

Space group (190) *P*-62*c*190
*hP*16

SrBe ₃ O ₄	<i>hP</i> 16	(190) <i>P</i> -62 <i>c</i> – gfdca
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SrBe₃O₄ [1]

Structural features: Close-packed O₃ and deficient triangle-mesh Sr□O layers alternate along [001]; Be in tetrahedral and trigonal voids. BeO₄ tetrahedra and BeO₃ trigonal units share vertices to form a 3D-framework.

Harris L.A., Yakel H.L. (1969) [1]

Be₃O₄Sr

$a = 0.45961$, $c = 0.893$ nm, $c/a = 1.943$, $V = 0.1634$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>g</i>	.2.	0.33371	0	0		coplanar triangle Be ₃
Be2	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.07075		tetrahedron O ₄
Sr3	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		9-vertex polyhedron O ₉
O4	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Be ₂
Be5	2 <i>a</i>	32.	0	0	0		coplanar triangle O ₃

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

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

Remarks: Identical to the phase called Sr₂Be₉O₁₁ in [2] and [3] and probably also to so-called SrBe₄O₅ in [4].

References: [1] Harris L.A., Yakel H.L. (1969), Acta Crystallogr. B 25, 1647-1651. [2] Mercer R.A., Miller R.P. (1964), Nature (London) 202, 581. [3] Mercer R.A., Miller R.P. (1966), J. Inorg. Nucl. Chem. 28, 61-76. [4] Levin E.M., Robbins C.R., McMurdie H.F. (1964), Phase Diagrams for Ceramists, Columbus (OH): The American Ceramic Society.

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*hP*16

Ag[NO ₃][NH ₃] ₃	<i>hP</i> 16	(190) <i>P</i> -62 <i>c</i> – h ² cb
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[Ag(NH₃)₃]NO₃ [1]

Structural features: Columns of superposed Ag(NH₃)₃ trigonal units (planar AgN₃ triangles, consecutive units rotated by 60°) and columns of superposed NO₃ trigonal units, all columns parallel to [001].

Zachwieja U., Jacobs H. (1989) [1]

AgH₉N₄O₃

$a = 0.8057$, $c = 0.584$ nm, $c/a = 0.725$, $V = 0.3283$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>h</i>	<i>m</i> ..	0.169	0.541	$\frac{1}{4}$		single atom N
(NH ₃)2	6 <i>h</i>	<i>m</i> ..	0.326	0.187	$\frac{1}{4}$		single atom Ag
N3	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle O ₃
Ag4	2 <i>b</i>	-6..	0	0	$\frac{1}{4}$		trigonal bipyramid (NH ₃) ₃ Ag ₂

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

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

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

References: [1] Zachwieja U., Jacobs H. (1989), *Z. Anorg. Allg. Chem.* 571, 37-50.

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hP16

Ba(Ba _{0.07} Pb _{0.93}) ₃ O ₄	hP16	(190) <i>P</i> -62c – hgdc
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Ba_{0.3}Pb_{0.7}O [1]

Structural features: :PbO₃ ψ -tetrahedra (partial substitution Ba/Pb) share vertices to form a 3D-framework.

Bodensohn B., Trömel M. (1999) [1]

Ba_{1.20}O₄Pb_{2.80}

$a = 0.7808$, $c = 0.6217$ nm, $c/a = 0.796$, $V = 0.3282$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	6h	$m..$	0.164	0.339	$\frac{1}{4}$		non-coplanar triangle O ₃
O2	6g	.2.	0.392	0	0		non-colinear Pb ₂
Ba3	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		8-vertex polyhedron O ₈
O4	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle Pb ₃

M1 = 0.933Pb + 0.067Ba

Transformation from published data: -x,-y,-z; origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, neutrons

Remarks: We assigned an approximate value to the Ba/Pb ratio of site M1 based on the nominal composition.

References: [1] Bodensohn B., Trömel M. (1999), *Z. Kristallogr. Suppl.* 16, 89.

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hP18

Mg ₂ Ga	hP18	(190) <i>P</i> -62c – hgfb
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Mg₂Ga [1]; Li₂Sb [2]

Structural features: Infinite columns of base-linked GaMg₆ trigonal prisms share edges to form a 3D-framework; single columns of base-linked GaMg₆ trigonal prisms in channels. Distorted derivative of Fe₂P.

Frank K., Schubert K. (1970) [1]

GaMg₂

$a = 0.7794$, $c = 0.6893$ nm, $c/a = 0.884$, $V = 0.3626$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mg1	6h	$m..$	0.399	0.380	$\frac{1}{4}$		tricapped pentagonal prism Ga ₅ Mg ₈
Mg2	6g	.2.	0.289	0	0		anticuboctahedron Ga ₄ Mg ₈
Ga3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.038		bicapped square prism Mg ₉ Ga
Ga4	2b	-6..	0	0	$\frac{1}{4}$		pseudo Frank-Kasper Mg ₉ Ga ₂

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.150$

References: [1] Frank K., Schubert K. (1970), *J. Less-Common Met.* 20, 215-221. [2] Müller W. (1977), *Z. Naturforsch. B* 32, 357-359.

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hP18

HfRhSn	hP18	(190) <i>P</i> -62c – hgfb
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HfRhSn [1]

Structural features: Infinite columns of base-linked RhHf₆ trigonal prisms share edges to form a 3D-framework; single columns of base-linked RhSn₆ trigonal prisms in channels. Ordering variant of Mg₂Ga.

Zumdick M.F., Pöttgen R. (1999) [1]

HfRhSn

$a = 0.732$, $c = 0.7148$ nm, $c/a = 0.977$, $V = 0.3317$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Hf1	6h	<i>m</i> ..	0.40598	0.38747	$\frac{1}{4}$		7-capped pentagonal prism Rh ₅ Sn ₆ Hf ₆
Sn2	6g	.2.	0.27054	0	0		14-vertex Frank-Kasper Rh ₄ Hf ₆ Sn ₄
Rh3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.03421		10-vertex polyhedron Sn ₃ Hf ₆ Rh
Rh4	2b	-6..	0	0	$\frac{1}{4}$		tricapped trigonal prism Sn ₆ Hf ₃

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.010$

Remarks: The average structure was refined in space group (189) *P*-62*m* with half cell volume. Preliminary data in [2].

References: [1] Zumdick M.F., Pöttgen R. (1999), Z. Kristallogr. 214, 90-97. [2] Zumdick M.F., Pöttgen R. (1998), Z. Kristallogr. Suppl. 15, 66.

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hP20

TbNiAlH _{0.3}	hP20	(190) <i>P</i> -62c – hgfcB
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TbNiAlH_{0.30} [1]

Structural features: Filled-up derivative of ZrNiAl with H in trigonal bipyramidal (Ni₂Tb₃) voids.

Hauback B.C. et al. (1999) [1]

AlD_{0.30}NiTb

$a = 0.70433$, $c = 0.77826$ nm, $c/a = 1.105$, $V = 0.3344$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Tb1	6h	<i>m</i> ..	0.4197	0.4053	$\frac{1}{4}$		single atom D
Al2	6g	.2.	0.2354	0	0		octahedron Ni ₄ Al ₂
Ni3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0125		single atom D
D4	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.91	colinear Ni ₂
Ni5	2b	-6..	0	0	$\frac{1}{4}$		tricapped trigonal prism Al ₆ Tb ₃

Experimental: powder, diffractometer, neutrons, X-rays, synchrotron, $R_p = 0.040$, $T = 298$ K

References: [1] Hauback B.C., Fjellvag H., Palhaugen L., Yartys V.A., Yvon K. (1999), J. Alloys Compd. 293/295, 178-184.

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hP20

Cs ₂ [S ₂ O ₆]	hP20	(190) <i>P</i> -62c – ifda
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Cs₂S₂O₆ [1]

Structural features: Cs atoms and O₃S-SO₃ units in a Ni₂In-type (ht-Co₂Ge) arrangement.

Hägg G. (1932) [1]

Cs₂O₆S₂

$a = 0.6326$, $c = 1.1535$ nm, $c/a = 1.823$, $V = 0.3998$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.107	0.44	0.125		single atom S
S2	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.23		
Cs3	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal prism O ₆
Cs4	2a	32.	0	0	0		octahedron O ₆

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

Experimental: powder, film, X-rays

Remarks: Short interatomic distances: d(S2-S2) = 0.046 nm. A different model in space group (182) $P6_322$ could not be rejected. The structure was later redetermined in space group (186) $P6_3mc$ [2].

References: [1] Hägg G. (1932), Z. Phys. Chem., Abt. B 18, 327-342. [2] Liminda R., Abrahams S.C., Bernstein J.L. (1980), J. Chem. Phys. 73, 1432-1438.

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hP24

YGe _{1.67}	hP24	(190) $P-62c - h^2gdc_b$
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Y₃Ge₅ hexagonal [1]

Structural features: 3D-framework of fused (Ge,□)Y₆ trigonal prisms. Derivative of AlB₂ with partly ordered Ge vacancies and splitting of the neighboring Ge site.

Venturini G. et al. (1999) [1]

Ge_{1.67}Y

$a = 0.6838$, $c = 0.8298$ nm, $c/a = 1.214$, $V = 0.3360$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	6h	$m..$	0.323	0.39	$\frac{1}{4}$	0.82	
Ge2	6h	$m..$	0.39	0.323	$\frac{1}{4}$	0.18	
Y3	6g	.2.	0.328	0	0		
Ge4	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.82	coplanar triangle Ge ₃
Ge5	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.18	coplanar triangle Ge ₃
Ge6	2b	-6..	0	0	$\frac{1}{4}$		

Experimental: single crystal, diffractometer, X-rays, R = 0.072

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

References: [1] Venturini G., Ijjaali I., Malaman B. (1999), J. Alloys Compd. 289, 116-119.

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hP24

FeS	hP24	(190) $P-62c - ihfa$
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Fe_{1-x}S rt [2], troilite

Structural features: Close-packed S layers in h stacking; Fe in octahedral voids. Derivative of NiAs with distortions towards the formation of Fe₃ trigonal clusters.

Keller Besrest F., Collin G. (1990) [1]

FeS

$a = 0.5965$, $c = 1.1756$ nm, $c/a = 1.971$, $V = 0.3623$ nm³, $Z = 12$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12i	1	0.3786	0.3233	0.1230		bicapped square prism S ₆ Fe ₄
S2	6h	$m..$	0.0030	0.3347	$1/4$		trigonal prism Fe ₆
S3	4f	3..	$1/3$	$2/3$	0.0200		trigonal prism Fe ₆
S4	2a	32.	0	0	0		trigonal prism Fe ₆

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.031$

Remarks: Phase stable at $T < \sim 410$ K, metastable for the stoichiometric composition. Refinements on material obtained by mechanochemical synthesis are reported in [3].

References: [1] Keller Besrest F., Collin G. (1990), J. Solid State Chem. 84, 194-210. [2] Bertaut E.F. (1954), J. Phys. Radium 15, 775. [3] Jiang J.Z., Larsen R.K., Lin R., Morup S., Chorkendorff I., Nielsen K., Hansen K., West K. (1998), J. Solid State Chem. 138, 114-125.

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hP24

Er ₂ RhSi ₃	hP24	(190) $P-62c - ihfb$
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Er₂RhSi₃ [1]; Sm₈Pt₁₁Si₅ [4]

Structural features: 3D-framework of fused RhEr₆ and SiEr₆ prisms. Planar hexagon-mesh RhSi₃ layers with Si₆ rings. Substitution derivative of AlB₂.

Chevalier B. et al. (1984) [1]

Er₂RhSi₃

$a = 0.8036$, $c = 0.7712$ nm, $c/a = 0.960$, $V = 0.4313$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	12i	1	0.167	0.333	0.0		tricapped trigonal prism Si ₂ RhEr ₆
Er2	6h	$m..$	0.019	0.481	$1/4$		pseudo Frank-Kasper Si ₈ Rh ₄ Er ₈
Rh3	4f	3..	$1/3$	$2/3$	0.0		tricapped trigonal prism Si ₃ Er ₆
Er4	2b	$-6..$	0	0	$1/4$		pseudo Frank-Kasper Si ₁₂ Er ₈

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

Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: The structure was later refined in space group (194) $P6_3/mmc$ [2]. Similar reliability factors were obtained for both space groups in [3], which indicates that the higher symmetry is probably correct. More important distortions are reported for Sm₈Pt₁₁Si₅ in [4] (Sm₂Pt(Pt,Si)₃).

References: [1] Chevalier B., Lejay P., Etourneau J., Hagenmuller P. (1984), Solid State Commun. 49, 753-760. [2] Gladyshevskii R.E., Cenxual K., Parthé E. (1992), J. Alloys Compd. 189, 221-228. [3] Bazela W., Wawrzynska E., Penc B., Stüsser N., Szytula A., Zygmunt A. (2003), J. Alloys Compd. 360, 76-80. [4] Barakatova Z.M., Aksel'rud L.G., Seropegin Y.D., Bodak O.I. (1995), Crystallogr. Rep. 40, 335-337 (Kristallografiya 40, 370-372).

190
hP26

AgCu[SCN] ₃ [NH ₃] ₂	hP26	(190) $P-62c - h^3fda$
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Cu(NH₃)₂Ag(SCN)₃ [1]

Structural features: Ag atoms and $\text{Cu}(\text{NCS})_3(\text{NH}_3)_2$ units (CuN_5 trigonal bipyramid, NCS linear units in equatorial positions) in a NiAs-type arrangement. See Fig. III.86.

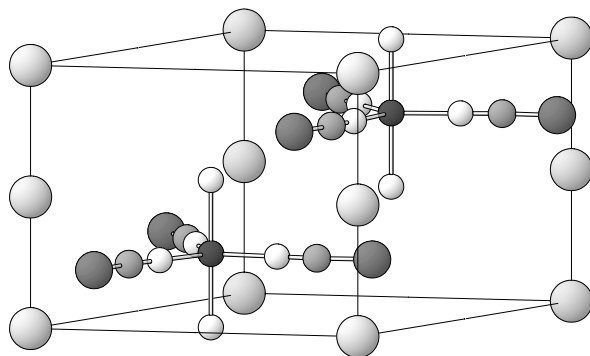


Fig. III.86. $\text{Cu}(\text{NH}_3)_2\text{Ag}(\text{SCN})_3$

Arrangement of $\text{Cu}(\text{SCN})_3(\text{NH}_3)_2$ units (Cu atoms small, S atoms dark, C atoms medium, N atoms light) and Ag atoms (large). For clarity, atoms located in the cell but belonging to units with the central Cu atom in a neighboring cell are omitted.

Huang J.L. et al. (1966) [1]

$\text{AgC}_3\text{CuH}_6\text{N}_5\text{S}_3$

$a = 0.922$, $c = 0.738$ nm, $c/a = 0.800$, $V = 0.5433$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	6h	$m..$	0.144	0.288	$\frac{1}{4}$		single atom C
C2	6h	$m..$	0.31	0.027	$\frac{1}{4}$		single atom N
N3	6h	$m..$	0.444	0.142	$\frac{1}{4}$		single atom C
$(\text{NH}_3)_4$	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.03		single atom Cu
Cu5	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal bipyramid $\text{N}_3(\text{NH}_3)_2$
Ag6	2a	32.	0	0	0		octahedron S_6

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

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

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In Table 2 of [1] the z -coordinates of the Cu and S sites are misprinted as $\frac{1}{4}$ instead of $\frac{3}{4}$ (checked on interatomic distances).

References: [1] Huang J.L., Li J.M., Lu J.X. (1966), Acta Chim. Sin. (Engl. Ed.) 32, 194-200.

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hP26

Sb_5IO_7	hP26	(190) $P\text{-}62c - \text{ihfda}$
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$\text{Sb}_5\text{O}_7\text{I}$ ht [1]

Structural features: SbO_3 ψ -tetrahedra share vertices to form infinite slabs with Sb_5O_6 cages.

Altenburger W. et al. (1987) [1]

IO_7Sb_5

$a = 0.6746$, $c = 1.2751$ nm, $c/a = 1.890$, $V = 0.5025$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.055	0.547	0.139		non-collinear Sb_2
Sb2	6h	$m..$	0.3576	0.0361	$\frac{1}{4}$		non-coplanar triangle O_3
Sb3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.05401		non-coplanar triangle O_3
O4	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		coplanar triangle Sb_3
I5	2a	32.	0	0	0		pseudo Frank-Kasper $\text{O}_{12}\text{Sb}_{12}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.028$, $T = 483$ K

Remarks: Structure type referred to as 2HA-SOI (2-layer polytype, Hexagonal, Acentrosymmetric, Sb-O-I). Phase stable at $T > 438$ K. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Space group (174) $P-6$ was tested and rejected ($R = 0.033$).

References: [1] Altenburger W., Hiller W., Jahn I.R. (1987), Z. Kristallogr. 181, 227-234.

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hP26

$\text{La}[\text{ClO}_2]_3[\text{H}_2\text{O}]_3$	<i>hP26</i>	(190) $P-62c - \text{ihgd}$
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$\text{La}(\text{ClO}_2)_3 \cdot 3\text{H}_2\text{O}$ [2]

Structural features: Layers containing ClO_2 non-linear units (approximately in the plane of the layer) and layers containing La atoms and H_2O molecules (perpendicular to the layer) alternate along [001].

Castellani Bisi C. (1984) [1]

$\text{Cl}_3\text{H}_6\text{LaO}_9$

$a = 0.8077$, $c = 0.8296$ nm, $c/a = 1.027$, $V = 0.4687$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.4358	0.1838	0.0149		single atom Cl
O2	6h	$m..$	0.0224	0.5798	$1/4$		single atom La
Cl3	6g	.2.	0.24	0	0		non-colinear O_2
La4	2d	-6..	$2/3$	$1/3$	$1/4$		tricapped trigonal prism O_9
H5	12i	1	0.341	0.44	0.153		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.029$, $T = 295$ K

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

References: [1] Castellani Bisi C. (1984), Acta Crystallogr. C 40, 1120-1121. [2] Coda A., Giuseppetti G., Tadini C. (1965), Period. Mineral. 34, 27-47.

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hP28

$\text{Rb}_3\text{Mo}_2\text{Cl}_8$	<i>hP28</i>	(190) $P-62c - \text{ihf}^2\text{b}$
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$\text{Rb}_3\text{Mo}_2\text{Cl}_8$ [1]

Structural features: Close-packed RbCl_3 layers (partial vacancies ignored) in hc_2 stacking; Mo in octahedral (Cl_6) voids leaving every third interlayer vacant. Units of two face-linked MoCl_6 octahedra (Mo_2 dumbbells), parallel to [001]. Derivative of $\text{Cs}_3\text{Cr}_2\text{Cl}_9$ with partly ordered vacancies and small distortions.

Bennett M.J. et al. (1969) [1]

$\text{Cl}_8\text{Mo}_2\text{Rb}_3$

$a = 0.719$, $c = 1.6662$ nm, $c/a = 2.317$, $V = 0.7460$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12i	1	0.1805	0.3491	0.0987		single atom Mo
Cl2	6h	$m..$	0.474	0.0166	$1/4$	0.667	non-colinear Mo_2
Mo3	4f	3..	$1/3$	$2/3$	0.1786		7-vertex polyhedron MoCl_6
Rb4	4f	3..	$1/3$	$2/3$	0.5721		cuboctahedron Cl_{12}

Rb5 2b -6.. 0 0 $\frac{1}{4}$ icosahedron Cl₁₂

Experimental: single crystal, diffractometer, X-rays, R = 0.061

Remarks: Space groups (186) *P*₆₃*mc* and (194) *P*₆₃/*mmc* were tested and rejected (R = 0.14 and 0.18, respectively).

References: [1] Bennett M.J., Brenic J.V., Cotton F.A. (1969), Inorg. Chem. 8, 1060-1065.

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hP28

Cs₃Fe₂F₉

hP28

(190) *P*-62*c* – ihfed

Cs₃Fe₂F₉ [1]

Structural features: Close-packed CsF₃ layers in h stacking; Fe in octahedral (F₆) voids, leaving every third interlayer vacant. Units of two face-linked FeF₆ octahedra, parallel to [001].

Wall F. et al. (1971) [1]

Cs₃F₉Fe₂

a = 0.6345, *c* = 1.4816 nm, *c/a* = 2.335, *V* = 0.5166 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12i	1	0.3005	0.1291	0.0963		single atom Fe
F2	6h	<i>m</i> ..	0.1164	0.2619	$\frac{1}{4}$		non-colinear Fe ₂
Cs3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0673		anticuboctahedron F ₁₂
Fe4	4e	3..	0	0	0.1505		octahedron F ₆
Cs5	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		anticuboctahedron F ₁₂

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

Experimental: single crystal, precession photographs, X-rays, R = 0.063

Remarks: The structure was later redetermined in space group (194) *P*₆₃/*mmc* [2].

References: [1] Wall F., Pausewang G., Babel D. (1971), J. Less-Common Met. 25, 257-270. [2] Dance J.M., Mur J., Darriet J., Hagenmuller P., Massa W., Kummer S., Babel D. (1986), J. Solid State Chem. 63, 446-451.

190
hP30

K₄Au₆S₅

hP30

(190) *P*-62*c* – ih²fa

K₄Au₆S₅ [1]

Structural features: Au₆S₅ cage units formed by six vertex-linked S-Au-S linear units (an Au₆ trigonal prism with one S atom above each triangular face and each edge between rectangular faces). See Fig. III.87.

Klepp K.O., Bronger W. (1988) [1]

Au₆K₄S₅

a = 0.9631, *c* = 0.9856 nm, *c/a* = 1.023, *V* = 0.7917 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Au1	12i	1	0.4513	0.1673	0.088		non-colinear S ₂
S2	6h	<i>m</i> ..	0.258	0.033	$\frac{1}{4}$		non-colinear Au ₂
K3	6h	<i>m</i> ..	0.347	0.416	$\frac{1}{4}$		8-vertex polyhedron S ₄ Au ₄
S4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.051		non-coplanar triangle Au ₃

K5 2a 32. 0 0 0 pseudo Frank-Kasper $S_6Au_6K_8$

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

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

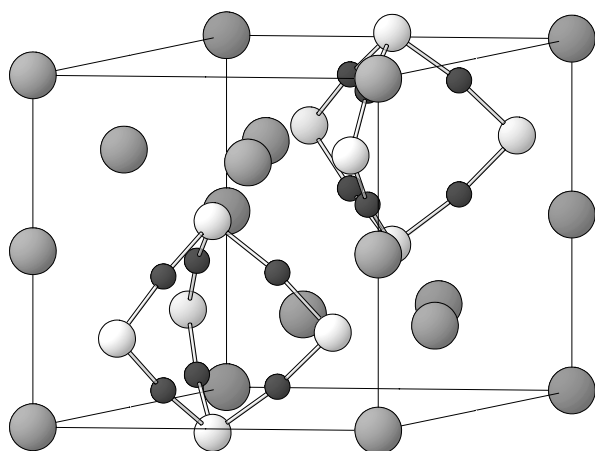


Fig. III.87. $K_4Au_6S_5$

Arrangement of Au_6S_5 cages (Au atoms dark, S atoms light) and K atoms (large).

References: [1] Klepp K.O., Bronger W. (1988), J. Less-Common Met. 137, 13-20.

190
hP30

$Ba_3CaRu_2O_9$

hP30

(190) $P-62c - ihf^2ba$

$Ba_3CaRu_2O_9$ [1], perovskite 6H; $Ba_3Cr_2WO_9$ 6H [2]

Structural features: Close-packed BaO_3 layers in hc_2 stacking; Ca and Ru in octahedral (O_6) voids. Pairs of face-linked RuO_6 octahedra (Ru_2 dumbbells) share vertices with single CaO_6 octahedra to form a 3D-framework. Derivative of $Ba_3(W_{0.5}Fe_{0.5})_2FeO_9$ with distorted O sublattice.

Wilkens J., Müller Buschbaum H. (1993) [1]

$Ba_3CaO_9Ru_2$

$a = 0.5891$, $c = 1.4571$ nm, $c/a = 2.473$, $V = 0.4379$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.1921	0.3581	0.0902		non-colinear RuCa
O2	6h	$m..$	0.031	0.503	$\frac{1}{4}$		non-colinear Ru_2
Ru3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.151		octahedron O_6
Ba4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5954		cuboctahedron O_{12}
Ba5	2b	-6..	0	0	$\frac{1}{4}$		anticuboctahedron O_{12}
Ca6	2a	32.	0	0	0		octahedron O_6

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

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

References: [1] Wilkens J., Müller Buschbaum H. (1993), Z. Anorg. Allg. Chem. 619, 517-520. [2] Shikano M., Ishiyama O., Inaguma Y., Nakamura T., Itoh M. (1995), J. Solid State Chem. 120, 238-243.

190
hP32

$Pt_9Ga_3B_4$

hP32

(190) $P-62c - ih^2gc$

Pt₉Ga₃B₄ [1]

Structural features: Infinite triple columns of edge-linked BPt₆ trigonal prisms (non-parallel prism axes) share vertices with single BPt₆ trigonal prisms to form a 3D-framework; Ga in channels of pentagonal cross-section parallel to [001].

Petry K. et al. (1994) [1]

B₄Ga₃Pt₉

$a = 0.87503$, $c = 0.63742$ nm, $c/a = 0.728$, $V = 0.4227$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pt1	12i	1	0.18733	0.4585	0.0167		pseudo Frank-Kasper B ₂ Ga ₄ Pt ₇
Pt2	6h	$m..$	0.1849	0.1778	$\frac{1}{4}$		square pyramid B ₄ Ga
Ga3	6h	$m..$	0.5566	0.043	$\frac{1}{4}$		non-coplanar triangle Pt ₃
B4	6g	.2.	0.174	0	0		square prism (cube) Pt ₆ B ₂
B5	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism Pt ₆

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.049$

References: [1] Petry K., Klünter W., Jung W. (1994), Z. Kristallogr. 209, 151-156.

190
hP34

Zr₆FeAl₂O_{0.1}H_{5.6} hP34 (190) $P-62c - h^2g^2f^2b$

Zr₆FeAl₂H_{5.6} (O) [1]

Structural features: Filled-up derivative of β_1 -K₂UF₆ antitype with O and H in tetrahedral (Zr₃Al and Zr₄, respectively) voids.

Yartys V.A. et al. (1999) [1]

Al₂D_{5.61}FeO_{0.14}Zr₆

$a = 0.80139$, $c = 0.69521$ nm, $c/a = 0.868$, $V = 0.3867$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	6h	$m..$	0.0383	0.4316	$\frac{1}{4}$		4-vertex polyhedron D ₄
D2	6h	$m..$	0.2836	0.4028	$\frac{1}{4}$	0.87	octahedron O ₂ Zr ₄
D3	6g	.2.	0.2757	0	0		tetrahedron Zr ₄
Zr4	6g	.2.	0.7517	0	0		tetrahedron D ₄
O5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.18	0.069	single atom O
Al6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.558		single atom O
Fe7	2b	-6..	0	0	$\frac{1}{4}$		trigonal prism Zr ₆

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

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

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

References: [1] Yartys V.A., Fjellvag H., Hauback B.C. (1999), J. Alloys Compd. 290, 157-163.

190
hP34

Re₃Cl₉[H₂O]₅ hP34 (190) $P-62c - ih^3f$

ReCl₃·1.67H₂O [1]

Structural features: $\text{Re}_3\text{Cl}_9(\text{OH}_2)_3$ clusters (a Re_3 triangle surrounded by a coplanar Cl_3 triangle, a Cl_6 trigonal prism and a large $(\text{OH}_2)_3$ triangle) in a Mg-type (h.c.p.) arrangement; additional H_2O between the units. See Fig. III.88.

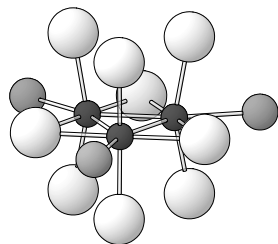


Fig. III.88. $\text{ReCl}_3 \cdot 1.67\text{H}_2\text{O}$

$\text{Re}_3\text{Cl}_9(\text{OH}_2)_3$ unit (Re atoms dark, Cl atoms light, O atoms medium).

Irmeler M., Meyer G. (1987) [1]

$\text{Cl}_9\text{H}_{10}\text{O}_5\text{Re}_3$

$a = 0.94489$, $c = 1.47007$ nm, $c/a = 1.556$, $V = 1.1367$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12i	1	0.5077	0.1107	0.0958		single atom Re
(OH ₂)2	6h	$m..$	0.1046	0.4073	$\frac{1}{4}$		single atom Re
Cl3	6h	$m..$	0.3438	0.2486	$\frac{1}{4}$		non-collinear Re_2
Re4	6h	$m..$	0.5447	0.16731	$\frac{1}{4}$		7-vertex polyhedron $\text{Cl}_4\text{Re}_2(\text{OH}_2)$
(OH ₂)5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1188		non-coplanar triangle $(\text{OH}_2)_3$

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.051$

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

References: [1] Irmeler M., Meyer G. (1987), Z. Anorg. Allg. Chem. 552, 81-89.

190
hP36

$\text{Tl}_3\text{Pb}_{0.5}\text{I}_5$	$hP36$	$(190)\ P-62c - h^2g^2fe$
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$\text{Tl}_6\text{PbI}_{10}$ [2]; $\text{Tl}_6\text{Ag}_2\text{I}_{10}$ [3]

Structural features: Infinite columns of face-linked I_6 octahedra, and I_4 linear segments parallel to $[001]$; Pb inside the octahedron columns (disorder), Tl between the columns.

Stoeger W. et al. (1977) [1]

$\text{I}_5\text{Pb}_{0.50}\text{Tl}_3$

$a = 1.0561$, $c = 1.3521$ nm, $c/a = 1.280$, $V = 1.3060$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	6h	$m..$	0.261	0.264	$\frac{1}{4}$		7-vertex polyhedron Pb_2Tl_5
Tl2	6h	$m..$	0.396	0.0312	$\frac{1}{4}$		tricapped trigonal prism I_9
I3	6g	.2.	0.258	0	0		non-collinear Pb_2
Tl4	6g	.2.	0.63	0	0		tricapped trigonal prism I_9
I5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.135		collinear I_2
I6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.6011		single atom I
Pb7	4e	3..	0	0	0.112	0.5	square prism (cube) Pb_2I_6

Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$

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

Remarks: The average structure was refined in space group (193) $P6_3/mcm$ (new axes $a, b, c/2$).

References: [1] Stoeger W., Schulz H., Rabenau A. (1977), Z. Anorg. Allg. Chem. 432, 5-16. [2] Rabenau A., Schulz H., Stoeger W. (1976), Naturwissenschaften 63, 245. [3] Stoeger W., Rabenau A. (1978), Z. Naturforsch. B 33, 740-744.

190
hP36

LaSiO ₃ F	hP36	(190) $P-62c - ih^2gfa$
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La₃F₃(Si₃O₉) [1]

Structural features: Si₃O₉ units consisting of three vertex-linked SiO₄ tetrahedra; La forms a simple hexagonal sublattice.

Müller Bunz H., Schleid T. (1999) [1]

FLaO₃Si

$a = 0.70832$, $c = 1.08948$ nm, $c/a = 1.538$, $V = 0.4734$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.3943	0.3187	0.1231		single atom Si
O2	6h	m..	0.0405	0.2354	$\frac{1}{4}$		non-colinear Si ₂
Si3	6h	m..	0.2713	0.2263	$\frac{1}{4}$		tetrahedron O ₄
La4	6g	.2.	0.35461	0	0		7-vertex polyhedron F ₃ O ₄
F5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0737		non-coplanar triangle La ₃
F6	2a	32.	0	0	0		coplanar triangle La ₃

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.017$, $T = 293$ K

Remarks: In table 2 of [1] the Wyckoff position of former F2 is misprinted as 4e instead of 4f.

References: [1] Müller Bunz H., Schleid T. (1999), Z. Anorg. Allg. Chem. 625, 1377-1383.

190
hP36

Ce[CO ₃]F	hP36	(190) $P-62c - ih^2gfa$
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CeCO₃F [2], bastnäsite-(Ce), Strukturbericht notation G7₁

Structural features: Ce atoms and CO₃ trigonal units (parallel to [001]) in a WC-type arrangement; F in trigonal (Ce₃) voids.

Ni Y. et al. (1993) [1]

CCeFO₃

$a = 0.71175$, $c = 0.97619$ nm, $c/a = 1.372$, $V = 0.4283$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.3828	0.3245	0.1354		single atom C
O2	6h	m..	0.109	0.316	$\frac{1}{4}$		single atom C
C3	6h	m..	0.29	0.322	$\frac{1}{4}$		coplanar triangle O ₃
Ce4	6g	.2.	0.33941	0	0		tricapped trigonal prism F ₃ O ₆
F5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.051		non-coplanar triangle Ce ₃
F6	2a	32.	0	0	0		coplanar triangle Ce ₃

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

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

Remarks: Natural specimen from Gallinas Mountains, New Mexico. The structure was refined independently in [4]. The average structure was refined in space group (189) $P\text{-}62m$ (new axes $a, b, c/2$) in [3].

References: [1] Ni Y., Hughes J.M., Mariano A.N. (1993), Am. Mineral. 78, 415-418. [2] Donnay G., Donnay J.D.H. (1953), Am. Mineral. 38, 932-963. [3] Oftedal I. (1931), Z. Kristallogr. 78, 462-469. [4] Terada Y., Nakai I., Kawashima T. (1993), Anal. Sci. 9, 561-562.

190
 $hP38$

$\text{Zr}_6\text{FeAl}_2\text{H}_{10}$	$hP38$	(190) $P\text{-}62c - h^3g^2fba$
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$\text{Zr}_6\text{FeAl}_2\text{H}_{10}$ [1]

Structural features: Filled-up derivative of $\beta_1\text{-K}_2\text{UF}_6$ antitype with H in tetrahedral (Zr_4 and Zr_3Fe) and trigonal bipyramidal (Fe_2Zr_3) voids.

Gingl F. et al. (1995) [1]

$\text{Al}_2\text{D}_{9.82}\text{FeZr}_6$

$a = 0.81354$, $c = 0.7094$ nm, $c/a = 0.872$, $V = 0.4066$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	6h	$m..$	0.1213	0.2457	$1/4$		single atom Fe
D2	6h	$m..$	0.4105	0.2895	$1/4$		tetrahedron Zr_4
Zr3	6h	$m..$	0.4256	0.0485	$1/4$		trigonal bipyramid D_5
D4	6g	$.2.$	0.2839	0	0	0.94	non-colinear Zr_2
Zr5	6g	$.2.$	0.7406	0	0		trigonal bipyramid D_5
Al6	4f	3..	$1/3$	$2/3$	0.054		pseudo Frank-Kasper AlD_9Zr_9
Fe7	2b	$-6..$	0	0	$1/4$		trigonal bipyramid D_5
D8	2a	32.	0	0	0		colinear Fe_2

Experimental: powder, diffractometer, neutrons, $R_p = 0.035$, $T = 293$ K

References: [1] Gingl F., Yvon K., Zavaliy I.Y., Yartys' V.A., Fischer P. (1995), J. Alloys Compd. 226, 1-4.

190
 $hP38$

$\text{K}_3\text{Na}[\text{UO}_2][\text{CO}_3]_3$	$hP38$	(190) $P\text{-}62c - h^4gfdc$
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$\text{K}_3\text{Na}(\text{UO}_2)(\text{CO}_3)_3$ [1], grimselite

Structural features: Single $\text{UO}_2(\text{CO}_3)_3$ units (a UO_8 hexagonal bipyramid sharing equatorial edges with three coplanar CO_3 trigonal units) in a Mg-type (h.c.p.) arrangement. See Fig. III.89.

Mazzi F., Rinaldi F. (1961) [1]

$\text{C}_3\text{K}_3\text{NaO}_{11}\text{U}$

$a = 0.929$, $c = 0.826$ nm, $c/a = 0.889$, $V = 0.6174$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6h	$m..$	0.034	0.509	$1/4$		single atom C
O2	6h	$m..$	0.215	0.367	$1/4$		single atom C
C3	6h	$m..$	0.36	0.382	$1/4$		coplanar triangle O_3
O4	6h	$m..$	0.37	0.25	$1/4$		single atom C
K5	6g	$.2.$	0.29	0	0		trigonal prism O_6

O6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.04	single atom U
Na7	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	trigonal bipyramid O ₅
U8	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	colinear O ₂

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

Experimental: single crystal, photographs, X-rays, R = 0.060

Remarks: H₂O may have been overlooked.

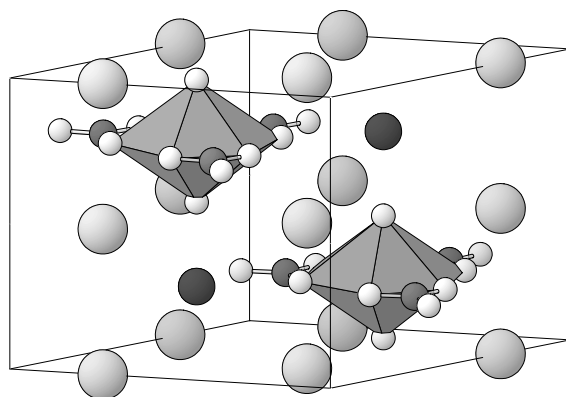
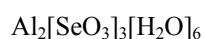


Fig. III.89. $\text{K}_3\text{Na}(\text{UO}_2)(\text{CO}_3)_3$

Arrangement of $\text{UO}_2(\text{CO}_3)_3$ units (UO_8 hexagonal bipyramids, C atoms dark, O atoms light), K (large) and Na (medium) atoms. For clarity, atoms located in the cell but belonging to units with the central U atom in a neighboring cell are omitted.

References: [1] Mazzi F., Rinaldi F. (1961), Period. Mineral. 30, 1-20.

190
hP40



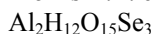
hP40

(190) $P\text{-}62c - i^2h^2f$

$\text{Al}_2(\text{SeO}_3)_3 \cdot 6\text{H}_2\text{O}$ [1]

Structural features: Single $\text{Al}_2(\text{SeO}_3)_3(\text{H}_2\text{O})_6$ units consisting of two $\text{Al}[\text{O}_3(\text{OH}_2)_3]$ octahedra interconnected via common vertices with three SeO_3 ψ -tetrahedra.

Morris R.E. et al. (1992) [1]



$a = 0.8802$, $c = 1.0707$ nm, $c/a = 1.216$, $V = 0.7184$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.1344	0.5131	0.1281		non-colinear SeAl
O2	12i	1	0.4826	0.3155	0.0713		single atom Al
Se3	6h	m..	0.12442	0.38176	$\frac{1}{4}$		non-coplanar triangle O ₃
O4	6h	m..	0.3247	0.0884	$\frac{1}{4}$		single atom Se
Al5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0333		octahedron O ₆
H6	12i	1	0.409	0.219	0.122		
H7	12i	1	0.6	0.08	0.08		

Transformation from published data: -x,-y,-z; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.026

Remarks: Supersedes a refinement in space group (159) $P31c$ [2], which does not take into consideration all symmetry elements of the proposed structure. Diffraction data from [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Morris R.E., Harrison W.T.A., Stucky G.D., Cheetham A.K. (1992), J. Solid State Chem. 99, 200. [2] Morris R.E., Harrison W.T.A., Stucky G.D., Cheetham A.K. (1991), J. Solid State Chem. 94, 227-235.

190
hP42

$\text{K}_3\text{Na}[\text{UO}_2][\text{CO}_3]_3[\text{H}_2\text{O}]$	<i>hP42</i>	(190) <i>P</i> -62 <i>c</i> – $\text{h}^4\text{gfd}c$
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$\text{K}_3\text{Na}(\text{UO}_2)(\text{CO}_3)_3 \cdot \text{H}_2\text{O}$ [1], grimselite

Structural features: Single $\text{UO}_2(\text{CO}_3)_3$ units consisting of a UO_8 hexagonal bipyramid sharing equatorial edges with three coplanar CO_3 trigonal units.

Li Y., Burns P.C. (2001) [1]

$\text{C}_3\text{H}_2\text{K}_3\text{NaO}_{12}\text{U}$

$a = 0.9302$, $c = 0.826$ nm, $c/a = 0.888$, $V = 0.6190$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>h</i>	<i>m</i> ..	0.0306	0.5103	$\frac{1}{4}$		single atom C
O2	6 <i>h</i>	<i>m</i> ..	0.217	0.3685	$\frac{1}{4}$		single atom C
C3	6 <i>h</i>	<i>m</i> ..	0.3601	0.3718	$\frac{1}{4}$		coplanar triangle O ₃
O4	6 <i>h</i>	<i>m</i> ..	0.3703	0.2429	$\frac{1}{4}$		single atom C
K5	6 <i>g</i>	.2.	0.2921	0	0		square prism (cube) O ₆ (OH ₂) ₂
O6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0327		colinear UNa
(OH ₂)7	4 <i>e</i>	3..	0	0	0.1277	0.5	colinear (OH ₂) ₂
Na8	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal bipyramid O ₅
U9	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear O ₂

Experimental: single crystal, diffractometer, X-rays, $R = 0.026$

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 (159) *P*31*c* was tested and rejected.

References: [1] Li Y., Burns P.C. (2001), Can. Mineral. 39, 1147-1151.

190
hP42

$\text{NaC}_2\text{N}_3[\text{H}_2\text{O}]$	<i>hP42</i>	(190) <i>P</i> -62 <i>c</i> – h^6g
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$\text{Na}_3\text{C}_6\text{N}_9 \cdot 3\text{H}_2\text{O}$ [2], Strukturbericht notation O8₅

Structural features: Triangle-mesh Na layers alternate with layers containing planar C_6N_9 units (a C_3N_3 hexagon with a linear NCN unit bonded to each C) and H_2O molecules.

Jürgens B. et al. (1998) [1]

$\text{C}_2\text{H}_2\text{N}_3\text{NaO}$

$a = 1.02353$, $c = 0.65085$ nm, $c/a = 0.636$, $V = 0.5905$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	6 <i>h</i>	<i>m</i> ..	0.0609	0.1478	$\frac{1}{4}$		coplanar triangle N ₃
N2	6 <i>h</i>	<i>m</i> ..	0.081	0.6074	$\frac{1}{4}$		single atom C
N3	6 <i>h</i>	<i>m</i> ..	0.1167	0.3	$\frac{1}{4}$		non-colinear C ₂
N4	6 <i>h</i>	<i>m</i> ..	0.1547	0.0907	$\frac{1}{4}$		non-colinear C ₂
C5	6 <i>h</i>	<i>m</i> ..	0.2642	0.3864	$\frac{1}{4}$		non-colinear N ₂
O6	6 <i>h</i>	<i>m</i> ..	0.4648	0.2009	$\frac{1}{4}$		non-colinear Na ₂
Na7	6 <i>g</i>	.2.	0.40446	0	0		octahedron N ₄ O ₂

H8	6h	m..	0.37	0.174	$\frac{1}{4}$
H9	6h	m..	0.515	0.293	$\frac{1}{4}$

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

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

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

References: [1] Jürgens B., Milius W., Morys P., Schnick W. (1998), *Z. Anorg. Allg. Chem.* 624, 91-97.
[2] Hoard J.L. (1938), *J. Am. Chem. Soc.* 60, 1194-1198.

190
hP42

BaCa _{0.5} Ce ₂ [CO ₃] ₄ F	hP42	(190) <i>P</i> -62c – i ² f ² edca
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BaCa_{0.5}Ce₂(CO₃)₄F [1], cordylite-(Ce)

Structural features: CO₃ trigonal units arranged in approximately planar layers where C forms a triangle mesh (BAABCAAC stacking). Ce(O₉F) polyhedra (an O₁₂ anticuboctahedron with one triangle replaced by a single F) share vertices to form infinite slabs; C in trigonal, Ca in trigonal prismatic voids in the slabs, Ba between the slabs.

Shen J., Mi J. (1992) [1]

Ba₄Ca_{0.50}Ce₂FO₁₂

$a = 0.5093$, $c = 2.3017$ nm, $c/a = 4.519$, $V = 0.5170$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.291	0.144	0.178		single atom C
O2	12i	1	0.498	0.043	0.0656		single atom C
Ce3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1458		10-vertex polyhedron FO ₉
C4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5656		coplanar triangle O ₃
C5	4e	3..	0	0	0.178		coplanar triangle O ₃
Ca6	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$	0.5	trigonal prism O ₆
F7	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Ce ₂
Ba8	2a	32.	0	0	0		trigonal prism O ₆

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

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

Remarks: Natural specimen from Bayan Obo, Inner Mongolia. Composition Ca_{0.398}Na_{0.255}Ba_{0.997}{Ce_{0.922}La_{0.652}Nd_{0.212}Pr_{0.057}}C_{4.130}O_{12.095}F_{0.905} from chemical analysis. The authors state that space group (194) *P*6₃/*mmc* was tested and rejected, however, only the coordinates of site O2 show a slight deviation from this symmetry. Additional reflections could be indexed with a 4-fold supercell (new axes 2a,2b,c).

References: [1] Shen J., Mi J. (1992), *J. China Univ. Geosci.* 3, 17-24.

190
hP42

NaV ₆ O ₁₁	hP42	(190) <i>P</i> -62c – i ² hfedc
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NaV₆O₁₁ rt [1]

Structural features: Close-packed NaO₃ and O₄ layers in h stacking; V in octahedral and trigonal bipyramidal voids. Infinite layers of edge-linked VO₆ octahedra (split V site) share vertices with slabs where units of two face-linked VO₆ octahedra (V₂ dumbbells) share vertices with VO₅ trigonal bipyramids.

De Roy M.E. et al. (1987) [1]

 $\text{NaO}_{11}\text{V}_6$ $a = 0.5699$, $c = 1.307$ nm, $c/a = 2.293$, $V = 0.3676$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
V1	12i	1	0.0135	0.505	0.0	0.5	
O2	12i	1	0.3408	0.173	0.0804		
O3	6h	m..	0.147	0.3051	$\frac{1}{4}$		non-coplanar triangle V ₃
O4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0902		7-vertex polyhedron V ₇
V5	4e	3..	0	0	0.1477		octahedron O ₆
Na6	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		anticuboctahedron O ₁₂
V7	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal bipyramid O ₅

Experimental: single crystal, diffractometer, X-rays, $R = 0.036$ Remarks: Short interatomic distances for partly occupied site(s). The structure was later redetermined in space group (194) $P6_3/mmc$ [2].

References: [1] De Roy M.E., Besse J.P., Chevalier R., Gasperin M. (1987), J. Solid State Chem. 67, 185-189. [2] Kanke Y., Kato K., Takayama Muromachi E., Isobe M. (1992), Acta Crystallogr. C 48, 1376-1380.

190
hP42

$\text{K}_3\text{Nb}_3[\text{Si}_2\text{O}_7]\text{O}_6$	hP42	(190) $P-62c - ih^2g^2fc$
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 $\text{K}_3\text{Nb}_3\text{O}_6(\text{Si}_2\text{O}_7)$ [1]Structural features: Infinite columns of vertex-linked NbO_6 octahedra share vertices with units of two vertex-linked SiO_4 tetrahedra to form a 3D-framework.

Jaulmes S. et al. (1995) [1]

 $\text{K}_3\text{Nb}_3\text{O}_{13}\text{Si}_2$ $a = 0.9012$, $c = 0.8027$ nm, $c/a = 0.891$, $V = 0.5646$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.486	0.31	0.017		non-colinear SiNb
O2	6h	m..	0.242	0.251	$\frac{1}{4}$		non-colinear Nb ₂
K3	6h	m..	0.4169	0.0323	$\frac{1}{4}$		12-vertex polyhedron O ₁₂
O4	6g	.2.	0.178	0	0		non-colinear Nb ₂
Nb5	6g	.2.	0.7626	0	0		octahedron O ₆
Si6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0473		tetrahedron O ₄
O7	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		colinear Si ₂

Transformation from published data: origin shift 0 0 $\frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.045$, $T = 293$ K

References: [1] Jaulmes S., Launay S., Mahe P., Quarton M. (1995), Acta Crystallogr. C 51, 794-796.

190
hP44

$\text{Rb}_4\text{Mn}[\text{MoO}_4]_3$	hP44	(190) $P-62c - ihf^4e^2b$
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 $\text{Rb}_4\text{Mn}(\text{MoO}_4)_3$ [2]Structural features: MnO_5 trigonal bipyramids share vertices with MoO_4 tetrahedra (including statistical occupation of two face-linked MoO_4 tetrahedra) to form infinite slabs.

Solodovnikov S.F. et al. (1988) [1]

$\text{MnMo}_3\text{O}_{12}\text{Rb}_4$

$a = 0.6088$, $c = 2.3676$ nm, $c/a = 3.889$, $V = 0.7600$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.3064	0.1241	0.0645		single atom Mo
O2	6h	m..	0.0562	0.3786	$\frac{1}{4}$		
Rb3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0282		7-vertex polyhedron O ₇
O4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1566	0.5	single atom Mo
Mo5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2279	0.5	
Rb6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.6576		octahedron O ₆
Mo7	4e	3..	0	0	0.0902		tetrahedron O ₄
O8	4e	3..	0	0	0.1647		colinear MoMn
Mn9	2b	-6..	0	0	$\frac{1}{4}$		trigonal bipyramid O ₅

Transformation from published data: $-x, -y, -z$; 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). The same data are reported in [2].

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). [2] Klevtsova R.F., Solodovnikov S.F., Klevtsov P.V. (1986), Izv. Akad. Nauk SSSR, Ser. Fiz. 50, 353-355.

190
hP46

$\text{Ca}_3\text{Mn}[\text{SO}_4]_2[\text{OH}]_6[\text{H}_2\text{O}]_3$	hP46	(190) $P\text{-}62c - i^2h^2f^2a$
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$\text{Ca}_3\text{Mn}(\text{SO}_4)_2(\text{OH})_6 \cdot 3\text{H}_2\text{O}$ [1], despujolsite

Structural features: $\text{Ca}[\text{O}_2(\text{OH})_4(\text{OH}_2)_2]$ square antiprisms share edges and vertices to form infinite slabs, which are interconnected via common vertices with $\text{Mn}(\text{OH})_6$ octahedra and SO_4 tetrahedra to form a 3D-framework.

Gaudefroy C. et al. (1968) [1]

$\text{Ca}_3\text{H}_{12}\text{MnO}_{17}\text{S}_2$

$a = 0.856$, $c = 1.076$ nm, $c/a = 1.257$, $V = 0.6828$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	12i	1	0.10037	0.20292	0.11114		single atom Mn
O2	12i	1	0.47747	0.22371	0.06805		single atom S
(OH ₂)3	6h	m..	0.01992	0.50189	$\frac{1}{4}$		octahedron Ca_2O_4
Ca4	6h	m..	0.30222	0.15669	$\frac{1}{4}$		square antiprism $\text{O}_2(\text{OH})_4(\text{OH}_2)_2$
O5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.11152		single atom S
S6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.52513		tetrahedron O ₄
Mn7	2a	32.	0	0	0		octahedron (OH) ₆

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

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.162$

Remarks: Natural specimen from Tachgagalt, Morocco. Ca/Mn ratio 3.10, S/Mn ratio 2.15 from electron microprobe analysis. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gaudefroy C., Granger M.M., Permingeat F., Protas J. (1968), Bull. Soc. Fr. Mineral. Cristallogr. 91, 43-50.

190
hP46

$\text{Ba}_3(\text{Hg}_{0.33}\text{Pt}_{0.67})_3\text{Pt}_2\text{O}_{11}$	<i>hP46</i>	(190) <i>P</i> -62 <i>c</i> – <i>i</i> ² <i>h</i> gf <i>d</i>
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Ba₃Pt₄HgO₁₁ [1]

Structural features: Units of two face-linked (Pt⁵⁺)O₆ octahedra (Pt₂ dumbbells) are interconnected via common vertices with O-Hg-O linear units or (Pt²⁺)O₄ squares (substitutional and partial orientational disorder).

Hansen T., Müller Buschbaum H. (1994) [1]

 $\text{Ba}_3\text{HgO}_{11}\text{Pt}_4$ $a = 0.6021$, $c = 1.7374$ nm, $c/a = 2.886$, $V = 0.5455$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.0055	0.4919	0.11691		non-colinear Pt ₂
O2	12 <i>i</i>	1	0.143	0.2527	0.0028	0.333	non-colinear O ₂
O3	6 <i>h</i>	<i>m</i> ..	0.182	0.3593	¹ / ₄		non-colinear Pt ₂
M4	6 <i>g</i>	.2.	0.4996	0	0		octahedron O ₆
Pt5	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.17215		octahedron O ₆
Ba6	4 <i>e</i>	3..	0	0	0.13226		15-vertex polyhedron O ₁₅
Ba7	2 <i>d</i>	-6..	² / ₃	¹ / ₃	¹ / ₄		anticuboctahedron O ₁₂

M4 = 0.667Pt + 0.333Hg

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

Remarks: $\text{Ba}_3(\text{Pt}^{2+})_2(\text{Pt}^{5+})_2(\text{Hg}^{2+})\text{O}_{11}$. Short interatomic distances for partly occupied site(s). A model for short-range order is proposed in space group (40) *Ama*2.

References: [1] Hansen T., Müller Buschbaum H. (1994), *Z. Anorg. Allg. Chem.* 620, 1471-1475.190
hP50

$\text{Pb}_3\text{Ge}[\text{SO}_4]_2[\text{OH}]_6[\text{H}_2\text{O}]_3$	<i>hP50</i>	(190) <i>P</i> -62 <i>c</i> – <i>i</i> ² <i>h</i> ² <i>f</i> ³ <i>a</i>
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Pb₃Ge(OH)₆(SO₄)₂·3H₂O [1], fleischerite

Structural features: $\text{Pb}[\text{O}_2(\text{OH})_4(\text{OH}_2)_2]$ square antiprisms share edges and vertices to form infinite slabs, which are interconnected via common vertices with $\text{Ge}(\text{OH})_6$ octahedra and SO_4 tetrahedra (partial disorder) to form a 3D-framework.

Otto H.H. (1975) [1]

 $\text{GeH}_{12}\text{O}_{17}\text{Pb}_3\text{S}_2$ $a = 0.8867$, $c = 1.0875$ nm, $c/a = 1.226$, $V = 0.7405$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.1946	0.0996	0.1079		single atom Ge
O2	12 <i>i</i>	1	0.217	0.492	0.027		single atom S
Pb3	6 <i>h</i>	<i>m</i> ..	0.15726	0.31726	¹ / ₄		10-vertex polyhedron O ₈ (OH ₂) ₂
(OH ₂)4	6 <i>h</i>	<i>m</i> ..	0.52	0.04	¹ / ₄		6-vertex polyhedron O ₄ Pb ₂
S5	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.021		trigonal bipyramid O ₅
O6	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.189	0.5	single atom O
O7	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.643	0.5	single atom S
Ge8	2 <i>a</i>	32.	0	0	0		octahedron O ₆
H9	12 <i>i</i>	1	0.3065	0.1561	0.0628		

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

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.039$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (182) $P6_322$ was tested and rejected ($R = 0.049$). Large difference between the interatomic distances within the SO_4 units.

References: [1] Otto H.H. (1975), Neues Jahrb. Mineral., Abh. 123, 160-190.

190
hP50

$\text{Na}_2\text{Ba}_5\text{Ru}_3\text{O}_{14}$	hP50	(190) $P-62c - i^2hf^3eda$
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Ba₅Ru₃Na₂O₁₄ ht [1], perovskite 10H

Structural features: Close-packed BaO_3 layers (partial vacancies ignored) in hc_4 stacking; Ru and Na in octahedral voids. Triple layers of vertex-linked NaO_6 and RuO_6 octahedra share vertices with units of two face-linked RuO_6 octahedra (Ru_2 dumbbells) to form a 3D-framework. Deformation derivative of $\text{Li}(\text{Li}_{0.5}\text{W}_{0.5})_2\text{Ba}_5\text{W}_2\text{O}_{15}$.

Quarez E., Mentré O. (2003) [1]

$\text{Ba}_5\text{Na}_2\text{O}_{14}\text{Ru}_3$

$a = 0.59261$, $c = 2.44$ nm, $c/a = 4.117$, $V = 0.7421$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.025	0.493	0.1531		non-colinear RuNa
O2	12i	1	0.307	0.13	0.0414	0.833	single atom Ru
O3	6h	m..	0.205	0.368	$\frac{1}{4}$		non-colinear Ru_2
Ba4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.05607		icosahedron O_{12}
Ru5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1942		octahedron O_6
Na6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5995		octahedron O_6
Ba7	4e	3..	0	0	0.16286		9-vertex polyhedron O_9
Ba8	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		anticuboctahedron O_{12}
Ru9	2a	32.	0	0	0		octahedron O_6

Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.065$, $T = 823$ K

Remarks: Phase stable at $T > 723$ K. Space groups (186) $P6_3mc$ and (194) $P6_3/mmc$ were tested and rejected ($R = 0.059$ but large number of refinable parameters for the former, $R = 0.071$ for the latter).

References: [1] Quarez E., Mentré O. (2003), Solid State Sci. 5, 1105-1116.

190
hP50

$\text{W}_6\text{Cl}_{18}\text{C}$	hP50	(190) $P-62c - i^3h^2c$
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CW₆Cl₁₈ [1]

Structural features: $\text{CW}_6\text{Cl}_{18}$ clusters consisting of a central C atom surrounded by a W_6 trigonal prism, a Cl_{12} anticuboctahedron and a large Cl_6 trigonal prism (six face-sharing $\text{W}(\text{Cl}_5\text{C})$ octahedra) in a Mg-type (h.c.p.) arrangement.

Zheng Y.Q. et al. (2003) [1]

$\text{CCl}_{18}\text{W}_6$

$a = 0.8923$, $c = 1.7503$ nm, $c/a = 1.962$, $V = 1.2069$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
W1	12i	1	0.14426	0.5037	0.16631		tricapped trigonal prism CCl_5W_3

Cl2	12i	1	0.3031	0.4387	0.0772	non-colinear W ₂
Cl3	12i	1	0.393	0.1053	0.102	single atom W
Cl4	6h	m..	0.0999	0.2674	¹ / ₄	non-colinear W ₂
Cl5	6h	m..	0.585	0.0652	¹ / ₄	non-colinear W ₂
C6	2c	-6..	¹ / ₃	² / ₃	¹ / ₄	trigonal prism W ₆

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

References: [1] Zheng Y.Q., Von Schnering H.G., Chang J.H., Grin Y., Engelhardt G., Heckmann G. (2003), Z. Anorg. Allg. Chem. 629, 1256-1264.

190
hP50

Zr ₆ NiAl ₂ H _{9,61}	hP50	(190) P-62c – ih ³ g ² fba
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Zr₆NiAl₂H_{9,61} [1]

Structural features: Filled-up derivative of β₁-K₂UF₆ antitype with H in tetrahedral (Zr₄ and Zr₃Al), trigonal bipyramidal (Zr₃Ni₂) and octahedral (Zr₄Al₂) voids.

Aksel'rud L.G. et al. (1999) [1]

Al₂H_{9,61}NiZr₆

$a = 0.813$, $c = 0.713$ nm, $c/a = 0.877$, $V = 0.4081$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
H1	12i	1	0.091	0.504	0.094	0.33	single atom Zr
H2	6h	m..	0.297	0.433	¹ / ₄	0.43	non-coplanar triangle H ₃
H3	6h	m..	0.364	0.253	¹ / ₄	0.78	coplanar square HZr ₃
Zr4	6h	m..	0.423	0.057	¹ / ₄		non-colinear H ₂
H5	6g	.2.	0.269	0	0		non-colinear H ₂
Zr6	6g	.2.	0.731	0	0		tricapped trigonal prism H ₉
Al7	4f	3..	¹ / ₃	² / ₃	0.059		non-coplanar triangle H ₃
Ni8	2b	-6..	0	0	¹ / ₄		colinear H ₂
H9	2a	32.	0	0	0		colinear Ni ₂

Transformation from published data: -x,-y,-z; origin shift 0 0 ¹/₂

Experimental: powder, diffractometer, neutrons, R_B = 0.063

Remarks: In table 6 of [1] the x-coordinate of former H4 is misprinted as 0.269 instead of -0.269 (better agreement with expected interatomic distances).

References: [1] Aksel'rud L.G., Fruchart D., Koblyuk N.D., Isnard O., Melnyk G.A., Skolozdra R.V. (1999), Int. J. Hydrogen Energy 24, 899-907.

190
hP50

Sr ₆ Ru ₃ O _{13,5}	hP50	(190) P-62c – ih ³ g ² fe
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Sr₄Ru₂O₉ [1]

Structural features: Units of two face-linked RuO₆ octahedra (partial disorder). Vacancy derivative of BaNiO₃ (perovskite 2H) with vacancies on both cation and anion sites.

Dussarrat C. et al. (1995) [1]

O_{13,50}Ru₃Sr₆

$a = 0.9642$, $c = 0.8104$ nm, $c/a = 0.840$, $V = 0.6525$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.4908	0.1742	0.0334		single atom Ru
Sr2	6h	m..	0.0176	0.3358	$\frac{1}{4}$		bicapped square antiprism O ₁₀
O3	6h	m..	0.1786	0.17	$\frac{1}{4}$		non-colinear Ru ₂
O4	6h	m..	0.3547	0.5154	$\frac{1}{4}$		non-colinear Ru ₂
O5	6g	.2.	0.1554	0	0	0.5	non-colinear Ru ₂
Sr6	6g	.2.	0.6639	0	0		bicapped square prism O ₁₀
Ru7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0784		octahedron O ₆
Ru8	4e	3..	0	0	0.1708	0.5	

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] Dussarrat C., Fompeyrine J., Darriet J. (1995), Eur. J. Solid State Inorg. Chem. 32, 3-14.

190
hP54

K ₉ Li ₃ [IO ₆] ₂ O	hP54	(190) <i>P</i> -62c – i ² h ² g ² fb
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K₉Li₃O(IO₆)₂ [1]

Structural features: IO₆ octahedra share edges with distorted LiO₄ tetrahedra to form infinite slabs separated by K₉O layers.

Untenecker H., Hoppe R. (1987) [1]

I₂K₉Li₃O₁₃

a = 0.9549, *c* = 1.1722 nm, *c/a* = 1.228, *V* = 0.9257 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.1551	0.5218	0.0998		non-colinear ILi
O2	12i	1	0.4897	0.3038	0.083		non-colinear ILi
K3	6h	m..	0.2814	0.3968	$\frac{1}{4}$		non-coplanar square O ₄
K4	6h	m..	0.453	0.1039	$\frac{1}{4}$		trigonal prism O ₆
K5	6g	.2.	0.2241	0	0		non-colinear O ₂
Li6	6g	.2.	0.539	0	0		tetrahedron O ₄
I7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0085		octahedron O ₆
O8	2b	-6..	0	0	$\frac{1}{4}$		coplanar triangle K ₃

Transformation from published data: -x,-y,-z; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, wR = 0.056

References: [1] Untenecker H., Hoppe R. (1987), Z. Anorg. Allg. Chem. 549, 129-138.

190
hP54

KAg ₅ S ₃	hP54	(190) <i>P</i> -62c – ih ⁵ gfa
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KAg₅S₃ [1]; RbAg₅S₃ (see remark)

Structural features: Close-packed S layers in h stacking; K in octahedral, Ag in trigonal and linear voids. AgS₃ trigonal units and AgS₂ linear units share vertices to form a 3D-framework; K in channels parallel to [001].

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

Ag_5KS_3

$a = 1.3196$, $c = 0.7943$ nm, $c/a = 0.602$, $V = 1.1978$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12i	1	0.1841	0.3344	0.0014		non-collinear S ₂
S2	6h	$m..$	0.1179	0.5329	$1/4$		6-vertex polyhedron Ag ₄ K ₂
S3	6h	$m..$	0.1366	0.2162	$1/4$		non-coplanar square Ag ₄
Ag4	6h	$m..$	0.2966	0.0041	$1/4$		tricapped trigonal prism S ₃ Ag ₆
Ag5	6h	$m..$	0.3688	0.3662	$1/4$		tricapped trigonal prism S ₃ Ag ₆
S6	6h	$m..$	0.4491	0.2217	$1/4$		non-coplanar square Ag ₄
Ag7	6g	.2.	0.4651	0	0		non-collinear S ₂
K8	4f	3..	$1/3$	$2/3$	0.0018		octahedron S ₆
K9	2a	32.	0	0	0		octahedron S ₆

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $1/2$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.040$, $T = 183$ K

Remarks: The authors of [1] state that the refinement of RbAg_5S_3 in space group (174) $P-6$ in [2] does not take into consideration all symmetry elements.

References: [1] Emirdag M., Schimek G.L., Kolis J.W. (1998), Acta Crystallogr. C 54, 1376-1378. [2] Wood P.T., Pennington W.T., Kolis J.W. (1994), Inorg. Chem. 33, 1556-1558.

190
hP56

Tl_3AuI_5	<i>hP56</i>	(190) $P-62c - h^3g^3f^3eba$
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$\text{Tl}_6\text{Au}_2\text{I}_{10}$ [1]

Structural features: Infinite columns of face-linked I₆ octahedra, and I₄ linear segments parallel to [001]; Au inside the octahedron columns (disorder), Tl between the columns.

Stoeger W., Rabenau A. (1979) [1]

AuI_5Tl_3

$a = 1.0569$, $c = 1.3431$ nm, $c/a = 1.271$, $V = 1.2993$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Au1	6h	$m..$	0.093	0.09	$1/4$	0.07	
I2	6h	$m..$	0.27	0.005	$1/4$		non-collinear Au ₂
Tl3	6h	$m..$	0.358	0.388	$1/4$		single atom Au
Au4	6g	.2.	0.08	0	0	0.07	
Tl5	6g	.2.	0.369	0	0		single atom Au
I6	6g	.2.	0.743	0	0		non-collinear Au ₂
I7	4f	3..	$1/3$	$2/3$	0.095	0.5	
I8	4f	3..	$1/3$	$2/3$	0.125	0.5	
I9	4f	3..	$1/3$	$2/3$	0.646		single atom I
Au10	4e	3..	0	0	0.145	0.13	
Au11	2b	-6..	0	0	$1/4$	0.66	
Au12	2a	32.	0	0	0	0.66	

Experimental: single crystal, diffractometer, X-rays, $R = 0.064$

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

References: [1] Stoeger W., Rabenau A. (1979), Z. Naturforsch. B 34, 685-692.

190
hP56

$\text{HLi}_2\text{Ba}_6[\text{Si}_2\text{O}_7][\text{SiO}_4]_2\text{Cl}$	<i>hP56</i>	(190) <i>P</i> -62c - i^2f^6 edcba
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 $\text{Li}_2\text{HBa}_6(\text{Si}_2\text{O}_7)(\text{SiO}_4)_2\text{Cl}$ [1]

Structural features: Slabs containing units of two vertex-linked SiO_4 tetrahedra and slabs containing single SiO_4 tetrahedra are interconnected via common vertices with LiO_6 octahedra to form composite slabs; Ba and Cl in voids in the slabs, additional Ba between the slabs. Ba forms an α -Nd type substructure.

Il'inets A.M. et al. (1982) [1]

 $a = 0.5704$, $c = 2.9402$ nm, $c/a = 5.155$, $V = 0.8285$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.179	0.357	0.0736		single atom Si
O2	12i	1	0.488	0.028	0.1748		single atom Si
M3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.002		single atom Si
Si4	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0568		tetrahedron O ₄
Li5	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.136		7-vertex polyhedron O ₆ Si
Ba6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5858		single atom O
Si7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.6942		tetrahedron O ₄
Ba8	4e	3..	0	0	0.1482		octahedron O ₆
O9	2d	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		colinear Si ₂
Ba10	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		trigonal prism O ₆
Cl11	2b	-6..	0	0	$\frac{1}{4}$		colinear Ba ₂
Ba12	2a	32.	0	0	0		octahedron O ₆

M3 = 0.5O + 0.5OH

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

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

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the *x*-coordinate of former O(1) is misprinted as -0.512 instead of 0.512 (checked on interatomic distances).

References: [1] Il'inets A.M., Iliukhin V.V., Belov N.V., Nevskii N.N. (1982), Dokl. Akad. Nauk SSSR 267, 1125-1127.

190
hP56

$\text{H}_2\text{Mg}[\text{SeO}_3]_2[\text{H}_2\text{O}]_3$	<i>hP56</i>	(190) <i>P</i> -62c - i^3h^2fe
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 $\text{Mg}(\text{HSeO}_3)_2 \cdot 3\text{H}_2\text{O}$ [1]

Structural features: $\text{Mg}[\text{O}_3(\text{OH})_2]_3$ octahedra share vertices with $:\text{Se}(\text{O}_2\text{OH})$ ψ -tetrahedra to form a 3D-framework; additional $:\text{Se}(\text{O}_2\text{OH})$ ψ -tetrahedra in channels (orientational disorder).

Boldt K. et al. (1999) [1]

 $a = 0.9434$, $c = 1.0492$ nm, $c/a = 1.112$, $V = 0.8087$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.1439	0.4932	0.1257		non-colinear SeMg
M2	12i	1	0.1641	0.1505	0.0484	0.5	single atom O
O3	12i	1	0.4988	0.3525	0.1014		single atom Mg

Se4	6h	m..	0.1607	0.3941	$\frac{1}{4}$	0.5	non-coplanar triangle O ₃
O5	6h	m..	0.2699	0.0434	$\frac{1}{4}$		single atom Se
Mg6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0147		octahedron O ₆
Se7	4e	3..	0	0	0.0207		
H8	12i	1	0.462	0.287	0.152		
H9	12i	1	0.574	0.07	0.106		
H10	6h	m..	0.21	0.046	$\frac{1}{4}$		

$$M2 = 0.667O + 0.333OH$$

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

Experimental: single crystal, diffractometer, X-rays, R = 0.016, T = 295 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. In table 2 of [1] the Wyckoff position of former O(11) is misprinted as 6g instead of 12i.

References: [1] Boldt K., Engelen B., Müller H., Panthöfer M., Unterderweide K. (1999), J. Mol. Struct. 475, 35-41.

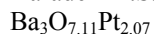
190
hP66

Ba ₃ Pt ₂ O ₇	hP66	(190) $P-62c - ih^4g^2f^2e^2a$
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Ba₃Pt₂O₇ [1]

Structural features: Close-packed Ba₃O₉ layers (partial vacancies ignored) and O-deficient triangle-mesh Ba₃O₆□₃ layers in hc stacking; Pt in octahedral, square and trigonal voids (disorder).

Haradem P.S. et al. (1977) [1]



$$a = 1.0108, c = 0.8638 \text{ nm}, c/a = 0.855, V = 0.7643 \text{ nm}^3, Z = 4$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.176	0.512	0.055		non-collinear Pt ₂
O2	6h	m..	0.17	0.14	$\frac{1}{4}$		non-collinear Pt ₂
Ba3	6h	m..	0.3337	0.0192	$\frac{1}{4}$		pentagonal pyramid O ₆
Pt4	6h	m..	0.3353	0.5975	$\frac{1}{4}$	0.17	
O5	6h	m..	0.525	0.357	$\frac{1}{4}$		non-collinear Pt ₂
O6	6g	.2.	0.156	0	0	0.74	single atom Pt
Ba7	6g	.2.	0.6646	0	0		10-vertex polyhedron O ₁₀
Pt8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1984	0.25	
Pt9	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5907		octahedron O ₆
Pt10	4e	3..	0	0	0.0877	0.18	
Pt11	4e	3..	0	0	0.1554	0.33	
Pt12	2a	32.	0	0	0	0.12	

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

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

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

References: [1] Haradem P.S., Chamberland B.L., Katz L., Gleizes A. (1977), J. Solid State Chem. 21, 217-223.

190
hP86

Pr ₂ Nb ₁₁ O ₃₀	hP86	(190) $P-62c - i^4hg^2f^5$
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Pr₂Nb₁₁O₃₀ [1]

Structural features: NbO₇ pentagonal bipyramids share edges to form simple and double infinite layers (also common vertices in the latter), which are interconnected via common vertices with NbO₆ octahedra to form a 3D-framework.

Kämmerer H. et al. (1998) [1]

Nb₁₁O₃₀Pr₂

$a = 0.6233$, $c = 3.2378$ nm, $c/a = 5.195$, $V = 1.0894$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Nb1	12i	1	0.00018	0.36132	0.19213		7-vertex polyhedron O ₇
O2	12i	1	0.25024	0.25103	0.18998		non-colinear Nb ₂
O3	12i	1	0.42448	0.05214	0.12875		non-colinear Nb ₂
O4	12i	1	0.43197	0.37664	0.05868		non-colinear Nb ₂
O5	6h	<i>m.</i>	0.04194	0.40839	¹ / ₄		non-colinear Nb ₂
O6	6g	.2.	0.24469	0	0		non-colinear Nb ₂
Nb7	6g	.2.	0.64379	0	0		7-vertex polyhedron O ₇
O8	4f	3..	¹ / ₃	² / ₃	0.01392		non-coplanar triangle Nb ₃
Pr9	4f	3..	¹ / ₃	² / ₃	0.09487		square prism (cube) O ₈
O10	4f	3..	¹ / ₃	² / ₃	0.17547		non-coplanar triangle Nb ₃
Nb11	4f	3..	¹ / ₃	² / ₃	0.59763		octahedron O ₆
O12	4f	3..	¹ / ₃	² / ₃	0.69754		non-coplanar triangle Nb ₃

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.019$

Remarks: In table 2 of [1] the *x*-coordinate of former O(7) is misprinted as ²/₃ instead of ¹/₃ (agreement with Wyckoff position 4f).

References: [1] Kämmerer H., Hofmann R., Gruehn R. (1998), Z. Anorg. Allg. Chem. 624, 1533-1537.

190
hP94

Cu ₅ Ta ₁₁ O ₃₀	hP94	(190) $P-62c - i^5hg^2f^3e$
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Cu₅Ta₁₁O₃₀ [1]

Structural features: TaO₇ pentagonal bipyramids share edges to form simple and double infinite layers (also common vertices in the latter), which are interconnected via common vertices with TaO₆ octahedra to form a 3D-framework; Cu in linear voids.

Jahnberg L. (1982) [1]

Cu₅O₃₀Ta₁₁

$a = 0.62297$, $c = 3.255$ nm, $c/a = 5.225$, $V = 1.0940$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	12i	1	0.0277	0.3317	0.192		7-vertex polyhedron O ₇
O2	12i	1	0.094	0.396	0.1296		non-coplanar triangle CuTa ₂
Cu3	12i	1	0.3333	0.1698	0.0952	0.833	non-colinear O ₂
O4	12i	1	0.371	0.433	0.0591		non-coplanar triangle CuTa ₂
O5	12i	1	0.417	0.331	0.1906		non-colinear Ta ₂
O6	6h	<i>m.</i>	0.038	0.307	¹ / ₄		non-colinear Ta ₂
O7	6g	.2.	0.252	0	0		non-colinear Ta ₂
Ta8	6g	.2.	0.6371	0	0		7-vertex polyhedron O ₇
Ta9	4f	3..	¹ / ₃	² / ₃	0.09705		octahedron O ₆
O10	4f	3..	¹ / ₃	² / ₃	0.1969		non-coplanar triangle Ta ₃

O11	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5096	non-coplanar triangle Ta ₃
O12	4e	3..	0	0	0.1818	non-coplanar triangle Ta ₃

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

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

References: [1] Jahnberg L. (1982), J. Solid State Chem. 41, 286-292.

190
hP104

KNa_{1.15}Mg_{4.66}Mn_{0.10}Fe_{0.12}Si₁₂O₃₀

hP104

(190) $P-62c - i^6h^2gf^3a$

KNa_{1.15}Mg_{4.66}Fe_{0.12}Mn_{0.10}Ti_{0.01}Si₁₂O₃₀ [1], roedderite

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with (Mg,Fe)O₆ octahedra and distorted (Mg,Fe)O₄ tetrahedra to form a 3D-framework; K inside the columns formed by superposed double 6-rings.

Armbruster T. (1989) [1]

Fe_{0.25}K_{0.94}Mg_{4.75}Na_{1.02}O₃₀Si₁₂

$a = 1.0141$, $c = 1.4286$ nm, $c/a = 1.409$, $V = 1.2723$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	12i	1	0.1145	0.3535	0.14031		tetrahedron O ₄
O2	12i	1	0.1534	0.4959	0.0771		non-coplanar triangle SiMg ₂
O3	12i	1	0.2235	0.2819	0.1193		non-colinear Si ₂
O4	12i	1	0.2713	0.0566	0.1138		non-colinear Si ₂
Si5	12i	1	0.3513	0.2356	0.13996		tetrahedron O ₄
O6	12i	1	0.499	0.3402	0.0796		non-coplanar triangle SiMg ₂
O7	6h	m..	0.1217	0.3916	$\frac{1}{4}$		non-colinear Si ₂
O8	6h	m..	0.3994	0.2567	$\frac{1}{4}$		non-colinear Si ₂
M9	6g	.2.	0.5031	0	0		tetrahedron O ₄
M10	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0035		octahedron O ₆
Na11	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2287	0.05	
Na12	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.7287	0.46	
K13	2a	32.	0	0	0	0.94	hexagonal prism O ₁₂

M9 = 0.95Mg + 0.05Fe; M10 = 0.95Mg + 0.05Fe

Transformation from published data: $-x, -y, -z$; origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.016, T = 300 K

Remarks: Natural specimen from Bellerberg, Eifel district, Germany. Small amounts of Ti ignored. Short interatomic distances for partly occupied site(s).

References: [1] Armbruster T. (1989), Eur. J. Mineral. 1, 715-718.

190
hP120

K_{1.67}Na_{0.33}B₄O₅[OH]₄[H₂O]₃

hP120

(190) $P-62c - i^7h^4gcba$

K_{1.67}Na_{0.33}B₄O₅(OH)₄·3H₂O [1]

Structural features: B₄O₅(OH)₄ units consisting of two B(O₃OH) tetrahedra and two B(O₂OH) trigonal units sharing vertices (two 6-membered rings, four endstanding OH).

Smykalla C., Behm H. (1988) [1]

B₄H₁₀K_{1.67}Na_{0.33}O₁₂

$a = 1.1278$, $c = 1.5806$ nm, $c/a = 1.401$, $V = 1.7411$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	12i	1	0.0627	0.49079	0.06606		tetrahedron O ₄
O2	12i	1	0.12337	0.18935	0.09736		single atom Na
O3	12i	1	0.13165	0.59582	0.12962		single atom B
O4	12i	1	0.16002	0.4546	0.02581		non-colinear B ₂
O5	12i	1	0.40767	0.25146	0.09625		single atom B
O6	12i	1	0.41397	0.04758	0.10868		non-colinear B ₂
B7	12i	1	0.42681	0.15223	0.05914		non-coplanar triangle O ₃
(OH ₂) ₈	6h	m..	0.0931	0.3235	1/4	0.366	single atom O
O9	6h	m..	0.26937	0.06644	1/4	0.634	single atom (OH ₂)
K10	6h	m..	0.43247	0.33447	1/4	0.366	
K11	6h	m..	0.60331	0.07839	1/4	0.634	
O12	6g	.2.	0.53275	0	0		non-colinear B ₂
K13	2c	-6..	1/3	2/3	1/4		trigonal prism O ₆
K14	2b	-6..	0	0	1/4		anticuboctahedron O ₉ (OH ₂) ₃
Na15	2a	32.	0	0	0		octahedron O ₆
H16	12i	1	0.116	0.198	0.057		
H17	12i	1	0.213	0.179	0.084		
H18	12i	1	0.325	0.084	0.205	0.634	
H19	12i	1	0.335	0.524	0.119		
H20	12i	1	0.412	0.311	0.058		

Experimental: single crystal, diffractometer, X-rays, R = 0.043, T = 293 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] Smykalla C., Behm H. (1988), Z. Kristallogr. 183, 51-61.

190
hP144

Fe ₂ (Fe _{0.5} Si _{0.5}) ₅ Pb ₁₁ Si ₁₀ Cl ₃ O ₄₁	hP144	(190) <i>P</i> -62 <i>c</i> - i ⁸ h ² gf ⁵ e ² b
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Pb₁₈Fe₄(Si₄(Si,Fe)₆)(Pb₄Si₁₆(Si,Fe)₄)O₈₂Cl₆ [1], jagoite

Structural features: SiO₄ and (Fe,Si)O₄ tetrahedra share vertices to form two kinds of infinite slab, which are interconnected via FeO₆ octahedra to form a 3D-framework.

Mellini M., Merlino S. (1981) [1]

Cl₃Fe_{4.50}O₄₁Pb₁₁Si_{12.50}

a = 0.8528, *c* = 3.333 nm, *c/a* = 3.908, *V* = 2.0992 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.011	0.198	0.181		non-colinear SiFe
Si2	12i	1	0.024	0.2903	0.1374		tetrahedron O ₄
O3	12i	1	0.112	0.225	0.106		single atom Si
O4	12i	1	0.14	0.51	0.142		non-colinear Si ₂
O5	12i	1	0.169	0.477	0.02		non-colinear SiFe
O6	12i	1	0.222	0.103	0.037		non-colinear Fe ₂
Pb7	12i	1	0.4114	0.3679	0.0757		4-vertex polyhedron O ₄
O8	12i	1	0.434	0.176	0.125		single atom Si
Pb9	6h	m..	0.1111	0.3883	1/4		monocapped trigonal prism Cl ₂ O ₅
Cl10	6h	m..	0.42	0.372	1/4		non-colinear Pb ₂
M11	6g	.2.	0.275	0	0		tetrahedron O ₄
Si12	4f	3..	1/3	2/3	0.0034		tetrahedron O ₄

Si13	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1613	tetrahedron O ₄
O14	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.204	single atom Si
O15	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.543	single atom Si
Pb16	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.6695	non-coplanar triangle O ₃
Fe17	4e	3..	0	0	0.0698	octahedron O ₆
M18	4e	3..	0	0	0.1969	tetrahedron O ₄
O19	2b	-6..	0	0	$\frac{1}{4}$	colinear Fe ₂

M11 = 0.5Fe + 0.5Si; M18 = 0.5Fe + 0.5Si

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

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

Remarks: Natural specimen from Långban, Sweden. General formula $X_6Pb^{2+}_{12}M_4(Si_4T_6)(Pb^{2+}_4Si_{16}T_4)_{-}O_{78}(O,OH)_4Cl_6$. Composition $(Pb_{3.43}Na_{1.33}K_{0.33}Ca_{0.71})Pb_{12}(Fe_{1.99}Ti_{0.09}Mg_{1.00}Mn_{0.84}Ca_{0.08})(Pb_4Si_{25.09}Be_{0.32}Al_{0.66}Fe_{3.93})O_{79.81}(OH)_{1.28}Cl_{6.18}$ from chemical analysis.

References: [1] Mellini M., Merlino S. (1981), Am. Mineral. 66, 852-858.

190
hP154

$Cu_{18.4}[SO_4]_{0.8}[NO_3]_{0.2}Cl_4[OH]_{31}[H_2O]_4$	hP154	(190) $P-62c - i^7h^8g^3ca$
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$Cu_{36.8}(NO_3)_{0.4}(SO_4)_{1.6}(OH)_{62}Cl_8(H_2O)_2 \cdot 6H_2O$ [1], buttgenbachite

Structural features: Cu(OH)₄ squares share vertices to form a 3D-framework; additional Cu in compressed trigonal antiprismatic voids, SO₄ tetrahedra and NO₃ trigonal units (substitutional and orientational disorder) and part of Cl atoms in large channels parallel to [001].

McLean W.J., Anthony J.W. (1972) [1]

$Cl_4Cu_{18.29}H_{39}N_{0.20}O_{38.80}S_{0.80}$

$a = 1.578$, $c = 0.91$ nm, $c/a = 0.577$, $V = 1.9624$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH)1	12i	1	0.077	0.451	0.092		non-colinear Cu ₂
(OH)2	12i	1	0.152	0.08	0.094		non-coplanar triangle Cu ₃
O3	12i	1	0.286	0.636	0.1184	0.267	non-colinear O ₂
(OH)4	12i	1	0.324	0.067	0.115		non-coplanar triangle Cu ₃
(OH)5	12i	1	0.329	0.254	0.099		non-coplanar triangle Cu ₃
(OH)6	12i	1	0.366	0.45	0.088		non-colinear Cu ₂
(OH ₂)7	12i	1	0.512	0.258	0.195	0.5	
Cu8	6h	m..	0.0149	0.3595	$\frac{1}{4}$		coplanar square (OH) ₄
Cl9	6h	m..	0.1418	0.2767	$\frac{1}{4}$		trigonal prism Cu ₆
O10	6h	m..	0.225	0.621	$\frac{1}{4}$	0.267	
O11	6h	m..	0.226	0.604	$\frac{1}{4}$	0.267	
O12	6h	m..	0.244	0.622	$\frac{1}{4}$	0.2	
Cu13	6h	m..	0.3349	0.1678	$\frac{1}{4}$		coplanar square (OH) ₄
Cu14	6h	m..	0.3451	0.3591	$\frac{1}{4}$		non-coplanar square (OH) ₄
M15	6h	m..	0.549	0.111	$\frac{1}{4}$		
Cu16	6g	.2.	0.2032	0	0		coplanar square (OH) ₄
Cu17	6g	.2.	0.5012	0	0		coplanar square (OH) ₄
Cu18	6g	.2.	0.7986	0	0		coplanar square (OH) ₄
M19	2c	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		coplanar triangle O ₃
Cu20	2a	32.	0	0	0	0.288	octahedron (OH) ₆

M15 = 0.334Cl + 0.333OH + 0.333OH₂; M19 = 0.8S + 0.2N

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

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

Remarks: Natural specimen from the Toughnut mine, Tombstone, Arizona. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. A more recent refinement on the same diffraction data is reported in [2]. In [1] the mineral is erroneously called connellite (see [2]).

References: [1] McLean W.J., Anthony J.W. (1972), *Am. Mineral.* 57, 426-438. [2] Hibbs D.E., Leverett P., Williams P.A. (2003), *Mineral. Mag.* 67, 47-60.