cu [1], Nowotny phase; Gd₅Bi₃Cu [3]; Mo₅Si₃C_x [2]; U₃TiSb₅ [4]; V₅Ge₃B [2]; Mo₅Ge₃C_x [5]

Structural features: SnHf₈Hf monocapped square antiprisms (SnHf₆Hf₃ tricapped trigonal prisms) share atoms to form a 3D-framework; Cu in octahedral voids. Infinite columns of face-sharing CuHf₆ octahedra along $0\ 0\ z$ and infinite linear -Hf- chains along $\frac{1}{3} \frac{2}{3} z$. Filled-up derivative of Mn₅Si₃ with Cu in octahedral voids. No B-B contact in V₅Ge₃B. See Fig. III.57.

Rieger W. et al. (1965) [1]

CuHf₅Sn₃

$a = 0.8527$, $c = 0.5822$ nm, $c/a = 0.683$, $V = 0.3666$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hf1	6g	$m2m$	0.27	0	$\frac{1}{4}$		7-vertex polyhedron Cu_2Sn_5
Sn2	6g	$m2m$	0.62	0	$\frac{1}{4}$		tricapped trigonal prism Hf_9
Hf3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		square prism (cube) Hf_2Sn_6
Cu4	2b	$-3.m$	0	0	0		square prism (cube) Hf_6Cu_2

Experimental: powder, film, X-rays

Remarks: We assigned an approximate value to the x-coordinate of site Sn2 in agreement with the Ti_5Ga_4 type, assigned by the authors. C was not located in [5]. Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [6], maximum 50% occupation of the C site is expected for carbides.

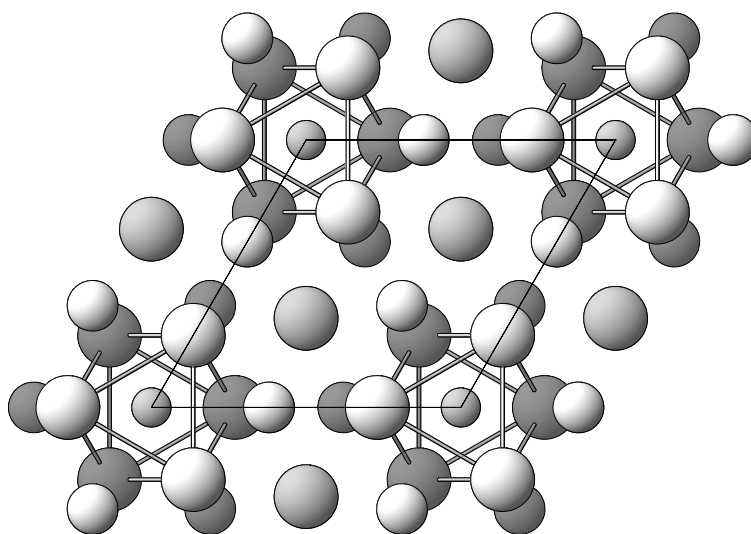


Fig. III.57. **$\text{Hf}_5\text{Sn}_3\text{Cu}$**

Arrangement of Hf (large), Sn (medium) and Cu (small) atoms viewed along [001].

References: [1] Rieger W., Nowotny H., Benesovsky F. (1965), Monatsh. Chem. 96, 98-103. [2] Parthé E., Jeitschko W., Sadagopan V. (1965), Acta Crystallogr. 19, 1031-1037. [3] Hohnke D., Parthé E. (1969), J. Less-Common Met. 17, 291-296. [4] Brylak M., Jeitschko W. (1994), Z. Naturforsch. B 49, 747-752. [5] Jeitschko W., Nowotny H., Benesovsky F. (1964), Monatsh. Chem. 95, 1242-1246. [6] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163.

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hP18

$\text{Gd}_3\text{Ti}_2\text{MnSi}_3$	<i>hP18</i>	(193) $P6_3/mcm - g^2db$
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$\text{Gd}_3\text{Ti}_2\text{MnSi}_3$ [1]; $\text{Ti}_3\text{Mo}_2\text{Si}_3\text{C}_x$ [2]

Structural features: $\text{Si}(\text{Gd}_4\text{Ti}_4)\text{Gd}$ monocapped square antiprisms (tricapped trigonal prisms) share atoms to form a 3D-framework; Mn in octahedral voids. Infinite columns of face-sharing MnGd_6 octahedra along $00z$ and infinite linear -Ti- chains along $\frac{1}{3}\frac{2}{3}z$. Ordering variant of Ti_5Ga_4 .

Morozkin A.V. (1999) [1]

$\text{Gd}_3\text{MnSi}_3\text{Ti}_2$

$a = 0.8508$, $c = 0.6418$ nm, $c/a = 0.754$, $V = 0.4023$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Gd1	6g	$m2m$	0.232	0	$1/4$		4-vertex polyhedron Si_2Mn_2
Si2	6g	$m2m$	0.669	0	$1/4$		non-colinear Gd_2
Ti3	4d	3.2	$1/3$	$2/3$	0		square prism (cube) Ti_2Si_6
Mn4	2b	$-3.m$	0	0	0		octahedron Gd_6

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

Remarks: Atom coordinates not determined for C-stabilized $\text{Ti}_3\text{Mo}_2\text{Si}_3$. Based on the occupation restriction rule for neighboring octahedral interstitial sites in close-packed structures [3], maximum 50% occupation of the C site is expected for carbides.

References: [1] Morozkin A.V. (1999), J. Alloys Compd. 292, 162-165. [2] Schachner H., Cerwenka E., Nowotny H. (1954), Monatsh. Chem. 85, 245-254. [3] Parthé E., Yvon K. (1970), Acta Crystallogr. B 26, 153-163.

193
hP20

$\text{Ti}_{4.73}\text{Pt}_{0.65}\text{Sb}_3$	hP20	(193) $P6_3/mcm - g^2dba$
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$\text{Ti}_{4.73}\text{Pt}_{0.65}\text{Sb}_3$ [1]

Structural features: Derivative of CuHf_5Sn_3 with partial vacancies on the Ti sites and Pt partly delocalized along 0 0 z.

Kaiser J.W. et al. (2001) [1]

$\text{Pt}_{0.65}\text{Sb}_3\text{Ti}_{4.73}$

$a = 0.8081$, $c = 0.5548$ nm, $c/a = 0.687$, $V = 0.3138$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ti1	6g	$m2m$	0.2682	0	$1/4$	0.937	single atom Pt
Sb2	6g	$m2m$	0.6134	0	$1/4$		tricapped trigonal prism Ti_9
Ti3	4d	3.2	$1/3$	$2/3$	0	0.959	square prism (cube) Ti_2Sb_6
Pt4	2b	$-3.m$	0	0	0	0.515	
Pt5	2a	$-62m$	0	0	$1/4$	0.136	

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

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

References: [1] Kaiser J.W., Haase M.G., Jeitschko W. (2001), Z. Anorg. Allg. Chem. 627, 2369-2376.

193
hP20

Ta_3SnS_6	hP20	(193) $P6_3/mcm - kcba$
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$\text{Sn}_{0.33}\text{TaS}_2$ [1]

Structural features: Close-packed S layers in ABBB stacking; Ta in trigonal prismatic, Sn in octahedral voids. TaS_6 trigonal prisms share edges to form infinite slabs.

Eppinga R., Wiegers G.A. (1980) [1]

S_6SnTa_3

$a = 0.5756$, $c = 1.451$ nm, $c/a = 2.521$, $V = 0.4163$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12k	..m	0.33333	0	0.16		non-coplanar triangle Ta ₃
Ta2	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism S ₆
Sn3	2b	-3.m	0	0	0		octahedron S ₆
Ta4	2a	-62m	0	0	$\frac{1}{4}$		trigonal prism S ₆

Transformation from published data (*P*6₃22): origin shift 0 0 $\frac{1}{4}$

Experimental: powder, diffractometer, X-rays

Remarks: Idealized *x*-coordinate for the S site. The description in space group (182) *P*6₃22 in [1] does not take into consideration all symmetry elements of the proposed structure.

References: [1] Eppinga R., Wiegers G.A. (1980), *Physica B+C* (Amsterdam) 99, 121-127.

193
*hP*20

LiAl ₂ Cl[OH] ₆	<i>hP</i> 20	(193) <i>P</i> 6 ₃ / <i>mcm</i> – kdba
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LiAl₂(OH)₆Cl [1]

Structural features: Infinite slabs of edge-linked Li(OH)₆ and Al(OH)₆ octahedra alternate with triangle-mesh Cl layers along [001].

Besserguenev A.V. et al. (1997) [1]

Al₂ClH₆LiO₆

a = 0.51, *c* = 1.42994 nm, *c/a* = 2.804, *V* = 0.3221 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	..m	0.365	0	0.0672		non-colinear Al ₂
Al2	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
Li3	2b	-3.m	0	0	0		octahedron O ₆
Cl4	2a	-62m	0	0	$\frac{1}{4}$		trigonal prism O ₆
H5	12k	..m	0.3121	0	0.1335		

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

Experimental: powder, diffractometer, neutrons, time-of-flight, *wR_p* = 0.016

Remarks: Refinement on combined X-ray synchrotron and neutron TOF powder diffraction data. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (176) *P*6₃/*m* was tested and rejected.

References: [1] Besserguenev A.V., Fogg A.M., Francis R.J., Price S.J., O'Hare D., Isupov V.P., Tolochko B.P. (1997), *Chem. Mater.* 9, 241-247.

193
*hP*22

Nb ₃ Bi ₂ S ₆	<i>hP</i> 22	(193) <i>P</i> 6 ₃ / <i>mcm</i> – hged
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Bi_{0.67}NbS₂β [1]

Structural features: Two directly superposed close-packed S₃ and hexagon-mesh Bi₂ layers alternate along [001]; Nb in trigonal prismatic (S₆) voids. NbS₆ trigonal prisms share edges to form infinite slabs.

Eppinga R., Wiegers G.A. (1980) [1]

Bi₂Nb₃S₆

a = 0.5743, *c* = 1.737 nm, *c/a* = 3.025, *V* = 0.4961 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.154		tetrahedron Nb ₃ Bi
Nb2	6g	m2m	0.33333	0	$\frac{1}{4}$		trigonal prism S ₆
S3	4e	3.m	0	0	0.154		non-coplanar triangle Nb ₃
Bi4	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal bipyramid S ₂ Bi ₃

Transformation from published data (*P*₆₃22): origin shift 0 0 $\frac{1}{4}$

Experimental: powder, diffractometer, X-rays

Remarks: Idealized coordinates. The description in space group (182) *P*₆₃22 in [1] does not take into consideration all symmetry elements of the proposed model.

References: [1] Eppinga R., Wiegers G.A. (1980), *Physica B+C* (Amsterdam) 99, 121-127.

193
hP22

Ta ₅ N ₆	hP22	(193) <i>P</i> ₆₃ / <i>mcm</i> – kgd
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Ta₅N₆ [2]; Nb₅N₆ [3]

Structural features: Close-packed N layers in AABB stacking; Ta in trigonal prismatic and octahedral voids. Layers of edge-linked TaN₆ trigonal prisms are interconnected via TaN₆ octahedra to form a 3D-framework. NTa₅ square pyramids share triangular faces and edges to form a 3D-framework.

Petrinin V.F. et al. (1980) [1]

N₆Ta₅

$a = 0.516$, $c = 1.027$ nm, $c/a = 1.990$, $V = 0.2368$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12k	..m	0.337	0	0.121		5-vertex polyhedron Ta ₅
Ta2	6g	m2m	0.670	0	$\frac{1}{4}$		trigonal prism N ₆
Ta3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron N ₆

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

Experimental: powder, diffractometer, neutrons

Remarks: The structure was studied jointly on X-ray and neutron diffraction data. Additional reflections indicate a possible superstructure for Nb₅N₆ [3]. Nb₅N₆ is identical to the phase called Nb(N,O) III in [4]. In [3] the position of the second Nb site is misprinted as 6Nb in 4d instead of 4Nb in 4d.

References: [1] Petrinin V.F., Sorokin N.I., Borovinskaya I.P., Pityulin A.N. (1980), *Sov. Powder Metall. Met. Ceram.* 19, 191-192 (Poroshk. Metall. 3, 62-64). [2] Fontbonne A., Gilles J.C. (1969), *Rev. Int. Hautes Temp. Refract.* 6, 181-192. [3] Terao N. (1971), *J. Less-Common Met.* 23, 159-169. [4] Terao N. (1965), *Jpn. J. Appl. Phys.* 4, 353-357.

193
hP22

Au ₆ Hg ₅	hP22	(193) <i>P</i> ₆₃ / <i>mcm</i> – kgd
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Au₆Hg₅ [2]

Structural features: Distorted Kagomé-mesh Hg₃ layers and hexagon-mesh Hg₂ layers alternate with Au₃ layers (Au forms triangles) along [001].

Lindahl T. (1970) [1]

Au₆Hg₅

$a = 0.69937$, $c = 1.0148$ nm, $c/a = 1.451$, $V = 0.4299$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Au1	12k	..m	0.2416	0	0.1098		bicapped square prism Au ₅ Hg ₅
Hg2	6g	m2m	0.5864	0	¹ / ₄		16-vertex Frank-Kasper Au ₈ Hg ₈
Hg3	4d	3.2	¹ / ₃	² / ₃	0		icosahedron Au ₆ Hg ₆

Experimental: single crystal, diffractometer, X-rays, wR = 0.075

Remarks: The atom distribution could not be determined in [2].

References: [1] Lindahl T. (1970), Acta Chem. Scand. 24, 946-952. [2] Berndt A.F., Cummins J.D. (1970), Acta Crystallogr. B 26, 864-867.

193
hP24

La ₅ Os ₃ C ₄	hP24	(193) P6 ₃ /mcm – g ² fdb
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La₅Os₃C_{4-x} [1]

Structural features: Filled-up derivative of Mn₅Si₃ with C in octahedral (La₆ and La₄Os₂) voids.

Wachtmann K.H. et al. (1997) [1]

C_{3.25}La₅Os₃

$a = 0.91957$, $c = 0.67386$ nm, $c/a = 0.733$, $V = 0.4935$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
La1	6g	m2m	0.24762	0	¹ / ₄		7-vertex polyhedron C ₄ Os ₃
Os2	6g	m2m	0.59867	0	¹ / ₄		non-colinear C ₂
C3	6f	..2/m	¹ / ₂	0	0		colinear Os ₂
La4	4d	3.2	¹ / ₃	² / ₃	0		coplanar triangle C ₃
C5	2b	-3.m	0	0	0	0.25	octahedron La ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.015

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for site C5.

References: [1] Wachtmann K.H., Hüfken T., Jeitschko W. (1997), J. Solid State Chem. 131, 49-53.

193
hP24

CeF ₃	hP24	(193) P6 ₃ /mcm – kgca
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CeF₃ [1], fluorite-(Ce), Strukturbericht notation D0₆

Structural features: CeF₃ trigonal bipyramids share vertices to form infinite layers.

Afanasiev M.L. et al. (1972) [1]

CeF₃

$a = 0.713$, $c = 0.729$ nm, $c/a = 1.022$, $V = 0.3209$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12k	..m	0.29	0	0.06		non-coplanar triangle F ₂ Ce
Ce2	6g	m2m	0.66667	0	¹ / ₄		pseudo Frank-Kasper F ₁₁
F3	4c	-6..	¹ / ₃	² / ₃	¹ / ₄		coplanar triangle Ce ₃
F4	2a	-62m	0	0	¹ / ₄		tricapped trigonal prism Ce ₃ F ₆

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

Remarks: Conclusions based on ^{19}F NMR spectroscopy. Cell parameters omitted; we took approximate values from the literature and assigned an idealized value to the x -coordinate of the Ce site.

References: [1] Afanasiev M.L., Habuda S.P., Lundin A.G. (1972), Acta Crystallogr. B 28, 2903-2905.

193
hP24

Ca_6GaN_5

hP24

(193) $P6_3/mcm$ – kgda

Ca_6GaN_5 [1]; Ca_6FeN_5 [1]

Structural features: Close-packed Ca layers in AABB stacking; Ga and N in trigonal prismatic, additional N in octahedral voids. Approximately planar layers containing single GaN_3 trigonal units alternate with infinite slabs of edge-linked NCa_6 octahedra along [001]. See Fig. III.58.

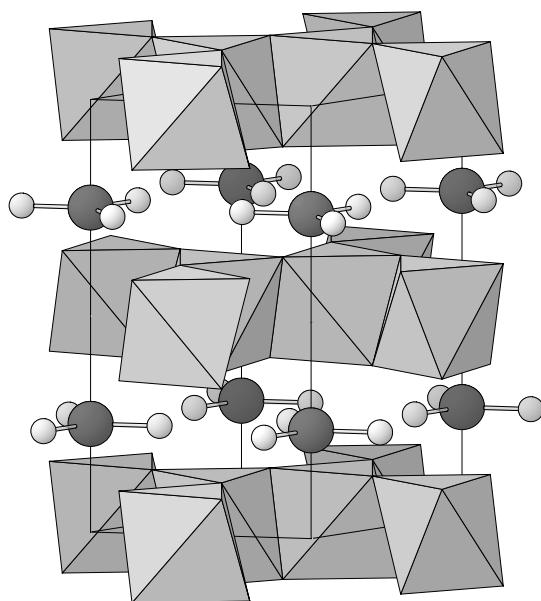


Fig. III.58. **Ca_6GaN_5**

Arrangement of NCa_6 octahedra and GaN_3 triangles (Ga atoms dark, N atoms light).

Cordier G. et al. (1990) [1]

Ca_6GaN_5

$a = 0.6277$, $c = 1.2198$ nm, $c/a = 1.943$, $V = 0.4162$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ca1	12k	$\dots m$	0.5935	0	0.1226		non-coplanar triangle N_3
N2	6g	$m2m$	0.3126	0	$\frac{1}{4}$		single atom Ga
N3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron Ca_6
Ga4	2a	$-62m$	0	0	$\frac{1}{4}$		coplanar triangle N_3

Experimental: single crystal, diffractometer, X-rays, $R = 0.090$

Remarks: Identical to the phase called $\text{Ca}_{21}\text{Ga}_3\text{N}_{17}$ in [2]. Preliminary data in [3].

References: [1] Cordier G., Höhn P., Kniep R., Rabenau A. (1990), Z. Anorg. Allg. Chem. 591, 58-66. [2] Verdier P., Marchand R., Lang J. (1976), Rev. Chim. Miner. 13, 214-218. [3] Cordier G., Rönninger S. (1988), Z. Kristallogr. 182, 60-61.

193
hP24

K_2PbO_3	<i>hP24</i>	(193) <i>P6₃/mcm</i> – kgdb
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 K_2PbO_3 β [1]

Structural features: Close-packed O layers in AABB stacking; Pb and K in octahedral, additional K in trigonal prismatic voids. PbO_6 octahedra share edges to form infinite layers.

Delmas C. et al. (1976) [1]

K_2O_3Pb

$a = 0.5958$, $c = 1.239$ nm, $c/a = 2.080$, $V = 0.3809$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>k</i>	.. <i>m</i>	0.585	0	0.098		non-colinear Pb_2
K2	6 <i>g</i>	<i>m2m</i>	0.27	0	$\frac{1}{4}$		8-vertex polyhedron O_6K_2
Pb3	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O_6
K4	2 <i>b</i>	-3. <i>m</i>	0	0	0		octahedron O_6

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

Experimental: powder, diffractometer, X-rays

Remarks: High-pressure phase.

References: [1] Delmas C., Demazeau G., Devalette M., Fouassier C., Hagenmuller P. (1976), J. Solid State Chem. 19, 87-94.

193
hP24

$Nb_5(N_{0.89}O_{0.11})_6$	<i>hP24</i>	(193) <i>P6₃/mcm</i> – kgdb
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 $Nb_5(N,O)_6$ [1]

Structural features: Close-packed (N,O) layers in AABB stacking; Nb in trigonal prismatic and octahedral voids. Layers of edge-linked $Nb(N,O)_6$ trigonal prisms are interconnected via $Nb(N,O)_6$ octahedra to form a 3D-framework. Derivative of Ta_5N_6 with partial disorder on the octahedral sites.

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

$N_{5.34}Nb_{4.98}O_{0.66}$

$a = 0.52018$, $c = 1.03676$ nm, $c/a = 1.993$, $V = 0.2429$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12 <i>k</i>	.. <i>m</i>	0.659	0	0.1198		
Nb2	6 <i>g</i>	<i>m2m</i>	0.3256	0	$\frac{1}{4}$		trigonal prism N_6
Nb3	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.975	octahedron N_6
Nb4	2 <i>b</i>	-3. <i>m</i>	0	0	0	0.026	octahedron N_6

$M1 = 0.89N + 0.11O$

Experimental: powder, diffractometer, X-rays, $R = 0.015$

Remarks: We assigned an approximate value to the N/O ratio of site M based on the nominal composition.

References: [1] Tyutyunnik A., Grins J., Svensson G. (1998), J. Alloys Compd. 278, 83-91.

193
hP24

$Nb_3(Nb_{0.5}Mn_{0.5})_2Mn(N_{0.9}O_{0.1})_6$	<i>hP24</i>	(193) <i>P6₃/mcm</i> – kgdb
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MnNb₂(N,O)₃ [1]

Structural features: Close-packed (N,O) layers in AABB stacking; Nb in trigonal prismatic, Mn and (Mn,Nb) in octahedral voids. Layers of edge-linked Nb(N,O)₆ trigonal prisms are interconnected via Mn(N,O)₆ and (Mn,Nb)(N,O)₆ octahedra to form a 3D-framework.

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

Mn_{2.13}N_{5.40}Nb_{3.87}O_{0.60}

$a = 0.52629$, $c = 1.0529$ nm, $c/a = 2.001$, $V = 0.2526$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12k	$\bar{3}m$	0.321	0	0.1231		octahedron Mn ₃ Nb ₃
Nb2	6g	$m\bar{2}m$	0.668	0	$\frac{1}{4}$		trigonal prism N ₆
M3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron N ₆
Mn4	2b	$\bar{3}m$	0	0	0		octahedron N ₆

M1 = 0.9N + 0.1O; M3 = 0.563Mn + 0.437Nb

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

Experimental: powder, diffractometer, X-rays, $R_p = 0.012$

Remarks: We assigned approximate values to the N/O and Mn/Nb ratios of sites M based on the nominal composition. In [1] the number of formula units per cell Z is misprinted as 3 instead of 4.

References: [1] Tyutyunnik A., Grins J., Svensson G. (1998), J. Alloys Compd. 278, 83-91.

193
hP26

Rb_{0.81}W₃O₉

hP26

(193) $P6_3/mcm$ – jgfb

Rb_{0.27}WO₃ [2], HTB (hexagonal tungsten bronze)

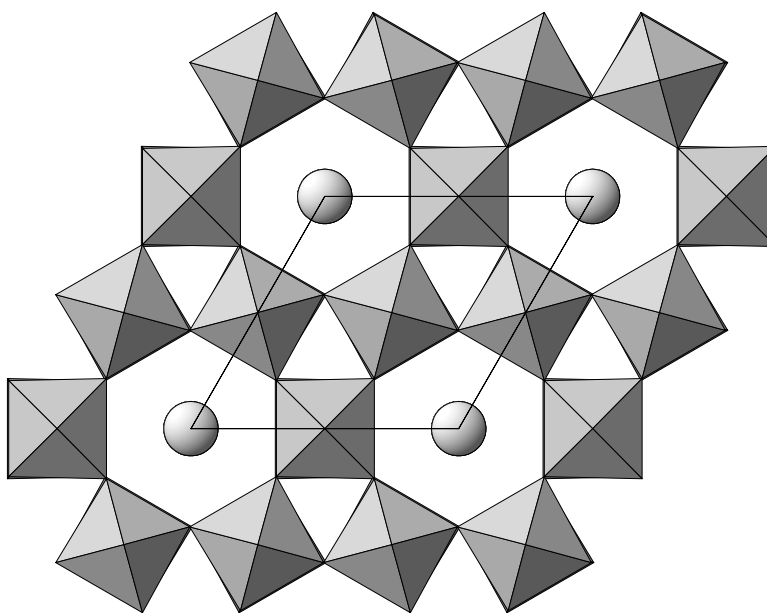


Fig. III.59. **Rb_{0.27}WO₃**

Arrangement of WO₆ octahedra and Rb atoms viewed along [001].

Structural features: WO_6 octahedra share vertices to form a 3D-framework; Rb in channels of hexagonal cross-section parallel to $[001]$. See Fig. III.59.

Brusetti R. et al. (2003) [1]

O_9RbW_3

$a = 0.73939$, $c = 0.75758$ nm, $c/a = 1.025$, $V = 0.3587$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	$m..$	0.216	0.423	$1/4$		non-colinear W_2
W2	6g	$m2m$	0.48241	0	$1/4$		octahedron O_6
O3	6f	$..2/m$	$1/2$	0	0		colinear W_2
Rb4	2b	$-3.m$	0	0	0		hexagonal prism O_{12}

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

Remarks: Additional reflections indicate lower symmetry; the structure was also refined in space groups (143) $P3$ and (173) $P6_3$ ($R = 0.037$ and 0.039 , respectively).

References: [1] Brusetti R., Bordet P., Marcus J. (2003), J. Solid State Chem. 172, 148-159. [2] Magnéli A. (1953), Acta Chem. Scand. 7, 315-324.

193
hP26

$\text{Ca}(\text{Al}_{0.5}\text{Si}_{0.5})_4\text{O}_8$	hP26	(193) $P6_3/mcm$ – khcb
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$\text{CaAl}_2\text{Si}_2\text{O}_8$ hexagonal [2]

Structural features: $(\text{Al},\text{Si})\text{O}_4$ tetrahedra share vertices to form infinite double slabs; Ca between the slabs in channels parallel to $[001]$.

Dimitrijevic R. et al. (1996) [1]

$\text{Al}_2\text{CaO}_8\text{Si}_2$

$a = 0.51175$, $c = 1.47716$ nm, $c/a = 2.886$, $V = 0.3350$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	$..m$	0.387	0	0.0974		non-colinear Al_2
M2	8h	3..	$1/3$	$2/3$	0.1403		tetrahedron O_4
O3	4c	$-6..$	$1/3$	$2/3$	$1/4$		colinear Al_2
Ca4	2b	$-3.m$	0	0	0		octahedron O_6

$\text{M2} = 0.50\text{Al} + 0.50\text{Si}$

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

References: [1] Dimitrijevic R., Dondur V., Kremenovic A. (1996), Zeolites 16, 294-300. [2] Takeuchi Y., Donnay G. (1959), Acta Crystallogr. 12, 465-470.

193
hP28

$\text{W}_3\text{Pb}_{0.87}\text{O}_9$	hP28	(193) $P6_3/mcm$ – jgfe
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$\text{Pb}_{0.29}\text{WO}_3$ [1], HTB (hexagonal tungsten bronze)

Structural features: WO_6 octahedra share vertices to form a 3D-framework; Pb in channels of hexagonal cross-section parallel to $[001]$.

Tatsumi K. et al. (1997) [1]

$\text{O}_9\text{Pb}_{0.87}\text{W}_3$

$a = 0.74073$, $c = 0.75646$ nm, $c/a = 1.021$, $V = 0.3594$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12j	<i>m.</i>	0.17	0.4	$\frac{1}{4}$		single atom W
W2	6g	<i>m2m</i>	0.505	0	$\frac{1}{4}$		octahedron O ₆
O3	6f	<i>..2/m</i>	$\frac{1}{2}$	0	0		colinear W ₂
Pb4	4e	<i>3.m</i>	0	0	0.207	0.435	

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.053$

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

References: [1] Tatsumi K., Hibino M., Kudo T. (1997), Solid State Ionics 96, 35-40.

193
hP28

Na _{0.67} (Mg _{0.25} Mn _{0.75})O ₂	hP28	(193) <i>P6₃/mcm</i> – kgdcb
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Na_{0.67}(Mg_{0.25}Mn_{0.75})O₂ form P2 [1]

Structural features: (Mn,Mg)O₆ octahedra share edges to form infinite slabs; Na in trigonal prismatic coordination between the slabs (in part split site). Variant of Na_{0.5}CoO₂.

Paulsen J.M. et al. (2000) [1]

Mg_{0.25}Mn_{0.75}Na_{0.54}O₂

$a = 0.5009$, $c = 1.1218$ nm, $c/a = 2.240$, $V = 0.2438$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	<i>..m</i>	0.646	0	0.08		non-coplanar triangle Mn ₂ Mg
Na2	6g	<i>m2m</i>	0.301	0	$\frac{1}{4}$	0.31	
M3	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
Na4	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.35	
M5	2b	-3.m	0	0	0		octahedron O ₆

M3 = 0.975Mn + 0.025Mg; M5 = 0.70Mg + 0.30Mn

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

Remarks: Refinement of the occupancy of site O1 gave 1.04 (standard uncertainty omitted). Refinement of an additional Na site in Wyckoff position 2a showed no significant deviation from zero occupancy. Short interatomic distances for partly occupied site(s).

References: [1] Paulsen J.M., Donaberger R.A., Dahn J.R. (2000), Chem. Mater. 12, 2257-2267.

193
hP30

Li[N ₃][H ₂ O]	hP30	(193) <i>P6₃/mcm</i> – jg ² db
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LiN₃·H₂O [1]

Structural features: Triangle-mesh Li layers and layers containing N₃ linear units and H₂O non-linear units (in the plane) alternate along [001].

Reckeweg O., Simon A. (2003) [1]

H₂LiN₃O

$a = 0.92401$, $c = 0.56006$ nm, $c/a = 0.606$, $V = 0.4141$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12j	<i>m.</i>	0.3328	0.47916	$\frac{1}{4}$		single atom N

O2	6g	<i>m2m</i>	0.17873	0	$\frac{1}{4}$	non-colinear Li ₂
N3	6g	<i>m2m</i>	0.59127	0	$\frac{1}{4}$	non-colinear N ₂
Li4	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0	octahedron N ₆
Li5	2b	-3. <i>m</i>	0	0	0	octahedron O ₆
H6	12j	<i>m..</i>	0.0789	0.2749	$\frac{1}{4}$	

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

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

References: [1] Reckeweg O., Simon A. (2003), Z. Naturforsch. B 58, 1097-1104.

193
hP30

WO ₃	<i>hP30</i>	(193) <i>P6₃/mcm</i> – kjg
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WO₃ hexagonal [1]

Structural features: WO₆ octahedra share vertices to form a 3D-framework (one split O site) with large channels of hexagonal cross-section.

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

O₃W

$a = 0.73244$, $c = 0.76628$ nm, $c/a = 1.046$, $V = 0.3560$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	<i>..m</i>	0.445	0	0.016	0.5	single atom W
O2	12 <i>j</i>	<i>m..</i>	0.183	0.3745	$\frac{1}{4}$		
W3	6g	<i>m2m</i>	0.4721	0	$\frac{1}{4}$		

Experimental: powder, diffractometer, X-rays, R = 0.068

Remarks: Metastable phase. Short interatomic distances: d(W-O) = 0.181 nm. Short interatomic distances for partly occupied site(s). Space group (182) *P6₃22* was tested and rejected.

References: [1] Oi J., Kishimoto A., Kudo T., Hiratani M. (1992), J. Solid State Chem. 96, 13-19.

193
hP32

Cs _{0.96} W ₃ O ₉	<i>hP32</i>	(193) <i>P6₃/mcm</i> – kjgb
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Cs_{0.32}WO₃ [2], HTB (hexagonal tungsten bronze); K_{0.32}WO₃ [2]

Structural features: WO₆ octahedra share vertices to form a 3D-framework (one split O site); Cs in channels of hexagonal cross-section parallel to [001].

Oi J. et al. (1993) [1]

Cs_{0.90}O₉W₃

$a = 0.74049$, $c = 0.76098$ nm, $c/a = 1.028$, $V = 0.3614$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	<i>..m</i>	0.493	0	0.01	0.5	non-colinear W ₂
O2	12 <i>j</i>	<i>m..</i>	0.2102	0.4185	$\frac{1}{4}$		
W3	6g	<i>m2m</i>	0.4857	0	$\frac{1}{4}$		
Cs4	2b	-3. <i>m</i>	0	0	0	0.9	hexagonal prism O ₁₂

Experimental: powder, diffractometer, X-rays, R_B = 0.024

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

References: [1] Oi J., Kishimoto A., Kudo T. (1993), J. Solid State Chem. 103, 176-185. [2] Kihlberg L., Hussain A. (1979), Mater. Res. Bull. 14, 667-674.

193
hP34

$(\text{Ta}_{0.5}\text{Nb}_{0.5})_8\text{N}_9$	<i>hP34</i>	(193) $P6_3/mcm - k^2dca$
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(Nb,Ta)₈N₉ [1]

Structural features: Close-packed N layers in hc_2 stacking; (Nb,Ta) in octahedral voids. N(Nb,Ta)₆ trigonal prisms and N(Nb,Ta)₅ square pyramids share atoms to form a 3D-framework.

Ettmayer P., Vendl A. (1980) [1]

$\text{N}_9\text{Nb}_4\text{Ta}_4$

$a = 0.5158$, $c = 1.610$ nm, $c/a = 3.121$, $V = 0.3710$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	12 <i>k</i>	.. <i>m</i>	0.333	0	0.078		square pyramid Nb ₅
M2	12 <i>k</i>	.. <i>m</i>	0.667	0	0.156		octahedron N ₆
M3	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron N ₆
N4	4 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Nb ₆
N5	2 <i>a</i>	-62 <i>m</i>	0	0	$\frac{1}{4}$		trigonal prism Nb ₆

M2 = 0.5Nb + 0.5Ta; M3 = 0.5Nb + 0.5Ta

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

Experimental: powder, diffractometer, X-rays

Remarks: We assigned an approximate value to the Nb/Ta ratio of the cation sites based on the compositions of two multiphase samples.

References: [1] Ettmayer P., Vendl A. (1980), J. Less-Common Met. 72, 209-217.

193
hP34

$\text{Tl}_{0.9}\text{W}_3\text{O}_9$	<i>hP34</i>	(193) $P6_3/mcm - kjge$
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Tl_{0.30}WO₃ [1], HTB (hexagonal tungsten bronze)

Structural features: WO₆ octahedra share vertices to form a 3D-framework (one split O site); Tl in channels of hexagonal cross-section parallel to [001] (split site).

Labbé P. et al. (1978) [1]

$\text{O}_9\text{Tl}_{0.90}\text{W}_3$

$a = 0.7381$, $c = 0.75091$ nm, $c/a = 1.017$, $V = 0.3543$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	.. <i>m</i>	0.4635	0	0.002	0.5	non-colinear W ₂
O2	12 <i>j</i>	<i>m</i> ..	0.2082	0.42	$\frac{1}{4}$		
W3	6 <i>g</i>	<i>m2m</i>	0.52256	0	$\frac{1}{4}$		
Tl4	4 <i>e</i>	3. <i>m</i>	0	0	0.0307	0.45	

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). Space group (185) $P6_3cm$ was tested and rejected. Average structure; additional reflections could be indexed with a 2-fold supercell (new axes $a, b, 2c$).

References: [1] Labbé P., Goreaud M., Raveau B., Monier J.C. (1978), Acta Crystallogr. B 34, 1433-1438.

193
hP36

$Nb_6(Nb_{0.2}Al_{0.8})_2Ir(Ir_{0.5}Al_{0.5})_6Al_3$	<i>hP36</i>	(193) $P6_3/mcm$ – kjgdb
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(AlIrNb) A' [1]

Structural features: Substitution derivative of $MgZn_2$. Tetrahedrally close-packed structure (Frank-Kasper phase).

Horyn R. (1977) [1]

$Al_{7.61}Ir_4Nb_{6.39}$

$a = 0.884$, $c = 0.822$ nm, $c/a = 0.930$, $V = 0.5563$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Nb1	12 <i>k</i>	.. <i>m</i>	0.3326	0	0.5645		16-vertex Frank-Kasper $Al_{11}IrNb_4$
M2	12 <i>j</i>	<i>m</i> ..	0.1634	0.496	$\frac{1}{4}$		icosahedron Al_6Nb_6
Al3	6 <i>g</i>	<i>m2m</i>	0.1704	0	$\frac{1}{4}$		icosahedron $Al_4Ir_2Nb_6$
M4	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron Al_6Nb_6
Ir5	2 <i>b</i>	-3. <i>m</i>	0	0	0		icosahedron Al_6Nb_6

$M2 = 0.5Al + 0.5Ir$; $M4 = 0.805Al + 0.195Nb$

Experimental: single crystal, diffractometer, X-rays, $R = 0.088$

References: [1] Horyn R. (1977), J. Less-Common Met. 56, 103-111.

193
hP38

$Ag_3Eu[CN]_6[H_2O]_3$	<i>hP38</i>	(193) $P6_3/mcm$ – k ² gfa
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Eu[Ag(CN)₂]₃·3H₂O [1]

Structural features: Single $Eu(CN)_6(OH_2)_3$ trigonal prismatic units (a central EuN_6O_3 tricapped trigonal prism) arranged in slabs separated by Kagomé-mesh Ag layers.

Assefa Z. et al. (1995) [1]

$Ag_3C_6EuH_6N_6O_3$

$a = 0.6688$, $c = 1.8479$ nm, $c/a = 2.763$, $V = 0.7158$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12 <i>k</i>	.. <i>m</i>	0.2609	0	0.1502		single atom C
C2	12 <i>k</i>	.. <i>m</i>	0.3461	0	0.0965		single atom N
(OH ₂)3	6 <i>g</i>	<i>m2m</i>	0.6334	0	$\frac{1}{4}$		single atom Eu
Ag4	6 <i>f</i>	.. <i>2/m</i>	$\frac{1}{2}$	0	0		colinear C ₂
Eu5	2 <i>a</i>	-62 <i>m</i>	0	0	$\frac{1}{4}$		tricapped trigonal prism (OH ₂) ₃ N ₆

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.035$, $T = 293$ K

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

References: [1] Assefa Z., Staples R.J., Fackler J.P. Jr., Patterson H.H., Shancle G. (1995), Acta Crystallogr. C 51, 2527-2529.

193
hP40

$\text{Ba}_{10}\text{Al}_3\text{Ge}_7$	<i>hP40</i>	(193) $P6_3/mcm - k^2gdca$
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$\text{Ba}_{10}\text{Al}_3\text{Ge}_7$ [1]

Structural features: Single propeller-like Al_3Ge_7 units where three AlGe_3 trigonal units share a common Ge atom.

Widera A., Schäfer H. (1977) [1]

$\text{Al}_3\text{Ba}_{10}\text{Ge}_7$

$a = 0.9749$, $c = 1.647$ nm, $c/a = 1.689$, $V = 1.3556$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ba1	12 <i>k</i>	.. <i>m</i>	0.2522	0	0.5982		15-vertex polyhedron $\text{Ge}_5\text{Al}_2\text{Ba}_8$
Ge2	12 <i>k</i>	.. <i>m</i>	0.3955	0	0.1168		single atom Al
Al3	6 <i>g</i>	<i>m2m</i>	0.273	0	$\frac{1}{4}$		tricapped trigonal prism Ge_3Ba_6
Ba4	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex Frank-Kasper Ge_6Ba_8
Ba5	4 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		17-vertex polyhedron $\text{Al}_3\text{Ge}_6\text{Ba}_8$
Ge6	2 <i>a</i>	-62 <i>m</i>	0	0	$\frac{1}{4}$		tricapped trigonal prism Al_3Ba_6

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.071$

References: [1] Widera A., Schäfer H. (1977), Z. Naturforsch. B 32, 619-624.

193
hP40

$\text{Na}_3\text{Sr}_7\text{P}_9\text{O}$	<i>hP40</i>	(193) $P6_3/mcm - k^2gdcb$
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$\text{Na}_3\text{Sr}_7(\text{P}_3)_3\text{O}$ [1]; $\text{Na}_3\text{Eu}_7(\text{P}_3)_3\text{O}$ [1]

Structural features: Non-linear P_3 chains and single OSr_6 octahedra; additional Sr and Na between the units.

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

$\text{Na}_3\text{OP}_9\text{Sr}_7$

$a = 0.8809$, $c = 1.3876$ nm, $c/a = 1.575$, $V = 0.9325$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	12 <i>k</i>	.. <i>m</i>	0.2432	0	0.60092		single atom O
P2	12 <i>k</i>	.. <i>m</i>	0.4124	0	0.1146		single atom P
P3	6 <i>g</i>	<i>m2m</i>	0.2739	0	$\frac{1}{4}$		non-colinear P_2
Na4	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron P_6
Sr5	4 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism P_9
O6	2 <i>b</i>	-3.. <i>m</i>	0	0	0		octahedron Sr_6

$M1 = 0.833\text{Sr} + 0.167\text{Na}$

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.035$, $T = 296$ K

References: [1] Lin J., Hönle W., Von Schnering H.G. (1992), J. Alloys Compd. 178, 455-465.

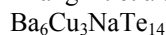
193
hP48

$\text{NaBa}_6\text{Cu}_3\text{Te}_{14}$	<i>hP48</i>	(193) $P6_3/mcm - k_j g^3 db$
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NaBa₆Cu₃Te₁₄ [1]

Structural features: Cu₃Te₁₄ units (rings of three vertex-linked CuTe₄ tetrahedra; the non-shared Te atoms and an additional Te above the tetrahedron edge form non-linear Te₃ chains) are loosely interconnected via longer Te-Te distances to form infinite columns parallel to [001]; Na in octahedral voids along the column axes, additional Te in Ba₆ trigonal prisms between the columns.

Zhang X. et al. (1995) [1]

 $a = 1.4123$, $c = 0.9075$ nm, $c/a = 0.643$, $V = 1.5676$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Te1	12 <i>k</i>	.. <i>m</i>	0.32036	0	0.0268		non-collinear CuTe
Ba2	12 <i>j</i>	<i>m</i> ..	0.2444	0.4509	$\frac{1}{4}$		10-vertex polyhedron Te ₉ Cu
Cu3	6 <i>g</i>	<i>m2m</i>	0.1924	0	$\frac{1}{4}$		tetrahedron Te ₄
Te4	6 <i>g</i>	<i>m2m</i>	0.4678	0	$\frac{1}{4}$		non-collinear Te ₂
Te5	6 <i>g</i>	<i>m2m</i>	0.8271	0	$\frac{1}{4}$		non-collinear Cu ₂
Te6	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		trigonal prism Ba ₆
Na7	2 <i>b</i>	-3. <i>m</i>	0	0	0		hexagonal prism Te ₆ Cu ₆

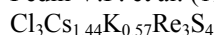
Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.037$, $T = 173$ KReferences: [1] Zhang X., Schindler J.L., Hogan T., Albritton Thomas J., Kannewurf C.R., Kanatzidis M.G. (1995), *Angew. Chem.* 107, 117-120.193
hP50

$(\text{Cs}_{0.72}\text{K}_{0.28})_2\text{Re}_3\text{S}_4\text{Cl}_3$	<i>hP50</i>	(193) $P6_3/mcm - k^3 ged$
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(Cs_{0.72}K_{0.28})₂Re₃S₄Cl₃ [1]

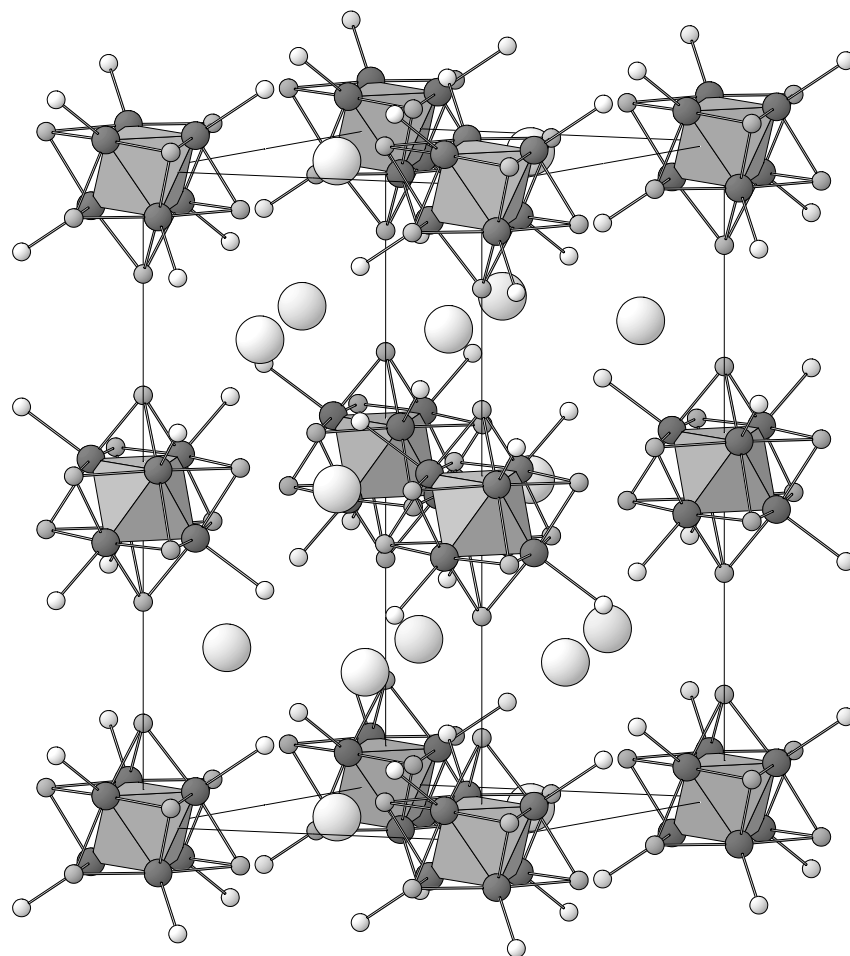
Structural features: Single Re₆S₈Cl₆ clusters (a central Re₆ octahedron surrounded by a S₈ cube and a large Cl₆ octahedron) in a simple hexagonal arrangement. See Fig. III.60.

Fedin V.P. et al. (1998) [1]

 $a = 0.9667$, $c = 1.853$ nm, $c/a = 1.917$, $V = 1.4996$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Re1	12 <i>k</i>	.. <i>m</i>	0.15435	0	0.05693		tricapped trigonal prism S ₄ ClRe ₄
S2	12 <i>k</i>	.. <i>m</i>	0.2866	0	0.5532		non-coplanar triangle Re ₃
Cl3	12 <i>k</i>	.. <i>m</i>	0.3592	0	0.1318		single atom Re
M4	6 <i>g</i>	<i>m2m</i>	0.6552	0	$\frac{1}{4}$	0.67	10-vertex polyhedron Cl ₆ S ₄
S5	4 <i>e</i>	3. <i>m</i>	0	0	0.1575		non-coplanar triangle Re ₃
M6	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron S ₆ Cl ₆

 $M4 = 0.673\text{Cs} + 0.327\text{K}$; $M6 = 0.763\text{Cs} + 0.237\text{K}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.039$ References: [1] Fedin V.P., Virovets A.A., Sykes A.G. (1998), *Inorg. Chim. Acta* 271, 228-230.

Fig. III.60. $(\text{Cs}_{0.72}\text{K}_{0.28})_2\text{Re}_3\text{S}_4\text{Cl}_3$

Arrangement of 20-atom clusters (Re_6 octahedron + S_8 cube + Cl_6 octahedron) and (Cs, K) atoms (large).

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hP54

$\text{Cs}_2\text{Re}_3\text{S}_4\text{Br}_3[\text{H}_2\text{O}]$

hP54

(193) $P6_3/mcm - k^3\text{gedc}$

$\text{Cs}_4[\text{Re}_6\text{S}_8\text{Br}_6] \cdot 2\text{H}_2\text{O}$ [1]

Structural features: Single $\text{Re}_6\text{S}_8\text{Br}_6$ clusters (a central Re_6 octahedron surrounded by a S_8 cube and a large Br_6 octahedron) in a simple hexagonal arrangement.

Yarovoi S.S. et al. (2003) [1]

$\text{Br}_3\text{Cs}_2\text{H}_2\text{ORe}_3\text{S}_4$

$a = 0.9762$, $c = 1.8763$ nm, $c/a = 1.922$, $V = 1.5485$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Re1	12 <i>k</i>	.. <i>m</i>	0.1532	0	0.0564		tricapped trigonal prism S_4BrRe_4
S2	12 <i>k</i>	.. <i>m</i>	0.2835	0	0.5526		non-coplanar triangle Re_3
Br3	12 <i>k</i>	.. <i>m</i>	0.3684	0	0.1351		single atom Re

Cs4	6g	<i>m2m</i>	0.6708	0	$\frac{1}{4}$	0.667	icosahedron O ₂ Br ₆ S ₄
S5	4e	3. <i>m</i>	0	0	0.1562		non-coplanar triangle Re ₃
Cs6	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		icosahedron S ₆ Br ₆
O7	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism Cs ₃ Br ₆
H8	24l	1	0.351	0.59	0.221	0.333	

Experimental: single crystal, diffractometer, X-rays, R = 0.027

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the occupancy of the H site is misprinted as implicit 1 instead of $\frac{1}{3}$ (from nominal composition).

References: [1] Yarovoi S.S., Solodovnikov S.F., Mironov Y.V., Fedorov V.E. (2003), J. Struct. Chem. 44, 318-321 (Zh. Strukt. Khim. 44, 355-358).

193
hP54

(Ce _{0.5} Ta _{0.5}) ₂ Ta ₆ O ₁₉	hP54	(193) <i>P6₃/mcm</i> – k ³ hgd
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CeTa₇O₁₉ [1]

Structural features: TaO₇ pentagonal bipyramids share edges and vertices to form double slabs.

Gatehouse B.M. (1979) [1]

CeO₁₉Ta₇

$a = 0.6226$, $c = 1.9976$ nm, $c/a = 3.208$, $V = 0.6706$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	.. <i>m</i>	0.241	0	0.656		non-collinear Ta ₂
Ta2	12 <i>k</i>	.. <i>m</i>	0.3606	0	0.1562		7-vertex polyhedron O ₇
O3	12 <i>k</i>	.. <i>m</i>	0.398	0	0.059		single atom Ta
O4	8 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.131		non-coplanar triangle Ta ₃
O5	6 <i>g</i>	<i>m2m</i>	0.396	0	$\frac{1}{4}$		non-collinear Ta ₂
M6	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		8-vertex polyhedron O ₈

M6 = 0.5Ce + 0.5Ta

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

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

Remarks: The structure was later redetermined in space group (188) *P-6c2* [2].

References: [1] Gatehouse B.M. (1979), J. Solid State Chem. 27, 209-213. [2] Johnson A.W.S., Gatehouse B.M. (1980), Acta Crystallogr. B 36, 523-526.

193
hP54

W ₃ InO ₉	hP54	(193) <i>P6₃/mcm</i> – lk ² g
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In_{0.33}WO₃ [1], HTB (hexagonal tungsten bronze)

Structural features: WO₆ octahedra share vertices to form a 3D-framework (split O sites); In in channels of hexagonal cross-section parallel to [001] (displaced from the channel axis, split site).

Labbe P. et al. (1979) [1]

In_{0.94}O₉W₃

$a = 0.73716$, $c = 0.75038$ nm, $c/a = 1.018$, $V = 0.3531$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.2091	0.4192	0.2192	0.5	
In2	12k	..m	0.0743	0	0.0	0.156	
O3	12k	..m	0.4547	0	0.0061	0.5	
W4	6g	m2m	0.51549	0	$\frac{1}{4}$		

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). Average structure; the authors state that true symmetry is probably not hexagonal.

References: [1] Labbé P., Goreaud M., Raveau B., Monier J.C. (1979), Acta Crystallogr. B 35, 1557-1564.

193
hP58

$\text{W}_3\text{In}_{0.63}\text{O}_9$	hP58	(193) $P6_3/mcm - lk^2ge$
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In_{0.21}WO₃ [2], HTB (hexagonal tungsten bronze)

Structural features: WO₆ octahedra share vertices to form a 3D-framework (split O sites); In in channels of hexagonal cross-section parallel to [001] (in part displaced from the channel axis, split sites).

Labbé P. et al. (1979) [1]

In_{0.65}O₉W₃

$a = 0.73883$, $c = 0.75065$ nm, $c/a = 1.016$, $V = 0.3549$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.2096	0.423	0.2261	0.5	
In2	12k	..m	0.0547	0	0.0	0.049	
O3	12k	..m	0.4702	0	0.0003	0.5	
W4	6g	m2m	0.52209	0	$\frac{1}{4}$		
In5	4e	3.m	0	0	0.0743	0.177	

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

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

Remarks: Homogeneity range In_xWO₃, 0.15 < x < 0.31. Short interatomic distances for partly occupied site(s). Average structure; additional reflections indicated a possible superstructure.

References: [1] Labbé P., Goreaud M., Raveau B., Monier J.C. (1979), Acta Crystallogr. B 35, 1557-1564. [2] Labbé P., Goreaud M., Raveau B., Monier J.C. (1978), Acta Crystallogr. B 34, 1433-1438.

193
hP60

$\text{Na}_{0.1}(\text{Zn}_{0.68}\text{Cr}_{0.32})[\text{SO}_4]_{0.21}[\text{OH}]_2[\text{H}_2\text{O}]_{1.5}$	hP60	(193) $P6_3/mcm - lk^2edba$
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Na_{0.098}[Zn_{0.68}Cr_{0.32}(OH)₂](SO₄)_{0.209}·1.47H₂O [1]

Structural features: Slabs of edge-linked (Zn,Cr)(OH)₆ octahedra and double layers containing a partly disordered arrangement of SO₄ tetrahedra, H₂O molecules and Na atoms alternate along [001].

Ennadi A. et al. (1994) [1]

Cr_{0.32}H_{4.64}Na_{0.10}O_{4.17}S_{0.21}Zn_{0.68}

$a = 0.5407$, $c = 2.2116$ nm, $c/a = 4.09$, $V = 0.5600$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24l	1	0.2399	0.3728	0.1781	0.33	non-colinear O(OH ₂)
O2	12k	..m	0.2507	0	0.1624	0.32	non-colinear (OH ₂) ₂
(OH)3	12k	..m	0.3365	0	0.5458		non-coplanar triangle Zn ₃
S4	4e	3.m	0	0	0.1851	0.32	tetrahedron O ₄
M5	4d	3.2	1/3	2/3	0		octahedron (OH) ₆
M6	2b	-3.m	0	0	0		octahedron (OH) ₆
M7	2a	-62m	0	0	1/4	0.94	colinear S ₂

M5 = 0.680Zn + 0.320Cr; M6 = 0.680Zn + 0.320Cr; M7 = 0.680O + 0.320Na

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

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

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Additional reflections could be indexed with a 3-fold supercell (new axes 2a+b, -a+b, c).

References: [1] Ennadi A., Khaldi M., De Roy A., Besse J.P. (1994), Mol. Cryst. Liq. Cryst. Sci. Technol. Sect. A 244, 373-378.

193
hP64

K ₃ Nb ₈ O ₂₁	hP64	(193) <i>P</i> 6 ₃ / <i>mcm</i> – lk ² g ² d
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K₃Nb₈O₂₁ [2]

Structural features: Units of six edge-linked NbO₆ octahedra share vertices to form infinite columns parallel to [001], which are interconnected via common vertices with additional NbO₆ octahedra to form a 3D-framework. See Fig. III.61.

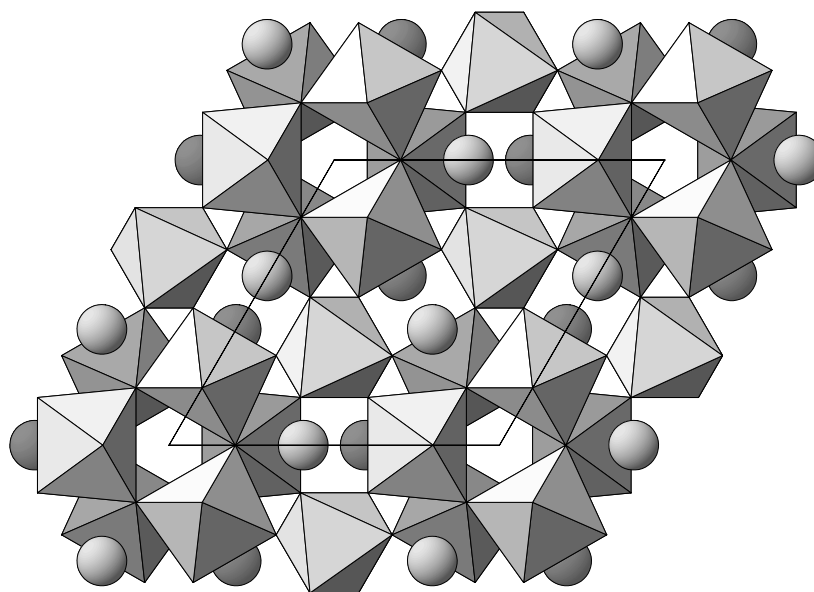


Fig. III.61. K₃Nb₈O₂₁

Arrangement of NbO₆ octahedra and K atoms viewed along [001].

Benabbas A. et al. (1993) [1]



$a = 0.91584$, $c = 1.20404$ nm, $c/a = 1.315$, $V = 0.8746$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.1675	0.4818	0.0958		non-collinear Nb ₂
O2	12k	..m	0.2006	0	0.574		non-coplanar triangle Nb ₃
Nb3	12k	..m	0.24888	0	0.09468		octahedron O ₆
O4	6g	m2m	0.207	0	$\frac{1}{4}$		non-collinear Nb ₂
K5	6g	m2m	0.5938	0	$\frac{1}{4}$		trigonal prism O ₆
Nb6	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.044, T = 294 K

References: [1] Benabbas A., Borel M.M., Grandin A., Leclaire A., Raveau B. (1993), Acta Crystallogr. C 49, 439-441. [2] Groult D., Chailleux J.M., Choynet J., Raveau B. (1976), J. Solid State Chem. 19, 235-244.

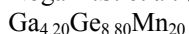
193
hP66

$\text{Mn}_{20}(\text{Ga}_{0.7}\text{Ge}_{0.3})_6\text{Ge}_7$	hP66	(193) $P6_3/mcm - j^2ig^3fdb$
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Mn₂₀Ga₄Ge₉ [1]

Structural features: Distorted derivative of ht-Co₂Ge with an ordered arrangement of vacancies, [(Mn₁₁Ge)(Mn₉□₃)][(Ga,Ge)₆Ge₆].

Noga A.S. et al. (1991) [1]



$a = 1.4384$, $c = 0.51805$ nm, $c/a = 0.360$, $V = 0.9282$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	12j	m..	0.1767	0.5007	$\frac{1}{4}$		pentacapped trigonal prism Ga ₄ GeMn ₆
M2	12j	m..	0.3299	0.4679	$\frac{1}{4}$		8-vertex polyhedron Mn ₈
Mn3	12i	..2	0.17	0.34	0		icosahedron Ga ₂ Ge ₄ Mn ₆
Mn4	6g	m2m	0.144	0	$\frac{1}{4}$		pentacapped trigonal prism Ge ₇ Mn ₄
Ge5	6g	m2m	0.329	0	$\frac{1}{4}$		15-vertex Frank-Kasper Mn ₉ Ge ₂ Ga ₄
Ge6	6g	m2m	0.7872	0	$\frac{1}{4}$		14-vertex Frank-Kasper Mn ₈ Ge ₄ Ga ₂
Mn7	6f	..2/m	$\frac{1}{2}$	0	0		icosahedron Mn ₆ Ga ₄ Ge ₂
Mn8	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		14-vertex Frank-Kasper Mn ₈ Ga ₆
Ge9	2b	-3.m	0	0	0		14-vertex Frank-Kasper Mn ₆ Ge ₈

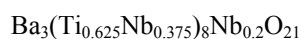
M2 = 0.7Ga + 0.3Ge

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

Experimental: single crystal, diffractometer, X-rays, R = 0.049

Remarks: Homogeneity range Mn₂₀(Ga_xGe_{1-x})₁₃, 0.23 < x < 0.35. In [1] the chemical formula is misprinted as Mn₂₀Ga₉Ge₄ instead of Mn₂₀Ga₄Ge₉ (better agreement with the refinement and with the graph for composition dependence in fig. 2).

References: [1] Noga A.S., Sichevich O.M., Zavodnik V.E., Grin Y.N. (1991), Sov. Phys. Crystallogr. 36, 794-796 (Kristallografiya 36, 1403-1407).

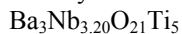


hP66

(193) $P6_3/mcm - \text{lk}^2\text{g}^2\text{da}$ **Ba₃Nb_{3.2}Ti₅O₂₁ [1]**

Structural features: Units of six edge-linked (Ti,Nb)O₆ octahedra share vertices to form infinite columns parallel to [001], which are interconnected via common vertices with additional (Ti,Nb)O₆ octahedra to form a 3D-framework; additional Nb in trigonal voids. Filled-up derivative of K₃Nb₈O₂₁.

Mercey C. et al. (1979) [1]


 $a = 0.902, c = 1.1796 \text{ nm}, c/a = 1.308, V = 0.8311 \text{ nm}^3, Z = 2$

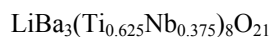
site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.177	0.501	0.105		non-colinear Ti ₂
O2	12k	..m	0.189	0	0.581		non-coplanar triangle Ti ₃
M3	12k	..m	0.246	0	0.095		octahedron O ₆
O4	6g	m2m	0.22	0	1/4		coplanar triangle Ti ₂ Nb
Ba5	6g	m2m	0.592	0	1/4		trigonal prism O ₆
M6	4d	3.2	1/3	2/3	0		octahedron O ₆
Nb7	2a	-62m	0	0	1/4	0.2	coplanar triangle O ₃

M3 = 0.625Ti + 0.375Nb; M6 = 0.625Ti + 0.375Nb

Experimental: powder, X-rays, R_B = 0.071

Remarks: Homogeneity range Ba₃Nb_{4-4x}Ti_{4+5x}O₂₁, 0 < x < 0.30. We assigned an approximate value to the Nb/Ti ratio of sites M based on the nominal composition.

References: [1] Mercey C., Groult D., Raveau B. (1979), Rev. Chim. Miner. 16, 165-173.

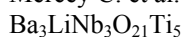


hP66

(193) $P6_3/mcm - \text{lk}^2\text{g}^2\text{da}$ **LiBa₃Nb₃Ti₅O₂₁ [1]**

Structural features: Units of six edge-linked (Ti,Nb)O₆ octahedra share vertices to form infinite columns parallel to [001], which are interconnected via common vertices with (Nb,Ti)O₆ octahedra to form a 3D-framework. Filled-up derivative of K₃Nb₈O₂₁ with Li in trigonal voids.

Mercey C. et al. (1978) [1]


 $a = 0.9072, c = 1.167 \text{ nm}, c/a = 1.286, V = 0.8318 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.169	0.483	0.108		non-colinear TiNb
O2	12k	..m	0.214	0	0.589		non-coplanar triangle Ti ₃
M3	12k	..m	0.242	0	0.094		octahedron O ₆
O4	6g	m2m	0.223	0	1/4		coplanar triangle Ti ₂ Li
Ba5	6g	m2m	0.596	0	1/4		trigonal prism O ₆
M6	4d	3.2	1/3	2/3	0		octahedron O ₆
Li7	2a	-62m	0	0	1/4		coplanar triangle O ₃

M3 = 0.75Ti + 0.25Nb; M6 = 0.75Nb + 0.25Ti

Experimental: powder, diffractometer, X-rays, R_B = 0.064

References: [1] Mercey C., Groult D., Raveau B. (1978), Mater. Res. Bull. 13, 797-804.

193
hP76

$\text{Th}_2\text{Ta}_9\text{O}_{26.5}$	<i>hP76</i>	(193) $P6_3/mcm - k^4hg^2dc$
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$\text{Th}_4\text{Ta}_{18}\text{O}_{53}$ [1]

Structural features: Triple layers of edge-linked TaO_7 pentagonal bipyramids (common vertices between the layers) share vertices with infinite layers of edge-linked ThO_6 octahedra to form a 3D-framework (partly ordered O vacancies).

Busche J., Gruehn R. (1996) [1]

$\text{O}_{26.50}\text{Ta}_9\text{Th}_2$

$a = 0.62554$, $c = 2.7709$ nm, $c/a = 4.430$, $V = 0.9390$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12k	..m	0.251	0	0.6105		non-colinear Ta ₂
Ta2	12k	..m	0.35729	0	0.11331		7-vertex polyhedron O ₇
O3	12k	..m	0.392	0	0.1797		non-colinear Ta ₂
O4	12k	..m	0.398	0	0.0395		non-coplanar triangle TaTh ₂
O5	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.102	0.875	non-coplanar triangle Ta ₃
Ta6	6g	m2m	0.3611	0	$\frac{1}{4}$		7-vertex polyhedron O ₇
O7	6g	m2m	0.755	0	$\frac{1}{4}$		non-colinear Ta ₂
Th8	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
O9	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Ta ₃

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

Experimental: single crystal, diffractometer, X-rays, R = 0.027

Remarks: Space group (188) $P-6c2$ was tested and rejected.

References: [1] Busche J., Gruehn R. (1996), Z. Anorg. Allg. Chem. 622, 640-648.

193
hP78

$\text{K}_3\text{Nd}[\text{Si}_2\text{O}_7]$	<i>hP78</i>	(193) $P6_3/mcm - lk^3gdcba$
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$\text{K}_3\text{NdSi}_2\text{O}_7$ [1]

Structural features: NdO_6 trigonal prisms and NdO_6 octahedra share vertices with units of two vertex-linked SiO_4 tetrahedra to form a 3D-framework. See Fig. III.62.

Hwang M.S. et al. (1987) [1]

$\text{K}_3\text{NdO}_7\text{Si}_2$

$a = 1.0025$, $c = 1.4526$ nm, $c/a = 1.449$, $V = 1.2643$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.1522	0.4742	0.0941		single atom Si
O2	12k	..m	0.1795	0	0.1432		single atom Si
Si3	12k	..m	0.3406	0	0.1437		tetrahedron O ₄
K4	12k	..m	0.6696	0	0.0898		8-vertex polyhedron O ₈
O5	6g	m2m	0.3988	0	$\frac{1}{4}$		non-colinear Si ₂
Nd6	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
K7	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		tricapped trigonal prism O ₉
K8	2b	-3.m	0	0	0		octahedron O ₆

Nd9 2a -62m 0 0 $\frac{1}{4}$ trigonal prism O₆

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.024, T = 298 K

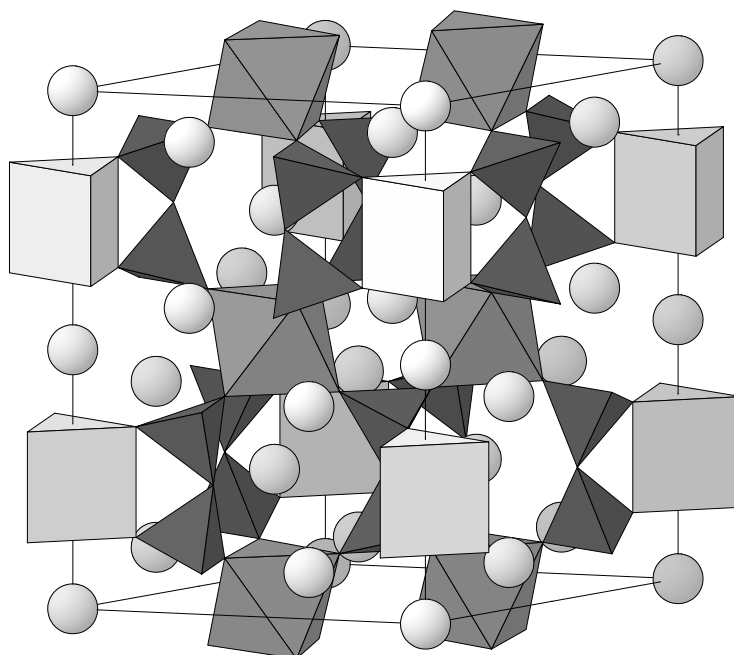


Fig. III.62. **K₃NdSi₂O₇**

Arrangement of NdO₆ trigonal prisms (light), NdO₆ octahedra (medium), SiO₄ tetrahedra (dark) and K atoms.

References: [1] Hwang M.S., Hong H.Y.P., Cheng M.C., Wang Y. (1987), Acta Crystallogr. C 43, 1241-1243.

193
hP80

Ce ₂ Ru ₃ Al ₁₅	hP80	(193) $P6_3/mcm - k^2j^2i^2ga$
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Ce₂Ru₃Al₁₅ [1]

Structural features: RuAl₁₀ pentagonal antiprisms share edges and vertices to form a 3D-framework; Ce in voids complete icosahedral coordination around Ru.

Tursina A.I. et al. (2004) [1]

Al₁₅Ce₂Ru₃

$a = 1.3122$, $c = 0.90964$ nm, $c/a = 0.693$, $V = 1.3564$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	..m	0.2026	0	0.0268		icosahedron Al ₇ Ru ₂ Ce ₃
Al2	12k	..m	0.6172	0	0.1024		pseudo Frank-Kasper Al ₉ Ru ₂ Ce ₂
Al3	12j	m..	0.1667	0.2868	$\frac{1}{4}$		pseudo Frank-Kasper Ru ₂ Al ₉ Ce ₂
Al4	12j	m..	0.2769	0.5238	$\frac{1}{4}$		icosahedron Ru ₂ Al ₉ Ce
Ru5	12i	..2	0.20355	0.4071	0		icosahedron Al ₁₀ Ce ₂

Al6	12i	..2	0.5911	0.1822	0	icosahedron Ru ₂ Al ₈ Ce ₂
Ce7	6g	<i>m2m</i>	0.39479	0	$\frac{1}{4}$	pseudo Frank-Kasper Al ₁₆ Ru ₄
Ce8	2a	-62 <i>m</i>	0	0	$\frac{1}{4}$	sixcapped hexagonal prism Al ₁₈

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

Experimental: single crystal, diffractometer, X-rays, R = 0.029, T = 293 K

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

References: [1] Tursina A.I., Nesterenko S.N., Murashova E.V., Chernyshev I.V., Noel H., Seropegin Y.D. (2004), *Acta Crystallogr. E* 60, i145-i146.

193
hP80

Ca ₃ Al[SO ₄] _{1.5} [OH] ₆ [H ₂ O] ₁₃	hP80	(193) <i>P6₃/mcm</i> – lk ² jhgdb
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Ca₆[Al(OH)₆]₂(SO₄)₃·26H₂O [1], ettringite

Structural features: Units of three edge-linked Ca[(OH)₄(OH₂)₂](OH₂)₂ bicapped trigonal prisms (common (OH)₂ edges between rectangular prisms faces) share other edges with single Al(OH)₆ octahedra to form infinite columns parallel to [001]; SO₄ units between the columns (partial orientational disorder).

Moore A., Taylor H.F.W. (1968) [1]

AlCa₃H₃₀O₂₄S_{1.50}

a = 1.123, *c* = 1.072 nm, *c/a* = 0.955, *V* = 1.1708 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.193	0.5965	0.0527	0.167	single atom O
(OH)2	12 <i>k</i>	.. <i>m</i>	0.1353	0	0.6088		single atom Al
(OH ₂)3	12 <i>k</i>	.. <i>m</i>	0.342	0	0.0877		non-coplanar triangle CaO ₂
(OH ₂)4	12 <i>j</i>	<i>m</i> ..	0.2557	0.4095	$\frac{1}{4}$		single atom Ca
O5	8 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1436		tetrahedron SO ₃
Ca6	6 <i>g</i>	<i>m2m</i>	0.1913	0	$\frac{1}{4}$		8-vertex polyhedron (OH ₂) ₄ (OH) ₄
S7	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0	0.75	8-vertex polyhedron O ₈
Al8	2 <i>b</i>	-3.. <i>m</i>	0	0	0		octahedron (OH) ₆

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

Remarks: Natural specimen from Scawt Hill, Northern Ireland. Partial substitution by H₂O on site S7 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. Average structure; the authors state that true symmetry is trigonal, space group (159) *P31c* or (163) *P-31c*.

References: [1] Moore A., Taylor H.F.W. (1968), *Nature* (London) 218, 1048-1049.

193
hP88

Y _{3.64} Re ₆ Al _{30.69}	hP88	(193) <i>P6₃/mcm</i> – k ² j ² i ² ge ² a
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Y_{7.28}Re₁₂Al_{61.38} [1]

Structural features: Re(Al₁₀Y₂) icosahedra share atoms to form a 3D-framework; additional Y and Al in partly disorderd arrangement along 0 0 *z*.

Niemann S., Jeitschko W. (1995) [1]

$\text{Al}_{30.69}\text{Re}_6\text{Y}_{3.64}$

$a = 1.3116$, $c = 0.9161$ nm, $c/a = 0.698$, $V = 1.3648$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12k	..m	0.207	0	0.029		
Al2	12k	..m	0.6145	0	0.1007		pseudo Frank-Kasper $\text{Al}_9\text{Re}_2\text{Y}_2$
Al3	12j	m..	0.1643	0.2855	$\frac{1}{4}$		
Al4	12j	m..	0.2723	0.522	$\frac{1}{4}$		icosahedron $\text{Re}_2\text{Al}_9\text{Y}$
Re5	12i	..2	0.20313	0.40626	0		icosahedron Al_{10}Y_2
Al6	12i	..2	0.58978	0.17956	0		icosahedron $\text{Re}_2\text{Al}_8\text{Y}_2$
Y7	6g	m2m	0.39158	0	$\frac{1}{4}$		pseudo Frank-Kasper $\text{Al}_{16}\text{Re}_4$
Al8	4e	3.m	0	0	0.097	0.345	
Y9	4e	3.m	0	0	0.1969	0.153	
Y10	2a	-62m	0	0	$\frac{1}{4}$	0.333	

Experimental: single crystal, diffractometer, X-rays, $R = 0.015$

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for sites Al8, Y9 and Y10. Short interatomic distances for partly occupied site(s).

References: [1] Niemann S., Jeitschko W. (1995), J. Alloys Compd. 221, 235-239.

193
hP100

$\text{Rh}_7\text{Pb}_3\text{O}_{15}$	hP100	(193) $P6_3/mcm - 1k^2jihg^2fb$
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Pb₃Rh₇O₁₅ [1]

Structural features: Infinite layers of edge-linked RhO_6 octahedra are interconnected via common vertices with units of two face-linked RhO_6 octahedra to form a 3D-framework.

Omaly J. et al. (1980) [1]

$\text{O}_{15}\text{Pb}_3\text{Rh}_7$

$a = 1.0342$, $c = 1.327$ nm, $c/a = 1.283$, $V = 1.2292$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.3341	0.492	0.0808		non-coplanar triangle Rh_3
O2	12k	..m	0.1706	0	0.5795		non-coplanar triangle Rh_3
O3	12k	..m	0.3343	0	0.0804		non-coplanar triangle Rh_3
O4	12j	m..	0.1784	0.5201	$\frac{1}{4}$		non-colinear Rh_2
Rh5	12i	..2	0.1684	0.3368	0		octahedron O_6
Rh6	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1489		octahedron O_6
Pb7	6g	m2m	0.2635	0	$\frac{1}{4}$		4-vertex polyhedron O_4
Pb8	6g	m2m	0.6048	0	$\frac{1}{4}$		non-colinear O_2
Rh9	6f	..2/m	$\frac{1}{2}$	0	0		octahedron O_6
Rh10	2b	-3.m	0	0	0		octahedron O_6

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

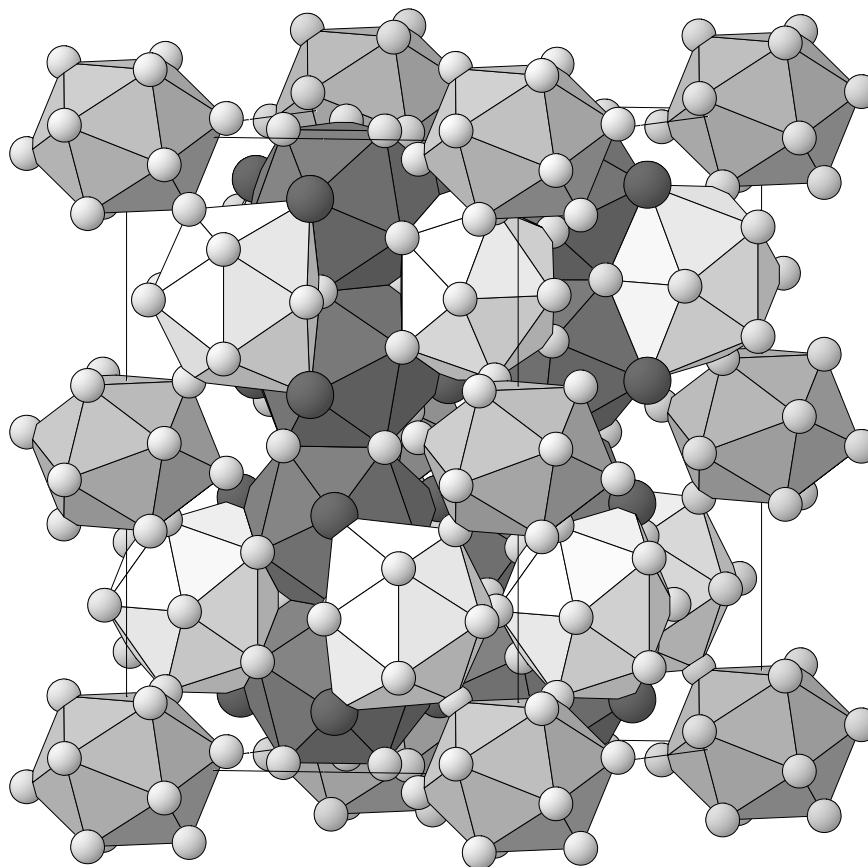
References: [1] Omaly J., Kohlmuller R., Batail P., Chevalier R. (1980), Acta Crystallogr. B 36, 1040-1044.

193
hP106

$\text{Ho}_6\text{Mo}_4\text{Al}_{43}$	hP106	(193) $P6_3/mcm - 1k^3jihg^2b$
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Ho₆Mo₄Al₄₃ [1]; Yb₆Cr_{4+x}Al_{43-x} [1]

Structural features: MoAl₁₂, Mo(Al₁₀Ho₂) and (Al₉Mo)(Al₉Ho₃) icosahedra share atoms to form a 3D-framework. See Fig. III.63.

Fig. III.63. **Ho₆Mo₄Al₂₃**

Arrangement of Mo(Ho₂Al₁₀) (light), MoAl₁₂ (medium) and (Al₉Mo)(Ho₃Al₉) (dark) icosahedra (Ho atoms large, Al atoms small).

Niemann S., Jeitschko W. (1994) [1]

Al_{42.89}Ho₆Mo_{4.11}

$a = 1.0968$, $c = 1.7666$ nm, $c/a = 1.611$, $V = 1.8404$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24l	1	0.15832	0.39459	0.16348		icosahedron Al ₉ MoHo ₂
Al2	12k	..m	0.1599	0	0.61438		12-vertex polyhedron Mo ₂ Al ₉ Ho
Al3	12k	..m	0.255	0	0.03009		12-vertex polyhedron Al ₉ MoHo ₂
Ho4	12k	..m	0.53102	0	0.0952		7-capped pentagonal prism Al ₁₅ HoMo
Al5	12j	m..	0.147	0.5959	$\frac{1}{4}$		icosahedron MoAl ₉ Ho ₂
Al6	12i	..2	0.24704	0.49408	0		icosahedron Al ₈ Ho ₄
M7	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.12624		icosahedron Al ₉ Ho ₃
Al8	6g	m2m	0.1481	0	$\frac{1}{4}$		12-vertex polyhedron Mo ₂ Al ₁₀
Mo9	6g	m2m	0.73038	0	$\frac{1}{4}$		icosahedron Al ₁₀ Ho ₂

Mo10 2b -3.m 0 0 0 icosahedron Al₁₂

M7 = 0.972Al + 0.028Mo

Experimental: single crystal, diffractometer, X-rays, R = 0.015

Remarks: An independent structure determination of Yb₆Cr_{4+x}Al_{43-x} (Yb₆Cr_{5.76}Al_{41.24}) is reported in [2].

References: [1] Niemann S., Jeitschko W. (1994), Z. Metallkd. 85, 345-349. [2] Yanson T.I., Manyako M.B., Bodak O.I., Zarechnyuk O.S., Gladyshevskii R.E., Cerny R., Yvon K. (1994), Acta Crystallogr. C 50, 1529-1531.

193
hP108

Mg ₁₃ Au ₄₁	hP108	(193) <i>P6₃/mcm</i> – k ³ i ³ g ³ db
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Mg₂₃Au₇₇ [1]

Structural features: Close-packed Mg₆Au₂₁ and Mg₇Au₂₀ layers in hc stacking. Ordering variant of α-Nd (d.h.c.p.).

Burkhardt V.K. et al. (1968) [1]

Au₄₁Mg₁₃

a = 1.4927, *c* = 0.9441 nm, *c/a* = 0.632, *V* = 1.8218 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Au1	12 <i>k</i>	..m	0.33	0	0.0		cuboctahedron Mg ₄ Au ₈
Au2	12 <i>j</i>	<i>m</i> ..	0.11	0.33	¹ / ₄		anticuboctahedron Mg ₄ Au ₈
Au3	12 <i>j</i>	<i>m</i> ..	0.22	0.56	¹ / ₄		anticuboctahedron Au ₉ Mg ₃
Au4	12 <i>j</i>	<i>m</i> ..	0.33	0.44	¹ / ₄		anticuboctahedron Au ₈ Mg ₄
Au5	12 <i>i</i>	..2	0.11	0.22	0		cuboctahedron Mg ₄ Au ₈
Mg6	12 <i>i</i>	..2	0.22	0.44	0		cuboctahedron Au ₁₂
Au7	12 <i>i</i>	..2	0.56	0.12	0		cuboctahedron Au ₈ Mg ₄
Au8	6 <i>g</i>	<i>m2m</i>	0.11	0	¹ / ₄		anticuboctahedron Au ₈ Mg ₄
Mg9	6 <i>g</i>	<i>m2m</i>	0.44	0	¹ / ₄		anticuboctahedron Au ₁₂
Mg10	6 <i>g</i>	<i>m2m</i>	0.78	0	¹ / ₄		anticuboctahedron Au ₁₂
Au11	4 <i>d</i>	3.2	¹ / ₃	² / ₃	0		cuboctahedron Au ₉ Mg ₃
Mg12	2 <i>b</i>	-3.m	0	0	0		cuboctahedron Au ₁₂

Experimental: bulk sample, electron diffraction

References: [1] Burkhardt V.K., Schubert K., Toth R.S., Sato H. (1968), Acta Crystallogr. B 24, 137-142.

193
hP108

Na _{3.16} Al ₅ (Al _{0.51} Ge _{0.49}) ₁₂ O ₃₀	hP108	(193) <i>P6₃/mcm</i> – l ² k ² jgfdcba
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Na_{2+x}Al₅[Al_{5+x}Ge_{7-x}O₃₀] [1]

Structural features: (Al,Ge)O₄ tetrahedra share vertices to form double 6-rings.

Fleet M.E. (1993) [1]

Al_{11.16}Ge_{5.84}Na_{2.90}O₃₀

a = 0.9716, *c* = 1.4192 nm, *c/a* = 1.461, *V* = 1.1602 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.1654	0.5105	0.0726		non-coplanar triangle Al ₃
M2	24 <i>l</i>	1	0.18194	0.36513	0.13477		tetrahedron O ₄

O3	12k	..m	0.1865	0	0.1275		non-colinear Al ₂
O4	12k	..m	0.3265	0	0.5829		non-coplanar triangle Al ₃
O5	12j	m..	0.2302	0.4189	$\frac{1}{4}$		non-colinear Al ₂
Na6	6g	m2m	0.5	0	$\frac{1}{4}$	0.094	non-colinear O ₂
Al7	6f	..2/m	$\frac{1}{2}$	0	0		octahedron O ₆
Al8	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron O ₆
Na9	4c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.31	coplanar triangle O ₃
Na10	2b	-3.m	0	0	0		octahedron O ₆
Na11	2a	-62m	0	0	$\frac{1}{4}$		trigonal prism O ₆

M2 = 0.513Al + 0.487Ge

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

Remarks: Homogeneity range Na_{2+x}Al_{10+x}Ge_{7-x}O₃₀, 0.94 < x < 1.38.

References: [1] Fleet M.E. (1993), Z. Kristallogr. 203, 215-224.

193
hP108

Al[PO ₄]	hP108	(193) $P6_3/mcm - l^2kji^2gf$
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AlPO₄ form 54 [1], zeolite VPI

Structural features: (Al,P)O₄ tetrahedra share vertices to form a VPI-type zeolite framework with channels delimited by 18-rings parallel to [001].

Richardson J.W. Jr. et al. (1989) [1]

AlO₄P

a = 1.8549, c = 0.8404 nm, c/a = 0.453, V = 2.5041 nm³, Z = 18

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24l	1	0.3397	0.5136	0.0486		tetrahedron O ₄
O2	24l	1	0.3464	0.4307	0.0227		non-colinear Al ₂
M3	12k	..m	0.4185	0	0.0533		tetrahedron O ₄
O4	12j	m..	0.3428	0.5056	$\frac{1}{4}$		non-colinear Al ₂
O5	12i	..2	0.2465	0.493	0		non-colinear Al ₂
O6	12i	..2	0.593	0.186	0		non-colinear Al ₂
O7	6g	m2m	0.4142	0	$\frac{1}{4}$		non-colinear Al ₂
O8	6f	..2/m	$\frac{1}{2}$	0	0		colinear Al ₂

M1 = 0.50Al + 0.50P; M3 = 0.50Al + 0.50P

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

Experimental: powder, diffractometer, neutrons, time-of-flight, wR_p = 0.042, T = 295 K

Remarks: Space group (185) $P6_3cm$ was tested and rejected.

References: [1] Richardson J.W. Jr., Smith J.V., Pluth J.J. (1989), J. Phys. Chem. 93, 8212-8219.

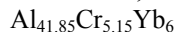
193
hP118

Yb ₆ Cr _{5.15} Al _{41.85}	hP118	(193) $P6_3/mcm - l^2k^3jhg^2b$
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Yb₆Cr_{4+x}Al_{43-x} [1]

Structural features: CrAl₁₂, Cr(Al₁₀Yb₂) and (Al,Cr)(Al₉Yb₃) icosahedra share atoms to form a 3D-framework. Partly disordered variant of Ho₆Mo₄Al₄₃.

Niemann S., Jeitschko W. (1994) [1]



$a = 1.086$, $c = 1.757$ nm, $c/a = 1.618$, $V = 1.7946$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24l	1	0.2341	0.3943	0.1636		
Al2	24l	1	0.2487	0.4974	0.0103	0.5	
Al3	12k	..m	0.1562	0	0.1149		pseudo Frank-Kasper Cr ₂ Al ₉
Al4	12k	..m	0.2531	0	0.5298		
Yb5	12k	..m	0.46712	0	0.09546		
Al6	12j	m..	0.1476	0.5466	$\frac{1}{4}$		icosahedron CrAl ₉ Yb ₂
M7	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1305		
Cr8	6g	m2m	0.2629	0	$\frac{1}{4}$		icosahedron Al ₁₀ Yb ₂
Al9	6g	m2m	0.8513	0	$\frac{1}{4}$		12-vertex polyhedron Cr ₂ Al ₁₀
Cr10	2b	-3.m	0	0	0		icosahedron Al ₁₂

M7 = 0.712Al + 0.288Cr

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

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

Remarks: Short interatomic distances for partly occupied site(s). An independent structure determination is reported in [2] (Yb₆Cr_{5.76}Al_{41.24}), where no site splitting was detected.

References: [1] Niemann S., Jeitschko W. (1994), Z. Metallkd. 85, 345-349. [2] Yanson T.I., Manyako M.B., Bodak O.I., Zarechnyuk O.S., Gladyshevskii R.E., Cerny R., Yvon K. (1994), Acta Crystallogr. C 50, 1529-1531.

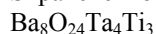
193
hP120

Ba ₈ (Ti _{0.43} Ta _{0.57}) ₇ O ₂₄	hP120	(193) $P6_3/mcm - lk^3jihg^2fedb$
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Ba₈Ta₄Ti₃O₂₄ [1], perovskite 8H; Ba₈Ta₄Ru_{2.67}Co_{0.67}O₂₄ [2]

Structural features: Close-packed BaO₃ layers in hc₃ stacking; Ta and Ti in octahedral voids. Units of two face-linked (Ti,Ta)O₆ octahedra share vertices with (Ta,Ti)O₆ and TaO₆ octahedra (statistical occupation of two face-sharing octahedra for the latter) to form a 3D-framework.

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



$a = 1.00314$, $c = 1.88694$ nm, $c/a = 1.881$, $V = 1.6444$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.165	0.498	0.1244		non-colinear TiTa
O2	12k	..m	0.177	0	0.111		single atom Ta
M3	12k	..m	0.3317	0	0.0617		octahedron O ₆
Ba4	12k	..m	0.6682	0	0.1368		cuboctahedron O ₁₂
O5	12j	m..	0.319	0.498	$\frac{1}{4}$		non-colinear Ti ₂
O6	12i	..2	0.176	0.352	0		non-colinear Ta ₂
M7	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1801	0.875	octahedron O ₆
Ba8	6g	m2m	0.3404	0	$\frac{1}{4}$		anticuboctahedron O ₁₂
O9	6g	m2m	0.857	0	$\frac{1}{4}$		non-colinear Ta ₂
O10	6f	..2/m	$\frac{1}{2}$	0	0		colinear Ta ₂
Ta11	4e	3.m	0	0	0.1959	0.5	7-vertex polyhedron O ₆ Ta
Ba12	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		cuboctahedron O ₁₂

Ba13 2b -3.m 0 0 0 cuboctahedron O₁₂

M3 = 0.667Ta + 0.333Ti; M7 = 0.714Ti + 0.286Ta

Experimental: powder, diffractometer, X-rays, R_B = 0.041

Remarks: Short interatomic distances for partly occupied site(s). For Ba₈Ta₄Ru_{2.67}Co_{0.67}O₂₄ [2] site M3 was found to be occupied exclusively by Ta, sites M7 and Ta11 by a mixture Ru/Co.

References: [1] Shpanchenko R.V., Nistor L., Van Tendeloo G., Van Landuyt J., Amelinckx S., Abakumov A.M., Antipov E.V., Kovba L.M. (1995), J. Solid State Chem. 114, 560-574. [2] Kopnin E.M., Belik A.A., Shpanchenko R.V., Antipov E.V., Izumi F., Takayama Muromachi E., Hadermann J. (2004), J. Solid State Chem. 177, 3499-3504.

193
hP148

Ba_{6.23}Nb₁₄[Si₂O₇]₂O₃₃ hP148 (193) P6₃/mcm – l²k⁶hg²dc

Ba_{6.23}Nb₁₄Si₄O₄₇ [1]; K_{6.5}Ca_{0.75}Nb₁₄Si₄O₄₇ [2]

Structural features: Units of six edge-linked NbO₆ octahedra share vertices with units of two vertex-linked SiO₄ tetrahedra and additional NbO₆ octahedra to form a 3D-framework.

Evans D.M., Katz L. (1973) [1]

Ba_{6.23}Nb₁₄O₄₇Si₄

a = 0.9034, c = 2.781 nm, c/a = 3.078, V = 1.9656 nm³, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24l	1	0.1729	0.4841	0.0438		non-colinear Nb ₂
O2	24l	1	0.1801	0.4898	0.1694		non-colinear SiNb
O3	12k	..m	0.1773	0	0.685		non-colinear Nb ₂
O4	12k	..m	0.2068	0	0.5326		non-coplanar triangle Nb ₃
O5	12k	..m	0.2203	0	0.1094		non-colinear Nb ₂
Nb6	12k	..m	0.2371	0	0.1833		octahedron O ₆
Nb7	12k	..m	0.2383	0	0.0434		octahedron O ₆
Ba8	12k	..m	0.5932	0	0.1076		pseudo Frank-Kasper O ₁₃
Si9	8h	3..	¹ / ₃	² / ₃	0.1918		tetrahedron O ₄
O10	6g	m2m	0.286	0	¹ / ₄		non-colinear Nb ₂
Ba11	6g	m2m	0.6117	0	¹ / ₄	0.076	trigonal bipyramid O ₅
Nb12	4d	3.2	¹ / ₃	² / ₃	0		octahedron O ₆
O13	4c	-6..	¹ / ₃	² / ₃	¹ / ₄		colinear Si ₂

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

Remarks: Partial ordering of K and Ca is reported for K_{6.5}Ca_{0.75}Nb₁₄Si₄O₄₇ [2].

References: [1] Evans D.M., Katz L. (1973), J. Solid State Chem. 8, 150-158. [2] Borel M.M., Chardon J., Grandin A., Leclaire A., Raveau B. (1993), Acta Crystallogr. C 49, 570-571.

193
hP264

Nd₅Fe₁₇ hP264 (193) P6₃/mcm – l⁵k³j⁵ig⁴fdb

Nd₅Fe₁₇ [1]

Structural features: Two kinds of primary layer with triangles, pentagons, hexagons and heptagons; additional Nd and Fe between polygons of neighboring layers. Infinite columns of close-packed Nd atoms in hc stacking parallel to [001].

Moreau J.M. et al. (1990) [1]

 $\text{Fe}_{17}\text{Nd}_5$ $a = 2.0214$, $c = 1.2329$ nm, $c/a = 0.610$, $V = 4.3628$ nm³, $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	24 <i>l</i>	1	0.1311	0.3792	0.062		14-vertex Frank-Kasper $\text{Fe}_{12}\text{Nd}_2$
Nd2	24 <i>l</i>	1	0.1587	0.5403	0.1153		7-capped pentagonal prism $\text{Fe}_{13}\text{Nd}_4$
Fe3	24 <i>l</i>	1	0.2352	0.3546	0.1477		icosahedron $\text{Fe}_{10}\text{Nd}_2$
Fe4	24 <i>l</i>	1	0.2792	0.4921	0.0817		icosahedron Fe_8Nd_4
Fe5	24 <i>l</i>	1	0.3667	0.4362	0.0779		icosahedron Fe_9Nd_3
Fe6	12 <i>k</i>	.. <i>m</i>	0.2622	0	0.148		icosahedron Fe_9Nd_3
Fe7	12 <i>k</i>	.. <i>m</i>	0.29	0	0.549		icosahedron Fe_9Nd_3
Fe8	12 <i>k</i>	.. <i>m</i>	0.3848	0	0.089		icosahedron Fe_9Nd_3
Fe9	12 <i>j</i>	<i>m</i> ..	0.0701	0.3913	$\frac{1}{4}$		icosahedron Fe_9Nd_3
Fe10	12 <i>j</i>	<i>m</i> ..	0.1158	0.2944	$\frac{1}{4}$		icosahedron Fe_8Nd_4
Fe11	12 <i>j</i>	<i>m</i> ..	0.2026	0.4423	$\frac{1}{4}$		icosahedron $\text{Fe}_{10}\text{Nd}_2$
Fe12	12 <i>j</i>	<i>m</i> ..	0.3098	0.585	$\frac{1}{4}$		icosahedron Fe_6Nd_6
Fe13	12 <i>j</i>	<i>m</i> ..	0.3388	0.4755	$\frac{1}{4}$		icosahedron Fe_9Nd_3
Nd14	12 <i>i</i>	.. <i>2</i>	0.1123	0.2246	0		7-capped pentagonal prism $\text{Fe}_{10}\text{Nd}_7$
Nd15	6 <i>g</i>	<i>m2m</i>	0.1202	0	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{Fe}_4\text{Nd}_{10}$
Nd16	6 <i>g</i>	<i>m2m</i>	0.5029	0	$\frac{1}{4}$		7-capped pentagonal prism $\text{Fe}_{13}\text{Nd}_4$
Fe17	6 <i>g</i>	<i>m2m</i>	0.653	0	$\frac{1}{4}$		14-vertex Frank-Kasper $\text{Fe}_{12}\text{Nd}_2$
Nd18	6 <i>g</i>	<i>m2m</i>	0.7999	0	$\frac{1}{4}$		15-vertex polyhedron Fe_9Nd_6
Fe19	6 <i>f</i>	.. <i>2/m</i>	$\frac{1}{2}$	0	0		icosahedron Fe_6Nd_6
Nd20	4 <i>d</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		pseudo Frank-Kasper $\text{Fe}_{12}\text{Nd}_6$
Nd21	2 <i>b</i>	-3. <i>m</i>	0	0	0		cuboctahedron Nd_{12}

Experimental: single crystal, diffractometer, X-rays, $R = 0.080$ Remarks: In table 2 of [1] the Wyckoff position of former Nd(1) is misprinted as 2*a* instead of 2*b*.

References: [1] Moreau J.M., Paccard L., Nozières J.P. (1990), J. Less-Common Met. 163, 245-251.

193
hP304

$\text{Ba}_5(\text{Ti}_{0.83}\text{Fe}_{0.17})_{12}\text{Fe}_2\text{O}_{31}$	<i>hP304</i>	(193) $P6_3/mcm - 1^5k^{10}j^3g^2e^3d$
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Ba₅Fe₄Ti₁₀O₃₁ [1]

Structural features: Close-packed Ba_3O_9 , Ba_2O_{10} , BaO_{11} and O_{12} layers in h_7c_2 stacking; (Ti,Fe) in octahedral, Fe in octahedral and tetrahedral voids (including statistical occupation of two face-sharing tetrahedra). (Ti,Fe) O_6 and FeO_6 octahedra and FeO_4 tetrahedra share atoms to form a 3D-framework.

Siegrist T. et al. (1998) [1]

 $\text{Ba}_5\text{Fe}_4\text{Ti}_{10}\text{O}_{31}$ $a = 0.99834$, $c = 4.2216$ nm, $c/a = 4.229$, $V = 3.6439$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>l</i>	1	0.1625	0.3412	0.1952		non-colinear Ti_2
O2	24 <i>l</i>	1	0.1635	0.3295	0.0841		non-coplanar triangle Ti_3
O3	24 <i>l</i>	1	0.1668	0.4976	0.0281		non-colinear TiFe
O4	24 <i>l</i>	1	0.1671	0.5022	0.1405		non-coplanar triangle Ti_3
M5	24 <i>l</i>	1	0.3126	0.4793	0.16786		octahedron O_6
O6	12 <i>k</i>	.. <i>m</i>	0.1651	0	0.133		non-coplanar triangle Ti_3
O7	12 <i>k</i>	.. <i>m</i>	0.168	0	0.0294		non-colinear FeTi

M8	12k	..m	0.1884	0	0.6087	octahedron O ₆
Ba9	12k	..m	0.33538	0	0.53019	cuboctahedron O ₁₂
M10	12k	..m	0.3364	0	0.0511	octahedron O ₆
M11	12k	..m	0.345	0	0.21627	octahedron O ₆
M12	12k	..m	0.3499	0	0.11849	octahedron O ₆
O13	12k	..m	0.4689	0	0.0835	non-coplanar Ti ₂
O14	12k	..m	0.517	0	0.1922	non-coplanar triangle Ti ₃
O15	12k	..m	0.672	0	0.142	non-coplanar triangle Ti ₃
O16	12j	m..	0.154	0.508	1/4	
Ba17	8h	3..	1/3	2/3	0.08653	anticuboctahedron O ₁₂
O18	8h	3..	1/3	2/3	0.191	tetrahedron FeTi ₃
Fe19	8h	3..	1/3	2/3	0.2374	0.5
O20	6g	m2m	0.217	0	1/4	non-coplanar Ti ₂
Ba21	6g	m2m	0.6866	0	1/4	anticuboctahedron O ₁₂
Fe22	4e	3.m	0	0	0.0412	tetrahedron O ₄
O23	4e	3.m	0	0	0.0857	tetrahedron FeTi ₃
Ba24	4e	3.m	0	0	0.18491	9-vertex polyhedron O ₉
Fe25	4d	3.2	1/3	2/3	0	octahedron O ₆

M5 = 0.833Ti + 0.167Fe; M8 = 0.833Ti + 0.167Fe; M10 = 0.833Ti + 0.167Fe; M11 = 0.833Ti + 0.167Fe; M12 = 0.833Ti + 0.167Fe

Experimental: single crystal, diffractometer, X-rays, wR = 0.060

Remarks: We assigned an approximate value to the Fe/Ti ratio of sites M based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Siegrist T., Vanderah T.A., Ramirez A.P., Geyer R.G., Roth R.S. (1998), J. Alloys Compd. 274, 169-178.

193
hP384

Mg ₆ Fe ₂ [CO ₃][OH] ₁₆ [H ₂ O] ₄	hP384	(193) P6 ₃ /mcm – 1 ⁷ k ⁵ j ⁶ i ⁴ g ³ fdcba
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Mg₆Fe₂(OH)₁₆CO₃·4H₂O [1], sjögrenite

Structural features: Infinite layers of edge-linked Mg(OH)₆ and Fe(OH)₆ octahedra and layers containing CO₃ trigonal units (perpendicular to [001]) and H₂O molecules alternate along [001].

Olowe A. (1995) [1]

CF₂H₂₄Mg₆O₂₃

a = 2.15675, *c* = 1.56084 nm, *c/a* = 0.724, *V* = 6.2877 nm³, *Z* = 12

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH)1	24l	1	0.083	0.25	0.0653		non-coplanar triangle Mg ₂ Fe
Mg2	24l	1	0.083	0.417	0.0		octahedron (OH) ₆
(OH)3	24l	1	0.083	0.5	0.0653		non-coplanar triangle FeMg ₂
(OH)4	24l	1	0.167	0.417	0.0653		non-coplanar triangle FeMg ₂
(OH)5	24l	1	0.25	0.333	0.0653		non-coplanar triangle Mg ₂ Fe
(OH)6	24l	1	0.25	0.583	0.0653		non-coplanar triangle Mg ₂ Fe
(OH)7	24l	1	0.333	0.5	0.0653		non-coplanar triangle Mg ₃
(OH)8	12k	..m	0.083	0	0.0653		non-coplanar triangle Mg ₂ Fe
(OH)9	12k	..m	0.167	0	0.5653		non-coplanar triangle Mg ₃
Mg10	12k	..m	0.25	0	0.0		octahedron (OH) ₆
(OH)11	12k	..m	0.333	0	0.0653		non-coplanar triangle Mg ₃
(OH)12	12k	..m	0.583	0	0.0653		non-coplanar triangle Mg ₂ Fe
(OH) ₂ 13	12j	m..	0.083	0.25	1/4		colinear (OH) ₂

(OH ₂)14	12j	<i>m..</i>	0.083	0.5	$\frac{1}{4}$	trigonal bipyramid (OH) ₂ (OH ₂) ₃
(OH ₂)15	12j	<i>m..</i>	0.167	0.417	$\frac{1}{4}$	trigonal bipyramid (OH) ₂ (OH ₂) ₃
O16	12j	<i>m..</i>	0.25	0.3089	$\frac{1}{4}$	single atom C
O17	12j	<i>m..</i>	0.2746	0.6076	$\frac{1}{4}$	single atom C
(OH ₂)18	12j	<i>m..</i>	0.333	0.5	$\frac{1}{4}$	colinear (OH) ₂
Mg19	12i	<i>..2</i>	0.083	0.166	0	octahedron (OH) ₆
Fe20	12i	<i>..2</i>	0.167	0.334	0	octahedron (OH) ₆
Mg21	12i	<i>..2</i>	0.25	0.5	0	octahedron (OH) ₆
Mg22	12i	<i>..2</i>	0.583	0.166	0	octahedron (OH) ₆
O23	6g	<i>m2m</i>	0.0589	0	$\frac{1}{4}$	single atom C
C24	6g	<i>m2m</i>	0.75	0	$\frac{1}{4}$	coplanar triangle O ₃
O25	6g	<i>m2m</i>	0.8089	0	$\frac{1}{4}$	single atom C
Fe26	6f	<i>..2/m</i>	$\frac{1}{2}$	0	0	octahedron (OH) ₆
Fe27	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0	octahedron (OH) ₆
C28	4c	<i>-6..</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	coplanar triangle O ₃
Fe29	2b	<i>-3.m</i>	0	0	0	octahedron (OH) ₆
C30	2a	<i>-62m</i>	0	0	$\frac{1}{4}$	coplanar triangle O ₃

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

Remarks: Diffraction data from the literature (JCPDS cards # 25-521 and 24-1091A; powder, X-rays). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Olowe A. (1995), Adv. X-Ray Anal. 38, 749-755.

193
hP564

Nd ₅ Fe ₁₇ H _{15.5}	hP564	(193) <i>P6₃/mcm</i> – $1^{14}k^7j^8ig^4fdb$
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Nd₅Fe₁₇H_{15.5} [1]

Structural features: Filled-up derivative of Nd₅Fe₁₇ with H in tetrahedral, octahedral and more unusual voids.

Chu Z. et al. (2001) [1]

D_{17,39}Fe₁₇Nd₅

$a = 2.1188$, $c = 1.28828$ nm, $c/a = 0.608$, $V = 5.0086$ nm³, $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	24l	1	0.044	0.569	0.171	0.612	
D2	24l	1	0.045	0.349	0.128	0.503	square pyramid Fe ₄ D
D3	24l	1	0.08	0.247	0.151	0.53	single atom Fe
Fe4	24l	1	0.1289	0.3736	0.0743		
Nd5	24l	1	0.1532	0.5314	0.1176		single atom D
D6	24l	1	0.173	0.199	0.071	0.605	
D7	24l	1	0.175	0.446	0.064		
D8	24l	1	0.207	0.273	0.122	0.862	single atom D
Fe9	24l	1	0.24	0.36	0.1458		
D10	24l	1	0.24	0.546	0.121	0.564	non-colinear DNd
D11	24l	1	0.266	0.415	0.202	0.846	
Fe12	24l	1	0.2779	0.4821	0.0836		square pyramid D ₅
D13	24l	1	0.319	0.577	0.058	0.644	single atom D
Fe14	24l	1	0.3566	0.4276	0.0758		
D15	12k	<i>..m</i>	0.116	0	0.089		single atom Nd
D16	12k	<i>..m</i>	0.116	0	0.637		non-colinear D ₂

D17	12k	..m	0.24	0	0.063	0.583	
Fe18	12k	..m	0.26	0	0.15		
Fe19	12k	..m	0.2836	0	0.555		non-coplanar triangle D ₃
Fe20	12k	..m	0.384	0	0.0857		non-coplanar D ₂
D21	12k	..m	0.624	0	0.088	0.801	non-coplanar Fe ₂
Fe22	12j	m..	0.0684	0.3752	$\frac{1}{4}$		non-coplanar D ₂
Fe23	12j	m..	0.1114	0.2984	$\frac{1}{4}$		non-coplanar D ₂
D24	12j	m..	0.114	0.589	$\frac{1}{4}$	0.739	single atom Fe
Fe25	12j	m..	0.1973	0.4289	$\frac{1}{4}$		non-coplanar D ₂
D26	12j	m..	0.203	0.504	$\frac{1}{4}$	0.651	single atom Fe
D27	12j	m..	0.266	0.425	$\frac{1}{4}$	0.281	
Fe28	12j	m..	0.3395	0.4653	$\frac{1}{4}$		
Fe29	12j	m..	0.3405	0.5731	$\frac{1}{4}$		non-coplanar DFe
Nd30	12i	..2	0.1078	0.2156	0		non-coplanar D ₂
Nd31	6g	m2m	0.1135	0	$\frac{1}{4}$		non-coplanar D ₂
Nd32	6g	m2m	0.5068	0	$\frac{1}{4}$		
Fe33	6g	m2m	0.6565	0	$\frac{1}{4}$		non-coplanar D ₂
Nd34	6g	m2m	0.7889	0	$\frac{1}{4}$		non-coplanar square D ₄
Fe35	6f	..2/m	$\frac{1}{2}$	0	0		coplanar square D ₄
Nd36	4d	3.2	$\frac{1}{3}$	$\frac{2}{3}$	0		octahedron D ₆
Nd37	2b	-3.m	0	0	0		hexagonal prism D ₁₂

Experimental: powder, diffractometer, neutrons

Remarks: Short interatomic distances: d(Nd4-D7) = 0.155 nm. Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies (D6-D6). There is discrepancy between the coordinates of former site D4 and the interatomic distances mentioned in [1].

References: [1] Chu Z., Yelon W.B., Murakami R.K., Da Silva P.S.M., Villas Boas V., Missell F.P. (2001), IEEE Trans. Magn. 37, 2172-2175.