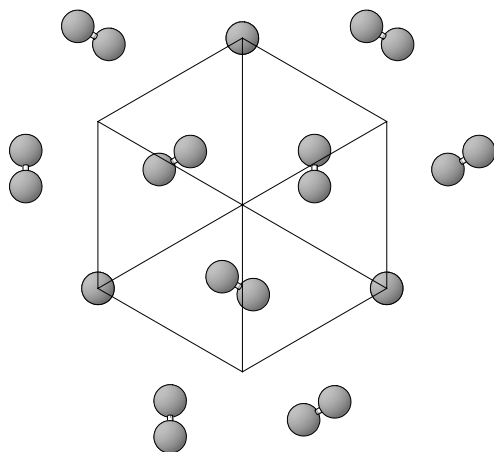


Space group (198) $P2_13$ 198
 $cP8$

[N ₂]	$cP8$	(198) $P2_13 - a^2$
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N₂ α [2]

Structural features: N₂ molecules in a Cu-type (cubic close-packed) arrangement. See Fig. II.69.

Fig. II.69. **N₂ α**

Arrangement of N₂ molecules in a layer perpendicular to $\langle 111 \rangle$.

La Placa S.J., Hamilton W.C. (1972) [1]

N₂

$a = 0.565 \text{ nm}$, $V = 0.1804 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	4a	.3.	0.1801	0.1801	0.1801		single atom N
N2	4a	.3.	0.2878	0.2878	0.2878		single atom N

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, photographs, X-rays, $R = 0.105$, $T = 20 \text{ K}$

Remarks: Refinement on diffraction data from [3], cell parameter from the same reference. The authors of [1] and [3] conclude in space group (198) $P2_13$, however, the authors of [4] and [5] (atom coordinates not refined) prefer the centrosymmetric space group (205) $Pa-3$.

References: [1] La Placa S.J., Hamilton W.C. (1972), Acta Crystallogr. B 28, 984-985. [2] (1931), Strukturberichte 1, 754. [3] Jordan T.H., Smith H.W., Streib W.E., Lipscomb W.N. (1964), J. Chem. Phys. 41, 756-759. [4] Schuchi A.F., Mills R.L. (1970), J. Chem. Phys. 52, 6000-6008. [5] Venables J.A., English C.A. (1974), Acta Crystallogr. B 30, 929-935.

198
 $cP8$

[CO]	$cP8$	(198) $P2_13 - a^2$
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CO α [1], Strukturbericht notation B21

Structural features: CO molecules in a Cu-type (cubic close-packed) arrangement.

Vegard L. (1930) [1]

CO

 $a = 0.563 \text{ nm}$, $V = 0.1785 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$4a$.3.	0.183	0.183	0.183		single atom C
C2	$4a$.3.	0.292	0.292	0.292		single atom O

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$ Experimental: powder, film, X-rays, $T = 77 \text{ K}$

Remarks: Phase stable at $T < 70 \text{ K}$ at ambient pressure. The authors of [2] prefer (205) Pa-3, however, the authors of [3] consider (198) $P2_13$ in their phase diagram.

References: [1] Vegard L. (1930), Z. Phys. 61, 185-190. [2] Krupskii I.N., Prokhvatilov A.I., Erenburg A.I., Yantsevich L.D. (1973), Phys. Status Solidi A 19, 519-527. [3] Mills R.L., Olinger B., Cromer D.T. (1986), J. Chem. Phys. 84, 2837-2845.

198
cP8

FeSi

cP8(198) $P2_13 - a^2$ **FeSi** [2], fersilicite, Strukturbericht notation B20

Structural features: 3D-framework of interpenetrating $\text{Fe}(\text{Si}_7\text{Fe}_6)$ and $\text{Si}(\text{Fe}_7\text{Si}_6)$ polyhedra. Heavily distorted derivative of CsCl. See Fig. II.70.

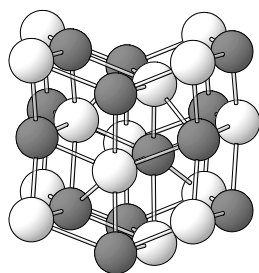


Fig. II.70. FeSi

Arrangement of Fe (light) and Si (dark) atoms.

Wartchow R. et al. (1997) [1]

FeSi

 $a = 0.4495 \text{ nm}$, $V = 0.0908 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	$4a$.3.	0.09262	0.09262	0.09262		pseudo Frank-Kasper Fe_7Si_6
Fe2	$4a$.3.	0.3865	0.3865	0.3865		pseudo Frank-Kasper Si_7Fe_6

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.014$, $T = 298 \text{ K}$

References: [1] Wartchow R., Gerighausen S., Binnewies M. (1997), Z. Kristallogr., New Cryst. Struct. 212, 320. [2] Wever F., Möller H. (1930), Z. Kristallogr. 75, 362-365.

PdF ₂	cP12	(198) $P2_13 - a^3$
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PdF₂ hp [1]

Structural features: Distorted PdF₆ octahedra share vertices to form a pyrite-type framework; F in trigonal coordination.

Tressaud A. et al. (1981) [1]

F₂Pd

$a = 0.5329$ nm, $V = 0.1513$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pd1	4a	.3.	0.000	0.000	0.000		octahedron F ₆
F2	4a	.3.	0.342	0.342	0.342		non-coplanar triangle Pd ₃
F3	4a	.3.	0.656	0.656	0.656		non-coplanar triangle Pd ₃

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

Experimental: powder, diffractometer, neutrons, $R = 0.055$, $T = 300$ K

Remarks: Phase stable at $p > \sim 1.5$ GPa at rt. Space group (205) $Pa-3$ was excluded based on the existence of two very weak diffraction lines.

References: [1] Tressaud A., Soubeyroux J.L., Touhara H., Demazeau G., Langlais F. (1981), Mater. Res. Bull. 16, 207-214.

NiSbS	cP12	(198) $P2_13 - a^3$
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NiSbS [2], ullmannite, Strukturbericht notation F0₁; "CoAsS cobaltite" (see remark); (Co,Ni)SbS [3]

Structural features: Ni(Sb₃S₃) octahedra share vertices to form a 3D-framework. Ni atoms and Sb-S dumbbells in a NaCl-type arrangement. Substitution derivative of pyrite. See Fig. II.71.

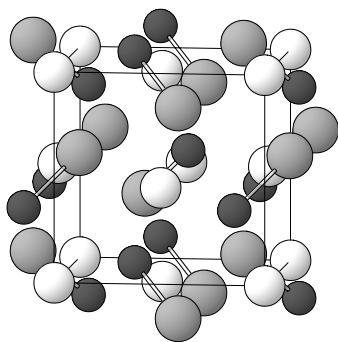


Fig. II.71. **NiSbS**

Arrangement of Ni (light), Sb (medium) and S (dark) atoms.

Foecker A.J., Jeitschko W. (2001) [1]

NiSSb

$a = 0.59341$ nm, $V = 0.2090$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	4a	.3.	0.01877	0.01877	0.01877		octahedron S ₃ Sb ₃
Sb2	4a	.3.	0.37326	0.37326	0.37326		tetrahedron SNi ₃

S3 4a .3. 0.61882 0.61882 0.61882 tetrahedron Ni₃Sb

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

Experimental: single crystal, diffractometer, X-rays, R = 0.009

Remarks: A structure proposal for CoAsS (cobaltite) with this structure type [4] is superseded (see [5]). Strukturbericht notation F0₁ was originally defined on cobaltite.

References: [1] Foecker A.J., Jeitschko W. (2001), J. Solid State Chem. 162, 69-78. [2] (1931), Strukturberichte 1, 269. [3] Pratt J.L., Bayliss P. (1980), Am. Mineral. 65, 154-156. [4] (1931), Strukturberichte 1, 269. [5] Giese R.F. Jr., Kerr P.F. (1965), Am. Mineral. 50, 1002-1014.

198
cP12

ZrSO	cP12	(198) P2 ₁ 3 – a ³
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ZrOS [2]; LaIrSi [3]

Structural features: Zr(S₄O₃) polyhedra (a S₂O₂ square facing a S₂O triangle) share atoms to form a 3D-framework. See Fig. II.72.

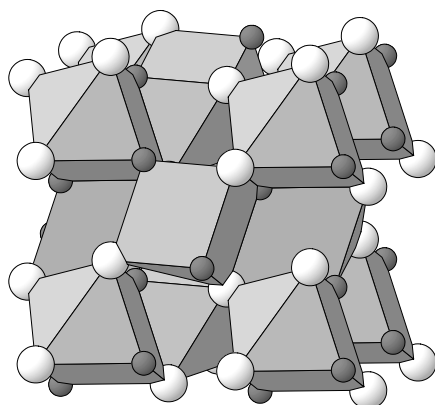


Fig. II.72. **ZrOS**

Arrangement of Zr(S₄O₃) polyhedra (S atoms light, O atoms dark).

Gleizes A. et al. (1974) [1]

OSZr

$a = 0.5696 \text{ nm}$, $V = 0.1848 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	4a	.3.	0.0701	0.0701	0.0701		7-vertex polyhedron O ₃ S ₄
S2	4a	.3.	0.3335	0.3335	0.3335		4-vertex polyhedron Zr ₄
O3	4a	.3.	0.6535	0.6535	0.6535		non-coplanar triangle Zr ₃

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

Remarks: The structure of LaIrSi was determined independently in [4].

References: [1] Gleizes A., Jeannin Y., Maire N. (1974), Bull. Soc. Chim. Fr. 1974, 1317-1321. [2] McCullough J.D., Brewer L., Bromley L.A. (1948), Acta Crystallogr. 1, 287-289. [3] Chevalier B., Lejay P., Cole A., Vlasse M., Etourneau J. (1982), Solid State Commun. 41, 801-804. [4] Klepp K., Parthé E. (1982), Acta Crystallogr. B 38, 1541-1544.

198
cP12

$(K_{0.5}Al_{0.5})ClO_{0.5}$	<i>cP12</i>	(198) $P2_13 - a^3$
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KAlOCl₂ [1]

Structural features: Close-packed Cl layers in c stacking; (K,Al) in octahedral (displaced from the center), O in tetrahedral voids (partial order).

Kuznetsov V.G. et al. (1973) [1]

 $a = 0.6276 \text{ nm}$, $V = 0.2472 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	4a	.3.	0.0	0.0	0.0		fourcapped trigonal prism O_4Al_6
O2	4a	.3.	0.25	0.25	0.25	0.5	square prism (cube) Al_4Cl_4
M3	4a	.3.	0.48	0.48	0.48		fourcapped trigonal prism O_4Cl_6

M3 = 0.50Al + 0.50K

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

Experimental: powder, Debye film, X-rays, R = 0.160

Remarks: Space group (208) $P4_232$ was tested and rejected.

References: [1] Kuznetsov V.G., Maksimova S.I., Morozov A.I. (1973), J. Struct. Chem. (Engl. Transl.) 14, 441-444.

198
cP16

SrBr[OH]	<i>cP16</i>	(198) $P2_13 - a^4$
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Sr(OH)Br cubic [2]

Structural features: $Sr([OH]_3Br_4)$ polyhedra (monocapped distorted octahedron) share atoms to form a 3D-framework, OH distributed over two sites (partial disorder).

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

 $a = 0.67488 \text{ nm}$, $V = 0.3074 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	4a	.3.	0.0799	0.0799	0.0799	0.838	
O2	4a	.3.	0.1233	0.1233	0.1233	0.162	
Br3	4a	.3.	0.4047	0.4047	0.4047		
Sr4	4a	.3.	0.6786	0.6786	0.6786		
H5	4a	.3.	0.204	0.204	0.204	0.162	
H6	4a	.3.	0.9951	0.9951	0.9951	0.838	

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

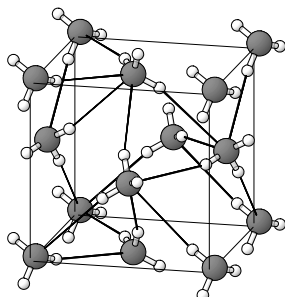
Experimental: powder, diffractometer, neutrons, T = 300 K

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] Peter S., Altorfer F., Bührer W., Lutz H.D. (2000), J. Solid State Chem. 151, 267-271. [2] Peter S., Lutz H.D. (1998), Z. Anorg. Allg. Chem. 624, 1067-1077.

198
cP16

[NH ₃]	<i>cP16</i>	(198) <i>P2₁3</i> – ba
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NH₃ [2], Strukturbericht notation D0₁Structural features: Single :NH₃ ψ -tetrahedra in a Cu-type (c.c.p.) arrangement, loosely interconnected via hydrogen bonding. See Fig. II.73.Fig. II.73. **NH₃**Arrangement of NH₃ molecules (N atoms dark, H atoms light).

Boese R. et al. (1997) [1]

H₃N $a = 0.51305 \text{ nm}$, $V = 0.1350 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	12 <i>b</i>	1	0.0063	0.4044	0.3797		single atom N
N2	4 <i>a</i>	.3.	0.0398	0.0398	0.0398		non-coplanar triangle H ₃

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.009$, $T = 160 \text{ K}$

References: [1] Boese R., Niederprüm N., Bläser D., Maulitz A., Antipin M.Y., Mallinson P.R. (1997), J. Phys. Chem. B 101, 5794-5799. [2] Mark H., Pohland E. (1925), Z. Kristallogr. 61, 532-537.

198
cP20

Au ₄ Al	<i>cP20</i>	(198) <i>P2₁3</i> – ba ²
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Au₄Al rt [2]; Mn₆₆Ni₂₀Si₁₄ β [3]Structural features: AlAu₁₂ icosahedra share atoms to form a 3D-framework. Substitution derivative of β-Mn.

Büchler H., Range K.J. (1990) [1]

AlAu₄ $a = 0.69227 \text{ nm}$, $V = 0.3318 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Au1	12 <i>b</i>	1	0.1172	0.2125	0.4507		14-vertex Frank-Kasper Al ₃ Au ₁₁
Al2	4 <i>a</i>	.3.	0.0597	0.0597	0.0597		icosahedron Au ₁₂
Au3	4 <i>a</i>	.3.	0.6827	0.6827	0.6827		icosahedron Al ₃ Au ₉

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.031$

Remarks: Phase stable at $T < 693$ K. In table 1 of [1] the cell volume is misprinted as 33.176 \AA^3 instead of 331.76 \AA^3 . Site occupancy $\text{Mn}_3(\text{Mn}_{0.28}\text{Ni}_{0.72})(\text{Ni}_{0.29}\text{Si}_{0.71})_2$ reported for β -(MnNiSi).

References: [1] Büchler H., Range K.J. (1990), J. Less-Common Met. 161, 347-354. [2] Ullner O.E. (1940), Ark. Kemi Mineral. Geol. 14A(3), 1-20. [3] Shoemaker C.B., Shoemaker D.P., Hopkins T.E., Yindepit S. (1978), Acta Crystallogr. B 34, 3573-3576.

198
cP20

$\text{Na}[\text{ClO}_3]$	<i>cP</i> 20	(198) $P2_13 - ba^2$
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NaClO₃ form I [2], Strukturbericht notation G0₃

Structural features: Single $:\text{ClO}_3$ ψ -tetrahedra and Na atoms in a distorted NaCl-type arrangement. NaO_6 octahedra are interconnected via common vertices and $:\text{ClO}_3$ ψ -tetrahedra to form a 3D-framework. See Fig. II.74.

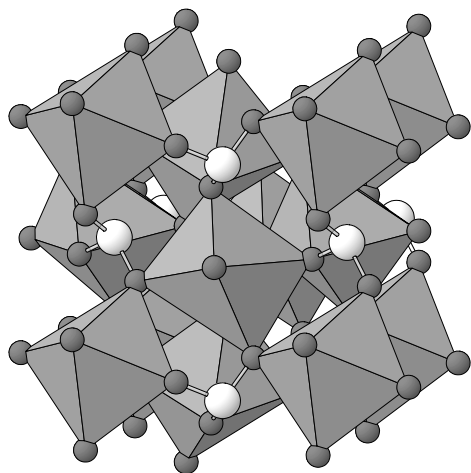


Fig. II.74. **NaClO₃ form I**

Arrangement of NaO_6 octahedra and $:\text{ClO}_3$ ψ -tetrahedra (Cl atoms large, O atoms small).

Sowa H. (1995) [1]

ClNaO_3

$a = 0.65718 \text{ nm}$, $V = 0.2838 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.0048	0.1967	0.4069		single atom Cl
Na2	4 <i>a</i>	.3.	0.069	0.069	0.069		octahedron O ₆
Cl3	4 <i>a</i>	.3.	0.4179	0.4179	0.4179		non-coplanar triangle O ₃

Experimental: single crystal, diffractometer, X-rays, $wR = 0.024$

References: [1] Sowa H. (1995), J. Solid State Chem. 118, 378-382. [2] (1931), Strukturberichte 1, 297.

198
cP24

SiO_2	<i>cP</i> 24	(198) $P2_13 - ba^3$
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SiO₂ cristobalite high [1], cristobalite high

Structural features: SiO_4 tetrahedra share vertices to form a 3D-framework where the Si atoms form a diamond-type sublattice.

Barth T.F.W. (1932) [1]

O₂Si

$a = 0.716 \text{ nm}$, $V = 0.3671 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.062	0.160	0.340		non-colinear Si ₂
Si2	4a	.3.	0.245	0.245	0.245		tetrahedron O ₄
O3	4a	.3.	0.375	0.375	0.375		colinear Si ₂
Si4	4a	.3.	0.508	0.508	0.508		tetrahedron O ₄

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

Experimental: powder, diffractometer, X-rays, $T = 773 \text{ K}$

Remarks: Phase stable at $1743 < T < 1983 \text{ K}$, may be maintained metastable down to $\sim 500 \text{ K}$. On page 353 of [3] the x -coordinate of former Si1 (u_1) is misprinted as 0.225 instead of 0.255 (given in the summary; checked on interatomic distances). Supersedes a structure proposal for idealized high-cristobalite with linear Si-O-Si sections in space group (227) $Fd\bar{3}m$. The structure was later redetermined in space group (227) $Fd\bar{3}m$ since no symmetry-forbidden reflections were observed (see [3]).

References: [1] Barth T.F.W. (1932), Am. J. Sci. 23, 350-356. [2] Wyckoff R.W.G. (1925), Z. Kristallogr. 62, 189-200. [3] Wright A.F., Leadbetter A.J. (1975), Philos. Mag. 31, 1391-1401.

198
cP24

Sn[WO ₄]	cP24	(198) $P2_13 - ba^3$
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SnWO₄ β [1]

Structural features: Single WO₄ tetrahedra and Sn atoms in a distorted NaCl-type arrangement. SnO₆ octahedra distorted to accommodate the electron lone-pair of Sn²⁺.

Jeitschko W., Sleight A.W. (1972) [1]

O₄SnW

$a = 0.72989 \text{ nm}$, $V = 0.3888 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.203	0.5229	0.3862		non-colinear WSn
Sn2	4a	.3.	0.0916	0.0916	0.0916		octahedron O ₆
W3	4a	.3.	0.4144	0.4144	0.4144		tetrahedron O ₄
O4	4a	.3.	0.5539	0.5539	0.5539		single atom W

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

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

Remarks: Phase stable at $T < 943 \text{ K}$.

References: [1] Jeitschko W., Sleight A.W. (1972), Acta Crystallogr. B 28, 3174-3178.

198
cP24

Sn ₂ ClF ₃	cP24	(198) $P2_13 - ba^3$
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Sn₂F₃Cl [1]

Structural features: :SnF₃ ψ-tetrahedra share vertices to form a 3D-framework; Cl in large voids.

Bergerhoff G., Goost L. (1974) [1]

ClF_3Sn_2

$a = 0.784 \text{ nm}$, $V = 0.4819 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12b	1	0.119	0.125	0.635		non-collinear Sn_2
Cl2	4a	.3.	0.011	0.011	0.011		15-vertex Frank-Kasper Sn_6F_9
Sn3	4a	.3.	0.351	0.351	0.351		non-coplanar triangle F_3
Sn4	4a	.3.	0.6824	0.6824	0.6824		non-coplanar triangle F_3

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

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

References: [1] Bergerhoff G., Goost L. (1974), Acta Crystallogr. B 30, 1362-1363.

198
cP24

CsCuTeS_3	<i>cP24</i>	(198) $P2_13 - ba^3$
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CsCuTeS₃ [1]

Structural features: Single TeS_3 ψ -tetrahedra and CuS_3 trigonal units share vertices to form a 3D-framework.

Zhang X., Kanatzidis M.G. (1994) [1]

CsCuS_3Te

$a = 0.9107 \text{ nm}$, $V = 0.7553 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12b	1	0.0346	0.3634	0.3133		non-collinear CuTe
Te2	4a	.3.	0.07091	0.07091	0.07091		non-coplanar triangle S_3
Cs3	4a	.3.	0.41793	0.41793	0.41793		7-vertex polyhedron CuS_6
Cu4	4a	.3.	0.6467	0.6467	0.6467		non-coplanar triangle S_3

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.038$, $T = 173 \text{ K}$

Remarks: We changed the y - and z -coordinates of the Cs and Te sites from 0.0821 and 0.4291 to 0.08207 and 0.42909, respectively, to be in agreement with Wyckoff position 4a.

References: [1] Zhang X., Kanatzidis M.G. (1994), J. Am. Chem. Soc. 116, 1890-1898.

198
cP28

$[\text{H}_2\text{S}]$	<i>cP28</i>	(198) $P2_13 - b^2a$
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H₂S form I' [1]

Structural features: Non-linear H_2S molecules in a Cu-type (cubic close-packed) arrangement (partial orientational disorder).

Fujihisa H. et al. (1998) [1]

H_2S

$a = 0.4931 \text{ nm}$, $V = 0.1199 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
H1	12b	1	0.002	0.2	0.192	0.333	single atom H

H2	12b	1	0.002	0.82	0.192	0.333	single atom H
S3	4a	.3.	0.01	0.01	0.01		trigonal prism H ₆

Transformation from published data: $1/4-y, 1/4-x, 1/4-z$

Experimental: powder, diffractometer, X-rays, $p = 9.5$ GPa

Remarks: Phase stable at $8.5 < p < 10.5$ GPa at rt.

References: [1] Fujihisa H., Yamawaki H., Sakashita M., Aoki K., Sasaki S., Shimizu H. (1998), Phys. Rev. B: Condens. Matter 57, 2651-2654.

198
cP28

Na₃AsS₃

cP28

(198) $P2_13 - ba^4$

Na₃AsS₃ [2]; K₃SbTe₃ [3]

Structural features: Single :AsS₃ ψ -tetrahedra and Na atoms in a distorted BiF₃-type arrangement. See Fig. II.75.

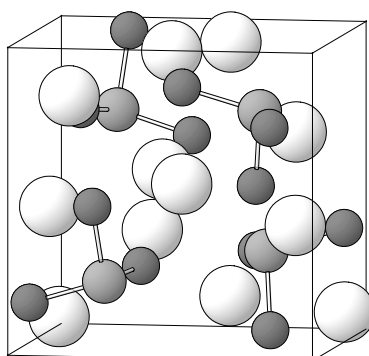


Fig. II.75. **Na₃AsS₃**

Arrangement of :AsS₃ ψ -tetrahedra (As atoms medium, S atoms dark) and Na atoms (light).

Sommer H., Hoppe R. (1977) [1]

AsNa₃S₃

$a = 0.8573$ nm, $V = 0.6301$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12b	1	0.028	0.2519	0.354		single atom As
Na2	4a	.3.	0.0604	0.0604	0.0604		11-vertex polyhedron S ₆ AsNa ₄
As3	4a	.3.	0.2781	0.2781	0.2781		non-coplanar triangle S ₃
Na4	4a	.3.	0.5681	0.5681	0.5681		octahedron S ₆
Na5	4a	.3.	0.8285	0.8285	0.8285		octahedron S ₆

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.069$

References: [1] Sommer H., Hoppe R. (1977), Z. Anorg. Allg. Chem. 430, 199-210. [2] Palazzi M. (1976), Acta Crystallogr. B 32, 3175-3177. [3] Jung J.S., Wu B., Stevens E.D., O'Connor C.J. (1991), J. Solid State Chem. 94, 362-367.

198
cP28

NaAl[SiO₄]

cP28

(198) $P2_13 - ba^4$

NaAlSiO₄ [1], carnegieite α , Strukturbericht notation S6₅

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a cristobalite-type framework (Al and Si form a zinc blende-type substructure); Na in large voids (displaced towards a face).

Barth F.W., Posnjak E. (1931) [1]

AlNaO_4Si

$a = 0.737 \text{ nm}$, $V = 0.4003 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.144	0.444	0.341		non-colinear SiAl
Si2	4 <i>a</i>	.3.	0.0	0.0	0.0		tetrahedron O_4
O3	4 <i>a</i>	.3.	0.125	0.125	0.125		non-colinear SiAl
Al4	4 <i>a</i>	.3.	0.258	0.258	0.258		tetrahedron O_4
Na5	4 <i>a</i>	.3.	0.744	0.744	0.744		non-coplanar triangle O_3

Experimental: powder, diffractometer, X-rays, $T = 1023 \text{ K}$

Remarks: Phase stable at $T > 1521 \text{ K}$, may be maintained metastable down to $\sim 963 \text{ K}$.

References: [1] Barth F.W., Posnjak E. (1931), *Z. Kristallogr.* 81, 135-141.

198
cP28

CaMgNiH_4	<i>cP28</i>	(198) $P2_13 - ba^4$
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CaMgNiH_4 [1]

Structural features: Ca and Mg form a distorted NaCl-type arrangement; a NiH_4 tetrahedron in every second distorted cubic void. See Fig. II.76.

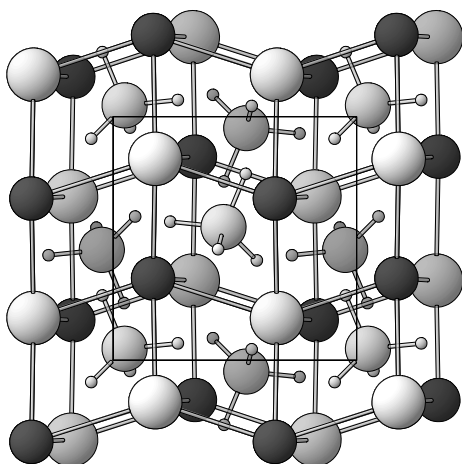


Fig. II.76. CaMgNiH_4

Arrangement of NiH_4 tetrahedra (Ni atoms large, H atoms small), Ca (light) and Mg (dark) atoms.

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

CaD_4MgNi

$a = 0.67301 \text{ nm}$, $V = 0.3048 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12 <i>b</i>	1	0.0444	0.431	0.2656		single atom Ni
Mg2	4 <i>a</i>	.3.	0.164	0.164	0.164		octahedron D_6
D3	4 <i>a</i>	.3.	0.4098	0.4098	0.4098		single atom Ni
Ni4	4 <i>a</i>	.3.	0.5468	0.5468	0.5468		tetrahedron D_4

Ca5 4a .3. 0.8271 0.8271 0.8271 octahedron D₆

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

Experimental: powder, diffractometer, neutrons, R_p = 0.047, T = 298 K

Remarks: The metal substructure was confirmed by X-ray diffraction on the hydride in [2].

References: [1] Huang B., Yvon K., Fischer P. (1992), J. Alloys Compd. 178, 173-179. [2] Gingl F., Yvon K. (1993), Z. Kristallogr. 207, 247-248.

198
cP32

Hg₃Cl₄O cP32 (198) P2₁3 – b²a²

Hg₃OCl₄ [2]

Structural features: Approximately planar Hg₃Cl₃O units consisting of three linear Cl-Hg-O units sharing a central O atom; additional Cl between the units.

Aurivillius K. (1964) [1]

Cl₄Hg₃O

a = 0.9236 nm, V = 0.7879 nm³, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	12b	1	0.0187	0.2312	0.3217		non-collinear OCl
Cl2	12b	1	0.1953	0.5274	0.334		single atom Hg
O3	4a	.3.	0.1783	0.1783	0.1783		non-coplanar triangle Hg ₃
Cl4	4a	.3.	0.5695	0.5695	0.5695		octahedron Hg ₆

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

Experimental: single crystal, diffractometer, neutrons, R = 0.064

References: [1] Aurivillius K. (1964), Ark. Kemi 22, 517-535. [2] Weiss A., Nagorsen G., Weiss A. (1953), Z. Anorg. Allg. Chem. 274, 151-168.

198
cP32

Ag₃S[NO₃] cP32 (198) P2₁3 – b²a²

Ag₃S(NO₃) [1]

Structural features: SAg₆ octahedra share vertices to form a 3D-framework; NO₃ trigonal units in voids.

Bergerhoff G. (1959) [1]

Ag₃NO₃S

a = 0.7929 nm, V = 0.4985 nm³, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.032	0.69	0.373		single atom N
Ag2	12b	1	0.136	0.19	0.503		non-coplanar triangle S ₂ O
N3	4a	.3.	0.089	0.089	0.089		non-coplanar triangle O ₃
S4	4a	.3.	0.367	0.367	0.367		octahedron Ag ₆

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

Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.190

References: [1] Bergerhoff G. (1959), Z. Anorg. Allg. Chem. 299, 328-337.

198
cP32

$\text{Na}_2\text{Ca}[\text{SiO}_4]$	<i>cP32</i>	(198) $P2_13 - ba^5$
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Na₂CaSiO₄ [1], Strukturbericht notation S6₅Structural features: CaO₄ and SiO₄ tetrahedra share vertices to form a cristobalite-type framework; Na in voids.

Barth F.W., Posnjak E. (1932) [1]

CaNa₂O₄Si $a = 0.748 \text{ nm}$, $V = 0.4185 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>b</i>	1	0.028	0.083	0.306		single atom Si
Na2	4 <i>a</i>	.3.	0.0	0.0	0.0		non-coplanar triangle O ₃
Ca3	4 <i>a</i>	.3.	0.2431	0.2431	0.2431		tetrahedron O ₄
O4	4 <i>a</i>	.3.	0.383	0.383	0.383		colinear SiCa
Si5	4 <i>a</i>	.3.	0.503	0.503	0.503		tetrahedron O ₄
Na6	4 <i>a</i>	.3.	0.75	0.75	0.75		non-coplanar triangle O ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: powder, diffractometer, X-rays

Remarks: Structure doubtful. In the summary of [1] the space group is misprinted as $P2_14$ instead of $P2_13$.

References: [1] Barth F.W., Posnjak E. (1932), Z. Kristallogr. 81, 370-375.

198
cP36

$\text{Ba}[\text{NO}_3]_2$	<i>cP36</i>	(198) $P2_13 - b^2a^3$
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Ba(NO₃)₂ [1]Structural features: Approximately planar NO₃ trigonal units; Ba atoms in a Cu-type (c.c.p.) arrangement.

Birnstock R. (1967) [1]

BaN₂O₆ $a = 0.811 \text{ nm}$, $V = 0.5334 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>b</i>	1	0.023	0.2186	0.0304		single atom N
O2	12 <i>b</i>	1	0.2653	0.4465	0.4521		single atom N
N3	4 <i>a</i>	.3.	0.0979	0.0979	0.0979		non-coplanar triangle O ₃
N4	4 <i>a</i>	.3.	0.3964	0.3964	0.3964		non-coplanar triangle O ₃
Ba5	4 <i>a</i>	.3.	0.75	0.75	0.75		cuboctahedron O ₁₂

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, neutrons, R = 0.070

References: [1] Birnstock R. (1967), Z. Kristallogr. 124, 310-334.

198
cP36

$\text{Hg}_3[\text{AsO}_4]\text{Cl}$	<i>cP36</i>	(198) $P2_13 - b^2a^3$
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Hg₃(AsO₄)Cl [2], kuznetsovite

Structural features: Cl atoms in a Cu-type (c.c.p.) arrangement; Hg₃ trigonal clusters and AsO₄ tetrahedra in large tetrahedral voids.

Weil M. (2001) [1]

AsClHg₃O₄

$a = 0.83983 \text{ nm}$, $V = 0.5923 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	12b	1	0.10802	0.64762	0.1956		non-collinear O ₂
O2	12b	1	0.1409	0.3731	0.1468		single atom As
Cl3	4a	.3.	0.0111	0.0111	0.0111		non-coplanar triangle Hg ₃
As4	4a	.3.	0.2656	0.2656	0.2656		tetrahedron O ₄
O5	4a	.3.	0.3791	0.3791	0.3791		single atom As

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: twinned crystal, diffractometer, X-rays, $R = 0.033$, $T = 295 \text{ K}$

Remarks: Identical with so-called Hg₆As₂Cl₂O₉ in [4]. Supersedes a structure proposal with an additional Hg site and unusual As-O distances in [3].

References: [1] Weil M. (2001), Z. Naturforsch. B 56, 753-758. [2] Romanenko G.V., Pervukhina N.V., Borisov S.V., Magarill S.A., Vasiliev V.I. (1999), J. Struct. Chem. (Engl. Transl.) 40, 270-275. [3] Solov'eva L.P., Tsybulya S.V., Zabolotnyi V.A., Pal'chik N.A. (1991), Sov. Phys. Crystallogr. (Engl. Transl.) 36, 731-732. [4] Vasiliev V.I., Lavrentiev I.G. (1980), Dokl. Akad. Nauk SSSR 255, 963-968.

198
cP36

CsXeF ₇	cP36	(198) $P2_13 - b^2a^3$
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CsXeF₇ [1]

Structural features: XeF₇ polyhedra and Cs atoms in a distorted NaCl-type arrangement.

Ellern A. et al. (1996) [1]

CsF₇Xe

$a = 0.846 \text{ nm}$, $V = 0.6055 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12b	1	0.1072	0.6976	0.1128		single atom Xe
F2	12b	1	0.182	0.3476	0.4145		single atom Xe
Cs3	4a	.3.	0.1011	0.1011	0.1011		15-vertex Frank-Kasper F ₁₅
Xe4	4a	.3.	0.4032	0.4032	0.4032		monocapped trigonal prism F ₇
F5	4a	.3.	0.5465	0.5465	0.5465		4-vertex polyhedron XeF ₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.035$, $T = 130 \text{ K}$

Remarks: In [1] the cell parameter is misprinted as 0.8960 nm instead of 0.8460 nm (from cell volume) and the number of formula units per unit cell Z as 8 instead of 4.

References: [1] Ellern A., Mahjoub A.R., Seppelt K. (1996), Angew. Chem. Int. Ed. Engl. 35, 1123-1125.

198
cP36

La _{0.89} Mo _{0.89} O ₄	cP36	(198) $P2_13 - b^2a^3$
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La₂Mo₂O₉ β [2], LAMOX

Structural features: Distorted (Mo, \square)O₄ tetrahedra (orientational disorder) and La atoms in a distorted NaCl-type arrangement.

Goutenoire F. et al. (2001) [1]

La_{0.89}Mo_{0.89}O₄

$a = 0.72342$ nm, $V = 0.3786$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.206	0.398	0.338	0.34	4-vertex polyhedron O ₃ Mo
O2	12 <i>b</i>	1	0.2408	0.587	0.429	0.66	non-colinear OMo
La3	4 <i>a</i>	.3.	0.1025	0.1025	0.1025	0.889	15-vertex Frank-Kasper O ₁₅
Mo4	4 <i>a</i>	.3.	0.4195	0.4195	0.4195	0.889	7-vertex polyhedron O ₇
O5	4 <i>a</i>	.3.	0.5679	0.5679	0.5679		single atom Mo

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$

Experimental: powder, diffractometer, neutrons, $R_B = 0.057$, $T = 943$ K

Remarks: Phase stable at $T > \sim 853$ K. Three different models with full occupancy of the cation sites were tested and rejected.

References: [1] Goutenoire F., Isnard O., Suard E., Bohnke O., Retoux R., Lacorre P. (2001), J. Mater. Chem. 11, 119-124. [2] Goutenoire F., Isnard O., Retoux R., Lacorre P. (2000), Chem. Mater. 12, 2575-2580.

198
cP40

SrZrO ₃	<i>cP40</i>	(198) $P2_13 - b^2a^4$
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SrZrO₃ rt [1], perovskite family

Structural features: ZrO₆ octahedra share vertices to form a 3D-framework; Sr in distorted cuboctahedral voids.

Van Roosmalen J.A.M. et al. (1992) [1]

O₃SrZr

$a = 0.8206$ nm, $V = 0.5526$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.0	0.205	0.205		non-colinear Zr ₂
O2	12 <i>b</i>	1	0.205	0.205	0.5		non-colinear Zr ₂
Sr3	4 <i>a</i>	.3.	0.0	0.0	0.0		non-coplanar triangle O ₃
Zr4	4 <i>a</i>	.3.	0.25	0.25	0.25		octahedron O ₆
Sr5	4 <i>a</i>	.3.	0.5	0.5	0.5		coplanar triangle O ₃
Zr6	4 <i>a</i>	.3.	0.75	0.75	0.75		octahedron O ₆

Transformation from published data: $1/4-y, 1/4-x, 1/4-z$

Experimental: powder, Guinier, X-rays, $T = 293$ K

Remarks: Phase stable below 1023 K. Idealized coordinates. The authors state that orthorhombic SrZrO₃, also observed at rt, may be stabilized by small amounts of impurities or deviations from the ideal cation ratio.

References: [1] Van Roosmalen J.A.M., Van Vlaanderen P., Cordfunke E.H.P. (1992), J. Solid State Chem. 101, 59-65.

198
cP40

$\text{TlCo}[\text{CO}]_4$	<i>cP40</i>	(198) $P2_13 - b^2a^4$
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 $\text{TlCo}(\text{CO})_4$ [2]

Structural features: $\text{Co}(\text{CO})_4$ tetrahedral units (linear Co-C-O segments) and Tl atoms in a distorted NaCl-type arrangement.

Klüfers P. (1983) [1]

$\text{C}_4\text{CoO}_4\text{Tl}$

$a = 0.8898 \text{ nm}$, $V = 0.7045 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>b</i>	1	0.1228	0.1858	0.5171		single atom C
C2	12 <i>b</i>	1	0.1485	0.1847	0.3889		single atom O
O3	4 <i>a</i>	.3.	0.008	0.008	0.008		single atom C
C4	4 <i>a</i>	.3.	0.0849	0.0849	0.0849		single atom O
Co5	4 <i>a</i>	.3.	0.1969	0.1969	0.1969		tetrahedron C_4
Tl6	4 <i>a</i>	.3.	0.68545	0.68545	0.68545		tricapped trigonal prism O_3C_6

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.025$, $T = 295 \text{ K}$

References: [1] Klüfers P. (1983), *Z. Kristallogr.* 165, 217-226. [2] Schussler D.P., Robinson W.R., Edgell W.F. (1974), *Inorg. Chem.* 13, 153-158.

198
cP40

$\text{TlFe}[\text{NO}][\text{CO}]_3$	<i>cP40</i>	(198) $P2_13 - b^2a^4$
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 $\text{TlFe}(\text{CO})_3(\text{NO})$ [1]

Structural features: $\text{Fe}([\text{CO}]_3[\text{NO}])$ tetrahedral units (linear Fe-C-O and Fe-N-O segments) and Tl atoms in a distorted NaCl-type arrangement. Ordering variant of $\text{TlCo}[\text{CO}]_4$. See Fig. II.77.

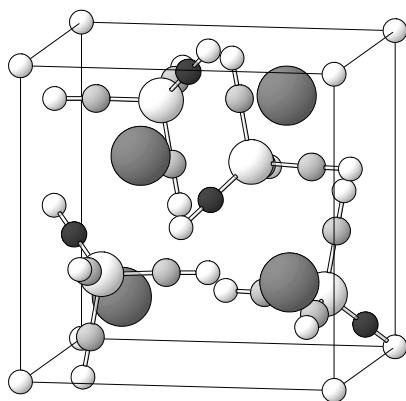


Fig. II.77. **$\text{TlFe}(\text{CO})_3(\text{NO})$**

Arrangement of $\text{Fe}(\text{CO})_3(\text{NO})$ units (N atoms dark, C atoms medium, O atoms light) and Tl atoms (large).

Clarkson L.M. et al. (1992) [1]

$\text{C}_3\text{FeNO}_4\text{Tl}$

$a = 0.8853 \text{ nm}$, $V = 0.6939 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>b</i>	1	0.1323	0.1869	0.52		single atom C

C2	12b	1	0.1561	0.1867	0.3922	single atom O
O3	4a	.3.	0.005	0.005	0.005	single atom N
N4	4a	.3.	0.0841	0.0841	0.0841	colinear OFe
Fe5	4a	.3.	0.19224	0.19224	0.19224	tetrahedron NC ₃
Tl6	4a	.3.	0.68432	0.68432	0.68432	non-coplanar triangle O ₃

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.020, T = 240 K

References: [1] Clarkson L.M., Clegg W., Hockless D.C.R., Norman N.C. (1992), Acta Crystallogr. C 48, 236-239.

198
cP44

Zr[WO ₄] ₂	cP44	(198) $P2_13 - b^2a^5$
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ZrW₂O₈ **a** [2]

Structural features: ZrO₆ octahedra and WO₄ tetrahedra share vertices to form a 3D-framework. See Fig. II.78.

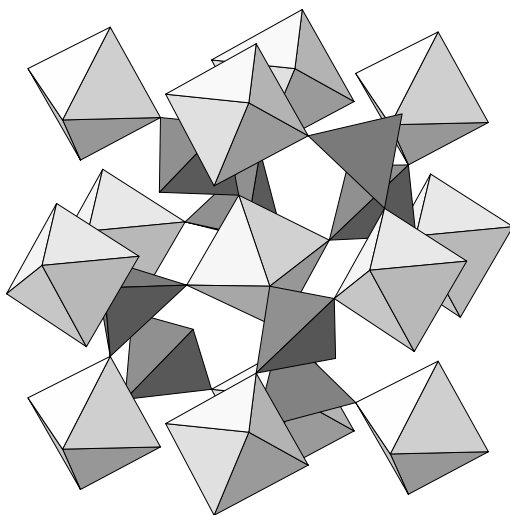


Fig. II.78. **ZrW₂O₈ **a****

Arrangement of WO₄ tetrahedra (dark) and ZrO₆ octahedra (light).

Mary T.A. et al. (1996) [1]

O₈W₂Zr

$a = 0.91599$ nm, $V = 0.7686$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.053	0.2929	0.0622		non-colinear WZr
O2	12b	1	0.0565	0.2124	0.5694		non-colinear WZr
O3	4a	.3.	0.0084	0.0084	0.0084		single atom W
W4	4a	.3.	0.1588	0.1588	0.1588		tetrahedron O ₄
O5	4a	.3.	0.2664	0.2664	0.2664		single atom W
Zr6	4a	.3.	0.4997	0.4997	0.4997		octahedron O ₆
W7	4a	.3.	0.8992	0.8992	0.8992		tetrahedron O ₄

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

Experimental: powder, diffractometer, neutrons, R_p = 0.074, T = 293 K

Remarks: Metastable phase observed at $T < 428$ K. Negative thermal expansion. The structure at 2 K is studied in [3].

References: [1] Mary T.A., Evans J.S.O., Vogt T., Sleight A.W. (1996), *Science* (Washington D.C.) 272, 90-92. [2] Auray M., Quarton M., Leblanc M. (1995), *Acta Crystallogr. C* 51, 2210-2213. [3] Evans J.S.O., David W.L.F., Sleight A.W. (1999), *Acta Crystallogr. B* 55, 333-340.

198
cP44

NaCa[PH ₂ O ₂] ₃	cP44	(198) $P2_13 - b^3a^2$
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NaCa(H₂PO₂)₃ [1]

Structural features: Single P(H₂O₂) tetrahedra. NaO₆ and CaO₆ octahedra share edges to form a 3D-framework.

Matsuzaki T., Iitaka Y. (1969) [1]

CaNaO₆P₃

$a = 0.972$ nm, $V = 0.9183$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	12b	1	0.0511	0.2323	0.405		non-colinear O ₂
O2	12b	1	0.0562	0.1098	0.3137		single atom P
O3	12b	1	0.1501	0.635	0.4619		single atom P
Ca4	4a	.3.	0.0773	0.0773	0.0773		octahedron O ₆
Na5	4a	.3.	0.6218	0.6218	0.6218		octahedron O ₆

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.097$

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

References: [1] Matsuzaki T., Iitaka Y. (1969), *Acta Crystallogr. B* 25, 1933-1938.

198
cP48

Hg ₃ [AsO ₄]Cl	cP48	(198) $P2_13 - b^3a^3$
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Hg₃(AsO₄)Cl [1], kuznetsovite

Structural features: Cl atoms in a Cu-type (c.c.p.) arrangement; Hg₃ trigonal clusters (partial orientational disorder) and AsO₄ tetrahedra in large tetrahedral voids.

Solov'eva L.P. et al. (1991) [1]

AsClHg₃O₄

$a = 0.84013$ nm, $V = 0.5930$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	12b	1	0.1026	0.329	0.5103	0.13	
Hg2	12b	1	0.1081	0.6508	0.1957	0.87	non-colinear OHg
O3	12b	1	0.132	0.386	0.177		single atom As
Cl4	4a	.3.	0.0198	0.0198	0.0198		
As5	4a	.3.	0.2616	0.2616	0.2616		tetrahedron O ₄
O6	4a	.3.	0.38	0.38	0.38		single atom As

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, diffractometer, X-rays, $R = 0.090$

Remarks: Natural specimen from the Arzaskii or Khaidarkan deposit. Composition $4\text{HgO} \cdot 2\text{HgCl} \cdot \text{As}_2\text{O}_5$ from electron microprobe analysis. Short interatomic distances for partly occupied site(s). A single, fully occupied Hg site was found in [2].

References: [1] Solov'eva L.P., Tsybulya S.V., Zabolotnyi V.A., Pal'chik N.A. (1991), Sov. Phys. Crystallogr. (Engl. Transl.) 36, 731-732. [2] Weil M. (2001), Z. Naturforsch. B 56, 753-758.

198
cP48

$\text{Co}[\text{CO}_3]\text{Cl}[\text{NH}_3]_6$	cP48	(198) $P2_13 - b^3a^3$
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[Co(NH₃)₆]CO₃Cl [1]

Structural features: Co[NH₃]₆ octahedral units in a Cu-type (c.c.p.) arrangement; planar CO₃ trigonal units and Cl atoms in "tetrahedral" voids.

Dahm M., Adam A. (2001) [1]

CClCoH₁₈N₆O₃

$a = 1.0005 \text{ nm}$, $V = 1.0015 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0483	0.5635	0.1005		single atom C
N2	12b	1	0.0634	0.2759	0.2415		single atom Co
N3	12b	1	0.2357	0.2799	0.4534		single atom Co
Cl4	4a	.3.	0.01238	0.01238	0.01238		tricapped trigonal prism N ₉
Co5	4a	.3.	0.25896	0.25896	0.25896		octahedron N ₆
C6	4a	.3.	0.4968	0.4968	0.4968		coplanar triangle O ₃
H7	12b	1	0.028	0.214	0.293		
H8	12b	1	0.036	0.356	0.273		
H9	12b	1	0.042	0.279	0.166		
H10	12b	1	0.177	0.343	0.464		
H11	12b	1	0.205	0.207	0.481		
H12	12b	1	0.295	0.491	0.307		

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

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

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

References: [1] Dahm M., Adam A. (2001), Z. Naturforsch. B 56, 1117-1122.

198
cP52

$\text{Pb}_3\text{P}_2\text{S}_8$	cP52	(198) $P2_13 - b^3a^4$
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Pb₃(PS₄)₂ [1]

Structural features: Single PS₄ tetrahedra.

Post E., Krämer V. (1984) [1]

P₂Pb₃S₈

$a = 1.09393 \text{ nm}$, $V = 1.3091 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12b	1	0.0052	0.2417	0.5922		single atom P

S2	12b	1	0.0476	0.2316	0.2847	single atom P
Pb3	12b	1	0.1376	0.4758	0.243	icosahedron S ₈ P ₄
S4	4a	.3.	0.0429	0.0429	0.0429	single atom P
P5	4a	.3.	0.1501	0.1501	0.1501	tetrahedron S ₄
P6	4a	.3.	0.4257	0.4257	0.4257	tetrahedron S ₄
S7	4a	.3.	0.5347	0.5347	0.5347	single atom P

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

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

References: [1] Post E., Krämer V. (1984), Mater. Res. Bull. 19, 1607-1612.

198
cP52

Ag ₄ Te[NO ₃] ₂	cP52	(198) P2 ₁ 3 – b ³ a ⁴
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Ag₄Te(NO₃)₂ β [1]

Structural features: TeAg₉ polyhedra share atoms to form a 3D-framework; NO₃ trigonal units in voids.

Schultze Rhonhof E., Bergerhoff G. (1969) [1]

Ag₄N₂O₆Te

$a = 0.8627$ nm, $V = 0.6421$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.08	0.28	0.21		non-colinear NO
Ag2	12b	1	0.0865	0.2116	0.5115		pseudo Frank-Kasper O ₄ Te ₂ Ag ₅ N ₂
O3	12b	1	0.09	0.71	0.31		non-colinear NO
Ag4	4a	.3.	0.023	0.023	0.023		4-vertex polyhedron O ₃ N
N5	4a	.3.	0.188	0.188	0.188		non-coplanar triangle O ₃
Te6	4a	.3.	0.316	0.316	0.316		single atom N
N7	4a	.3.	0.688	0.688	0.688		non-coplanar triangle O ₃

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

Experimental: single crystal, diffractometer, X-rays, R = 0.112

References: [1] Schultze Rhonhof E., Bergerhoff G. (1969), Acta Crystallogr. B 25, 2645-2648.

198
cP56

Cu ₂ [SeO ₃] ₂ O	cP56	(198) P2 ₁ 3 – b ³ a ⁵
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Cu₂O(SeO₃) form I [1]

Structural features: :SeO₃ ψ-tetrahedra, CuO₅ square pyramids and CuO₅ trigonal bipyramids share atoms to form a 3D-framework.

Effenberg H., Pertlik F. (1986) [1]

Cu₂O₄Se

$a = 0.8925$ nm, $V = 0.7109$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0199	0.7794	0.2666		non-coplanar triangle SeCu ₂
O2	12b	1	0.021	0.2187	0.5608		non-coplanar triangle SeCu ₂
Cu3	12b	1	0.1219	0.3711	0.3835		square pyramid O ₅
O4	4a	.3.	0.0121	0.0121	0.0121		tetrahedron Cu ₄

Cu5	4a	.3.	0.136	0.136	0.136	square pyramid O ₅
O6	4a	.3.	0.2605	0.2605	0.2605	tetrahedron Cu ₄
Se7	4a	.3.	0.4613	0.4613	0.4613	non-coplanar triangle O ₃
Se8	4a	.3.	0.709	0.709	0.709	non-coplanar triangle O ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: powder, diffractometer, X-rays, wR = 0.028

References: [1] Effenberger H., Pertlik F. (1986), Monatsh. Chem. 117, 887-896.

198
cP56

Sr[MnO ₄] ₂ [H ₂ O] ₃	cP56	(198) $P2_13 - b^3a^5$
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Sr(MnO₄)₂·3H₂O [1]

Structural features: Single MnO₄ tetrahedra, non-linear H₂O units and Sr atoms.

Ferrari A. et al. (1966) [1]

H₆Mn₂O₁₁Sr

$a = 0.9611$ nm, $V = 0.8878$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0371	0.3826	0.3973		single atom Mn
O2	12b	1	0.0883	0.4042	0.1043		single atom Mn
(OH ₂) ₃	12b	1	0.3053	0.3078	0.5346		single atom Sr
Mn4	4a	.3.	0.0138	0.0138	0.0138		tetrahedron O ₄
O5	4a	.3.	0.1113	0.1113	0.1113		single atom Mn
Sr6	4a	.3.	0.2715	0.2715	0.2715		10-vertex polyhedron (OH ₂) ₃ O ₇
Mn7	4a	.3.	0.5724	0.5724	0.5724		tetrahedron O ₄
O8	4a	.3.	0.6698	0.6698	0.6698		single atom Mn

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.160

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

References: [1] Ferrari A., Braibanti A., Bigliardi G., Manotti Lanfredi A.M. (1966), Acta Crystallogr. 21, 681-685.

198
cP56

Ag ₇ AsS ₆	cP56	(198) $P2_13 - b^3a^5$
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Ag₇AsS₆ [1], billingsleyite, argyrodite family

Structural features: S forms a tetrahedrally close-packed (MgCu₂-type) framework; As in tetrahedral, Ag in tetrahedral, trigonal and linear coordination. Single AsS₄ tetrahedra.

Pertlik F. (1994) [1]

Ag₇AsS₆

$a = 1.0475$ nm, $V = 1.1494$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12b	1	0.0746	0.4034	0.2651		7-vertex polyhedron S ₄ Ag ₃
S2	12b	1	0.1234	0.6279	0.1425		tetrahedron AsAg ₃
Ag3	12b	1	0.2267	0.4815	0.491		non-coplanar triangle S ₃

S4	4a	.3.	0.0132	0.0132	0.0132	monocapped trigonal prism Ag ₇
Ag5	4a	.3.	0.146	0.146	0.146	colinear S ₂
S6	4a	.3.	0.2798	0.2798	0.2798	4-vertex polyhedron Ag ₄
S7	4a	.3.	0.6264	0.6264	0.6264	tetrahedron AsAg ₃
As8	4a	.3.	0.7473	0.7473	0.7473	tetrahedron S ₄

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$; origin shift $1/2 \ 1/2 \ 1/2$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.028$, $T = 298$ K

Remarks: Phase stable at $T < 533$ K. The orthorhombic cell reported for natural billingsleyite in [2] is stated to be doubtful (similar diffraction patterns).

References: [1] Pertlik F. (1994), J. Solid State Chem. 112, 170-175. [2] Frondel C., Honea R.M. (1968), Am. Mineral. 53, 1791-1798.

198
cP56

Ag ₆ Hg _{0.82} GeS _{5.82}	cP56	(198) $P2_13 - b^3a^5$
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Ag₆Hg_{0.82}GeS_{5.82} [1], argyrodite family

Structural features: S forms a tetrahedrally close-packed (MgCu₂-type) framework (partial vacancies ignored); Ge in tetrahedral, Ag in tetrahedral and trigonal voids, Hg in linear coordination. Single GeS₄ tetrahedra and S-Hg-S linear units.

Gulay L.D., Parasyuk O.V. (2001) [1]

Ag₆GeHg_{0.82}S_{5.82}

$a = 1.05547$ nm, $V = 1.1758$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12b	1	0.0757	0.4079	0.2603		pseudo Frank-Kasper S ₅ Ag ₃ Hg ₂ Ge
S2	12b	1	0.133	0.638	0.1458		tetrahedron GeAg ₃
Ag3	12b	1	0.2281	0.4948	0.4996		non-coplanar triangle S ₃
S4	4a	.3.	0.002	0.002	0.002	0.82	tetrahedron HgAg ₃
Hg5	4a	.3.	0.1311	0.1311	0.1311	0.82	colinear S ₂
S6	4a	.3.	0.26	0.26	0.26		4-vertex polyhedron HgAg ₃
S7	4a	.3.	0.622	0.622	0.622		tetrahedron GeAg ₃
Ge8	4a	.3.	0.7472	0.7472	0.7472		tetrahedron S ₄

Transformation from published data: $1/4-y, 1/4-x, 1/4-z$; origin shift $1/2 \ 1/2 \ 1/2$

Experimental: powder, diffractometer, X-rays, $R_B = 0.087$

Remarks: In table 1 of [1] the cell volume is misprinted as 1.1779 nm³ instead of 1.1759 nm³.

References: [1] Gulay L.D., Parasyuk O.V. (2001), J. Alloys Compd. 327, 100-103.

198
cP56

Li ₂ ZnMn ₃ O ₈	cP56	(198) $P2_13 - b^3a^5$
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Li₂ZnMn₃O₈ [1], spinel AA'[A'B₃]O₈

Structural features: Close-packed O layers in c stacking, Mn and part of Li in octahedral voids, Zn and remaining Li in tetrahedral voids. Substitution derivative of MgAl₂O₄ (spinel).

Joubert J.C., Durif A. (1964) [1]

Li₂Mn₃O₈Zn

$a = 0.8192$ nm, $V = 0.5498$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	12b	1	0.125	0.125	0.375		octahedron O ₆
O2	12b	1	0.125	0.125	0.625		tetrahedron Li ₂ Mn ₂
O3	12b	1	0.125	0.375	0.375		tetrahedron ZnMn ₂ Li
Zn4	4a	.3.	0.0	0.0	0.0		tetrahedron O ₄
O5	4a	.3.	0.125	0.125	0.125		tetrahedron ZnMn ₃
Li6	4a	.3.	0.375	0.375	0.375		octahedron O ₆
O7	4a	.3.	0.625	0.625	0.625		tetrahedron LiMn ₃
Li8	4a	.3.	0.75	0.75	0.75		tetrahedron O ₄

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

Experimental: powder, film, X-rays

References: [1] Joubert J.C., Durif A. (1964), C. R. Hebd. Seances Acad. Sci. 258, 4482-4485.

198
cP60

Ba ₈ Ga ₇	cP60	(198) $P2_13 - b^4a^3$
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Ba₈Ga₇ [1]; Sr₈Al₇ [1]

Structural features: Tetrahedral Ga₄ and trigonal Ga₃ clusters in Ba₆ and Ba₁₃ cages, respectively.

Fornasini M.L. (1983) [1]

Ba₈Ga₇

$a = 1.2990$ nm, $V = 2.1919$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	12b	1	0.0011	0.2987	0.4421		7-capped pentagonal prism Ga ₈ Ba ₉
Ba2	12b	1	0.0613	0.5186	0.2025		15-vertex Frank-Kasper Ga ₆ Ba ₉
Ga3	12b	1	0.0760	0.2390	0.1941		tricapped trigonal prism Ga ₃ Ba ₆
Ga4	12b	1	0.2467	0.3133	0.5831		tricapped trigonal prism Ga ₂ Ba ₇
Ga5	4a	.3.	0.0689	0.0689	0.0689		tricapped trigonal prism Ga ₃ Ba ₆
Ba6	4a	.3.	0.3127	0.3127	0.3127		15-vertex Frank-Kasper Ga ₆ Ba ₉
Ba7	4a	.3.	0.6852	0.6852	0.6852		pseudo Frank-Kasper Ga ₉ Ba ₉

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

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

Remarks: Supersedes a structure proposal for so-called SrAl (α InCl-type structure) in [2].

References: [1] Fornasini M.L. (1983), Acta Crystallogr. C 39, 943-946. [2] Fornasini M.L., Merlo F. (1976), Acta Crystallogr. B 32, 1864-1867.

198
cP64

InCl	cP64	(198) $P2_13 - b^4a^4$
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InCl α [2]; "SrAl" (see remark)

Structural features: Approximately close-packed Cl layers in c stacking; In in heavily distorted octahedral voids ($:\text{InCl}_3$ ψ -tetrahedra and $:\text{InCl}_4$ trigonal ψ -bipyramids). Distorted derivative of NaCl. See Fig. II.79.

Van Der Vorst C.P.J.M. et al. (1978) [1]

ClIn

$a = 1.2373$ nm, $V = 1.8942$ nm³, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	12b	1	0.00270	0.27948	0.02805		tricapped trigonal prism Cl ₆ In ₃
Cl2	12b	1	0.0498	0.239	0.3049		non-coplanar triangle In ₃
Cl3	12b	1	0.1996	0.5505	0.2505		octahedron In ₆
In4	12b	1	0.22119	0.46978	0.49873		tricapped trigonal prism Cl ₆ In ₃
Cl5	4a	.3.	0.0486	0.0486	0.0486		non-coplanar triangle In ₃
In6	4a	.3.	0.28016	0.28016	0.28016		bicapped square prism Cl ₇ In ₃
Cl7	4a	.3.	0.4561	0.4561	0.4561		non-coplanar triangle In ₃
In8	4a	.3.	0.71731	0.71731	0.71731		tricapped trigonal prism Cl ₆ In ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: single crystal, diffractometer, X-rays, wR = 0.030, T = 293 K

Remarks: Phase stable at T < 390 K. The same data are also reported in [3]. A similar structure proposal for so-called SrAl in [4] is superseded (see [5]; the composition was corrected to Sr₈Al₇).

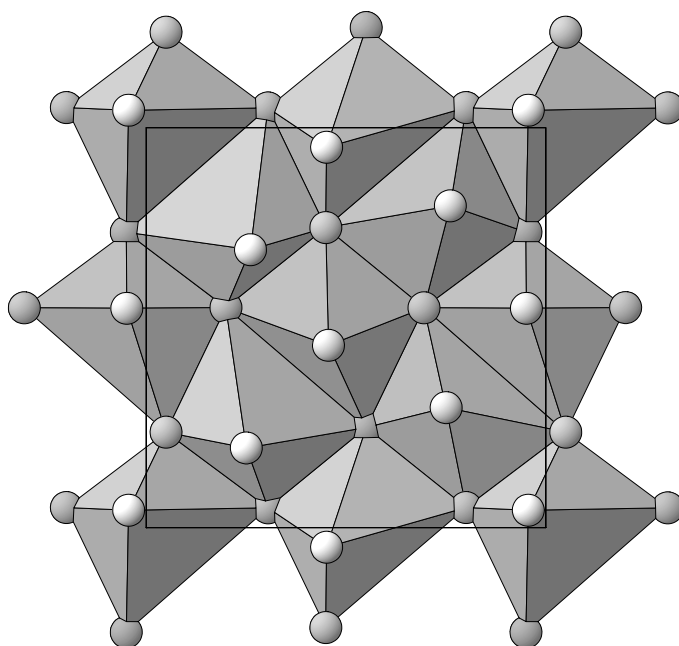


Fig. II.79. **InCl α**

Arrangement of InCl₆ octahedra (In atoms at $x = 0.22$ and 0.28).

References: [1] Van Der Vorst C.P.J.M., Verschoor G.C., Maaskant W.J.A. (1978), Acta Crystallogr. B 34, 3333-3335. [2] Van Den Berg J.M. (1966), Acta Crystallogr. 20, 905-910. [3] Van Der Vorst C.P.J.M., Maaskant W.J.A. (1980), J. Solid State Chem. 34, 301-313. [4] Fornasini M.L., Merlo F. (1976), Acta Crystallogr. B 32, 1864-1867. [5] Fornasini M.L. (1983), Acta Crystallogr. C 39, 943-946.

198
cP64

Ag₉GaSe₆

cP64

(198) $P2_13 - b^4a^4$

Ag₉GaSe₆ β [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu₂-type) framework; Ga in tetrahedral, Ag in trigonal voids. Single GaSe₄ tetrahedra.

Deloume J.P. et al. (1978) [1]

Ag_9GaSe_6

$a = 1.1126 \text{ nm}$, $V = 1.3773 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12b	1	0.0313	0.2272	0.2308		tricapped trigonal prism Se_4Ag_5
Se2	12b	1	0.1232	0.1328	0.6025		pentagonal pyramid GaAg_5
Ag3	12b	1	0.1466	0.3308	0.4651		bicapped square prism Se_4Ag_6
Ag4	12b	1	0.1727	0.5697	0.3622		9-vertex polyhedron Se_4Ag_5
Se5	4a	.3.	0.0192	0.0192	0.0192		9-vertex polyhedron Ag_9
Se6	4a	.3.	0.2628	0.2628	0.2628		6-vertex polyhedron Ag_6
Ga7	4a	.3.	0.508	0.508	0.508		tetrahedron Se_4
Se8	4a	.3.	0.6304	0.6304	0.6304		tetrahedron GaAg_3

Experimental: single crystal, diffractometer, X-rays, $R = 0.044$, $T = 268 \text{ K}$

Remarks: Phase stable at $T < 281 \text{ K}$.

References: [1] Deloume J.P., Faure R., Loiseleur H., Roubin M. (1978), Acta Crystallogr. B 34, 3189-3193.

198
cP64

$\text{Cs}_{2.29}\text{Fe}_{1.57}[\text{CN}]_6$	cP64	(198) $P2_13 - b^4a^4$
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$\text{Cs}_{16}\text{Fe}_4[\text{Fe}(\text{CN})_6]_7$ [1]

Structural features: $\text{Fe}^{2+}[\text{CN}]_6$ octahedral units in a Cu-type (c.c.p) arrangement; (Fe^{3+} , Cs) in "octahedral", additional Cs in "tetrahedral" voids.

Kuznetsov V.G. et al. (1970) [1]

$\text{C}_6\text{Cs}_{2.29}\text{Fe}_{1.57}\text{N}_6$

$a = 1.032 \text{ nm}$, $V = 1.0991 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	12b	1	0.0	0.193	0.02		single atom N
N2	12b	1	0.0	0.202	0.485		single atom C
C3	12b	1	0.0	0.307	0.52		single atom N
N4	12b	1	0.015	0.5	0.202		single atom C
(Fe^{2+})5	4a	.3.	0.0	0.0	0.0		octahedron C_6
Cs6	4a	.3.	0.25	0.25	0.25		cuboctahedron C_6N_6
M7	4a	.3.	0.5	0.5	0.5		octahedron N_6
Cs8	4a	.3.	0.75	0.75	0.75	0.86	cuboctahedron C_6N_6

$\text{M7} = 0.57\text{Fe}^{3+} + 0.43\text{Cs}$

Experimental: powder, film, X-rays

Remarks: Correct symmetry is space group (205) $Pa-3$ if sites Cs6 and Cs8 have the same occupancy.

References: [1] Kuznetsov V.G., Popova Z.V., Seifer G.B. (1970), Russ. J. Inorg. Chem. 15, 1407-1410.

198
cP68

Cu_7PSe_6	cP68	(198) $P2_13 - b^4a^5$
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$\text{Cu}_7\text{PSe}_6 \beta$ [1], argyrodite family

Structural features: Se forms a tetrahedrally close-packed (MgCu₂-type) framework; P in tetrahedral, Cu in tetrahedral and trigonal voids (partial disorder). Single PSe₄ tetrahedra.

Gaudin E. et al. (2000) [1]

Cu₇PSe₆

$a = 1.0108 \text{ nm}$, $V = 1.0328 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	12b	1	0.0139	0.3078	0.1864	0.32	
Cu2	12b	1	0.0295	0.2534	0.2476	0.68	
Se3	12b	1	0.12645	0.62079	0.36917		single atom P
Cu4	12b	1	0.1608	0.178	0.4804		trigonal bipyramid CuSe ₄
P5	4a	.3.	0.0015	0.0015	0.0015		tetrahedron Se ₄
Se6	4a	.3.	0.25921	0.25921	0.25921		tetrahedron Cu ₄
Cu7	4a	.3.	0.3892	0.3892	0.3892		colinear Se ₂
Se8	4a	.3.	0.51399	0.51399	0.51399		single atom Cu
Se9	4a	.3.	0.87523	0.87523	0.87523		tetrahedron PCu ₃

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.030$, $T = 293 \text{ K}$

Remarks: Phase stable at $T < 320 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Gaudin E., Boucher F., Petricek V., Taulelle F., Evain M. (2000), Acta Crystallogr. B 56, 402-408.

198
cP68

Na ₃ AlP ₃ NO ₉	<i>cP68</i>	(198) $P2_13 - b^4a^5$
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Na₃AlP₃O₉N [2]

Structural features: :N(PO₃)₃ ψ -tetrahedral units (three P(NO₃) tetrahedra sharing the N atom); Al octahedrally coordinated by the O atoms of three ψ -tetrahedral units.

Conanec R. et al. (1994) [1]

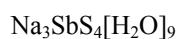
AlNNa₃O₉P₃

$a = 0.9274 \text{ nm}$, $V = 0.7976 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0024	0.1	0.3701		non-colinear PAl
O2	12b	1	0.0317	0.8438	0.2354		non-colinear PAl
P3	12b	1	0.07818	0.23952	0.32864		tetrahedron O ₃ N
O4	12b	1	0.1615	0.3084	0.4484		single atom P
Na5	4a	.3.	0.01256	0.01256	0.01256		trigonal prism O ₆
N6	4a	.3.	0.1922	0.1922	0.1922		non-coplanar triangle P ₃
Na7	4a	.3.	0.39138	0.39138	0.39138		octahedron O ₆
Al8	4a	.3.	0.58176	0.58176	0.58176		octahedron O ₆
Na9	4a	.3.	0.79865	0.79865	0.79865		non-coplanar triangle O ₃

Experimental: single crystal, diffractometer, X-rays, $R = 0.014$

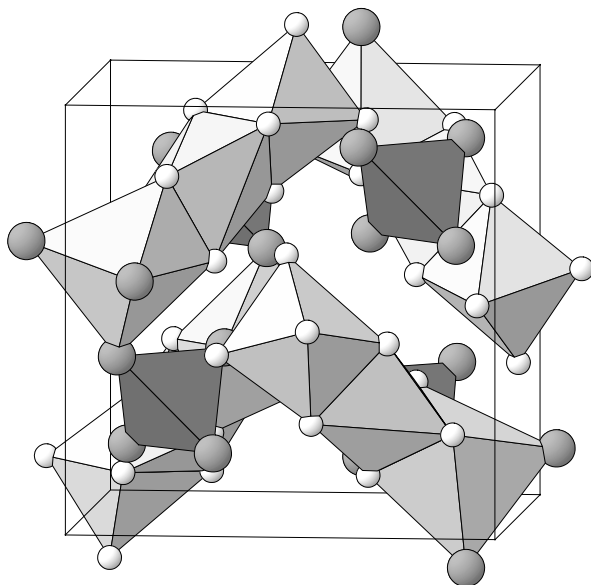
References: [1] Conanec R., L'Haridon P., Feldmann W., Marchand R., Laurent Y. (1994), Eur. J. Solid State Inorg. Chem. 31, 13-24. [2] Ronis J., Bondars B., Vitola A., Millers T. (1993), Latv. Kim. Z. 6, 662-665.



cP68

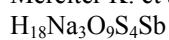
(198) $P2_13 - b^4a^5$ **$\text{Na}_3\text{SbS}_4 \cdot 9\text{H}_2\text{O}$** [2], Schlippe's salt

Structural features: Single SbS_4 tetrahedra and $\text{Na}_3\text{S}_3(\text{H}_2\text{O})_9$ units (one $\text{Na}([\text{OH}_2]_3\text{S}_3)$ and two $\text{Na}(\text{OH}_2)_6$ octahedra sharing faces) share S atoms to form a 3D-framework. See Fig. II.80.

Fig. II.80. **$\text{Na}_3\text{SbS}_4 \cdot 9\text{H}_2\text{O}$**

Arrangement of SbS_4 tetrahedra (dark), $\text{Na}(\text{S}_3(\text{OH}_2)_3)$ and $\text{Na}(\text{OH}_2)_6$ octahedra (S atoms large, O atoms small).

Mereiter K. et al. (1979) [1]

 $a = 1.1957 \text{ nm}$, $V = 1.7095 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.05462	0.06613	0.24246		non-collinear Na_2
S2	12b	1	0.10152	0.17188	0.60195		single atom Sb
O3	12b	1	0.14881	0.57875	0.49383		non-collinear NaO
O4	12b	1	0.17575	0.38291	0.27612		non-collinear Na_2
Na5	4a	.3.	0.0417	0.0417	0.0417		octahedron O_6
Na6	4a	.3.	0.19999	0.19999	0.19999		octahedron O_6
Na7	4a	.3.	0.35606	0.35606	0.35606		7-vertex polyhedron $\text{O}_3\text{S}_3\text{Na}$
S8	4a	.3.	0.67492	0.67492	0.67492		single atom Sb
Sb9	4a	.3.	0.78724	0.78724	0.78724		tetrahedron S_4
H10	12b	1	0.0015	0.7693	0.4114		
H11	12b	1	0.0073	0.5835	0.2095		
H12	12b	1	0.0196	0.3053	0.4819		
H13	12b	1	0.1102	0.3902	0.3219		
H14	12b	1	0.1776	0.4451	0.2254		
H15	12b	1	0.1907	0.6202	0.4393		

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.018$

Remarks: The same data are quoted in [3], where the structure at 105 K is studied on a deuterated sample. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Mereiter K., Preisinger A., Guth H. (1979), Acta Crystallogr. B 35, 19-25. [2] Grund A., Preisinger A. (1950), Acta Crystallogr. 3, 363-366. [3] Mereiter K., Preisinger A., Guth H., Heger G., Hiebl K., Mikenda W. (1979), Z. Kristallogr. 150, 215-229.

198
cP72

$K_9Ni_2O_7$	cP72	(198) $P2_13 - b^4a^6$
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$K_9Ni_2O_7$ [1]

Structural features: Single NiO_4 tetrahedra and NiO_3 trigonal units.

Zentgraf H., Hoppe R. (1980) [1]

$K_9Ni_2O_7$

$a = 1.091$ nm, $V = 1.2986$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	12b	1	0.0339	0.2866	0.4187		15-vertex Frank-Kasper $O_6K_7Ni_2$
O2	12b	1	0.0679	0.1996	0.6693		single atom Ni
K3	12b	1	0.0834	0.5385	0.2511		16-vertex Frank-Kasper $O_6K_8Ni_2$
O4	12b	1	0.0883	0.314	0.1663		single atom Ni
O5	4a	.3.	0.0519	0.0519	0.0519		single atom Ni
Ni6	4a	.3.	0.1552	0.1552	0.1552		tetrahedron O_4
K7	4a	.3.	0.3197	0.3197	0.3197		7-capped pentagonal prism $O_6K_{10}Ni$
K8	4a	.3.	0.4828	0.4828	0.4828		14-vertex Frank-Kasper O_6K_8
K9	4a	.3.	0.6548	0.6548	0.6548		7-capped pentagonal prism O_6NiK_{10}
Ni10	4a	.3.	0.8229	0.8229	0.8229		non-coplanar triangle O_3

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.099$

References: [1] Zentgraf H., Hoppe R. (1980), Z. Anorg. Allg. Chem. 462, 80-91.

198
cP72

$Hg_7As_4SnI_6$	cP72	(198) $P2_13 - b^4a^6$
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$Hg_7SnAs_4I_6$ [1]

Structural features: As_2Hg_7 units (two vertex-linked $AsHg_4$ tetrahedra), $Hg_3As-AsHg_3$ units (an As_2 dumbbell in a Hg_6 octahedron) and I atoms are interconnected to form a 3D-framework; single $:SnI_3$ ψ -tetrahedra in voids.

Olenev A.V. et al. (2000) [1]

$As_4Hg_7I_6Sn$

$a = 1.31117$ nm, $V = 2.2541$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	12b	1	0.0012	0.7507	0.3177		non-colinear As_2
I2	12b	1	0.0389	0.3043	0.4356		single atom Sn
Hg3	12b	1	0.0643	0.1774	0.657		non-colinear As_2
I4	12b	1	0.0681	0.5085	0.2196		non-colinear Hg_2
Sn5	4a	.3.	0.0171	0.0171	0.0171		non-coplanar triangle I_3

As6	4a	.3.	0.1758	0.1758	0.1758	tetrahedron Hg ₄
Hg7	4a	.3.	0.2842	0.2842	0.2842	colinear As ₂
As8	4a	.3.	0.3928	0.3928	0.3928	tetrahedron Hg ₄
As9	4a	.3.	0.6815	0.6815	0.6815	tetrahedron AsHg ₃
As10	4a	.3.	0.787	0.787	0.787	tetrahedron AsHg ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: single crystal, diffractometer, X-rays, R = 0.046

References: [1] Olenov A.V., Baranov A.I., Shevelkov A.V., Popovkin B.A. (2000), Eur. J. Inorg. Chem. 2000, 265-270.

198
cP76

$\text{K}_2\text{Mg}_2[\text{SO}_4]_3$

cP76

(198) $P2_13 - b^5a^4$

$\text{K}_2\text{Mg}_2(\text{SO}_4)_3$ [2], langbeinite

Structural features: MgO_6 octahedra and SO_4 tetrahedra share vertices to form a 3D-framework; K in tricapped trigonal prismatic and icosahedral voids. See Fig. II.81.

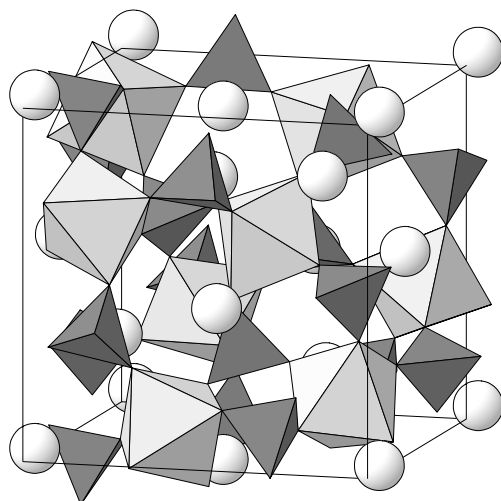


Fig. II.81. $\text{K}_2\text{Mg}_2(\text{SO}_4)_3$

Arrangement of SO_4 tetrahedra (dark), MgO_6 octahedra (light) and K atoms.

Speer D., Salje B. (1986) [1]

$\text{K}_2\text{Mg}_2\text{O}_{12}\text{S}_3$

$a = 0.9923 \text{ nm}$, $V = 0.9771 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0092	0.0755	0.3291		single atom S
S2	12b	1	0.0179	0.2161	0.3757		tetrahedron O ₄
O3	12b	1	0.0421	0.8042	0.2269		single atom S
O4	12b	1	0.1582	0.2533	0.4024		single atom S
O5	12b	1	0.2656	0.4988	0.4407		single atom S
K6	4a	.3.	0.0482	0.0482	0.0482		tricapped trigonal prism O ₉
Mg7	4a	.3.	0.3353	0.3353	0.3353		octahedron O ₆
Mg8	4a	.3.	0.5992	0.5992	0.5992		octahedron O ₆
K9	4a	.3.	0.8166	0.8166	0.8166		icosahedron O ₁₂

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

Remarks: A model with splitting of all O sites (see [3]) was tested and rejected.

References: [1] Speer D., Salje B. (1986), Phys. Chem. Miner. 13, 17-24. [2] Zemmann A., Zemmann J. (1957), Acta Crystallogr. 10, 409-413. [3] Yamada N., Maeda M., Adachi H. (1981), J. Phys. Soc. Jpn. 50, 907-913.

198
cP80

$\text{Na}_3\text{P}_6\text{N}_{11}$

cP80

(198) $P2_13 - b^5a^5$

$\text{Na}_3\text{P}_6\text{N}_{11}$ [1]

Structural features: PN_4 tetrahedra share vertices to form a 3D-framework.

Ronis J. et al. (1990) [1]

$\text{N}_{11}\text{Na}_3\text{P}_6$

$a = 1.0112 \text{ nm}$, $V = 1.0340 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12b	1	0.0331	0.3789	0.2967		non-colinear P_2
N2	12b	1	0.0392	0.6322	0.2271		non-colinear P_2
P3	12b	1	0.0607	0.4889	0.1745		tetrahedron N_4
P4	12b	1	0.0729	0.2298	0.3131		tetrahedron N_4
N5	12b	1	0.1121	0.2154	0.4632		non-colinear P_2
Na6	4a	.3.	0.0045	0.0045	0.0045		non-coplanar triangle N_3
N7	4a	.3.	0.2049	0.2049	0.2049		coplanar triangle P_3
Na8	4a	.3.	0.3652	0.3652	0.3652		colinear N_2
N9	4a	.3.	0.5344	0.5344	0.5344		non-coplanar triangle P_3
Na10	4a	.3.	0.7131	0.7131	0.7131		non-coplanar triangle N_3

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

Experimental: powder, diffractometer, X-rays, $R = 0.087$

References: [1] Ronis J., Bondars B., Vitola A., Millers T. (1990), Latv. PSR Zinat. Akad. Vestis, Kim. Ser. 1990, 299-301.

198
cP80

$\text{Ce}_4\text{Si}_4\text{N}_6\text{O}_5$

cP80

(198) $P2_13 - b^5a^5$

$\text{Ce}_4[\text{Si}_4\text{O}_4\text{N}_6]\text{O}$ [1]

Structural features: $\text{Si}(\text{N}_3\text{O})$ tetrahedra share vertices to form hyperbolically corrugated layers; OCe_4 tetrahedra (disorder on one of the Ce sites) in voids.

Irran E. et al. (2000) [1]

$\text{Ce}_4\text{N}_6\text{O}_5\text{Si}_4$

$a = 1.03367 \text{ nm}$, $V = 1.1044 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ce1	12b	1	0.03068	0.31849	0.29155		7-vertex polyhedron O_4N_3
N2	12b	1	0.07	0.562	0.3514		non-colinear Si_2
N3	12b	1	0.1192	0.1597	0.677		non-colinear Si_2
O4	12b	1	0.1742	0.2081	0.4306		single atom Si
Si5	12b	1	0.1952	0.5749	0.2452		tetrahedron ON_3
Si6	4a	.3.	0.0757	0.0757	0.0757		tetrahedron ON_3
O7	4a	.3.	0.1681	0.1681	0.1681		single atom Si

Ce8	4a	.3.	0.3921	0.3921	0.3921	0.177	
Ce9	4a	.3.	0.46979	0.46979	0.46979	0.823	
O10	4a	.3.	0.5927	0.5927	0.5927		tetrahedron Ce ₄

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.041$, $T = 292$ K

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

References: [1] Irran E., Köllisch K., Leoni S., Nesper R., Henry P.F., Weller M.T., Schnick W. (2000), Chem. Eur. J. 6, 2714-2720.

198
cP88

Ba _{1.5} Eu _{1.5} YbSi ₆ N ₁₁	cP88	(198) $P2_13 - b^5a^7$
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BaEu(Ba_{0.5}Eu_{0.5})YbSi₆N₁₁ [1]

Structural features: SiN₄ tetrahedra share vertices to form a 3D-framework; Ba, Eu and Yb in voids (distinct positions for Ba and Eu for a site with statistical mixture Ba/Eu).

Huppertz H., Schnick W. (1998) [1]

Ba_{1.50}Eu_{1.50}N₁₁Si₆Yb

$a = 1.04364$ nm, $V = 1.1367$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12b	1	0.021	0.3927	0.2624		non-collinear Si ₂
Si2	12b	1	0.0664	0.2436	0.3044		tetrahedron N ₄
N3	12b	1	0.0761	0.6565	0.2151		non-collinear Si ₂
Si4	12b	1	0.0838	0.5019	0.1565		tetrahedron N ₄
N5	12b	1	0.1182	0.2392	0.4599		non-collinear Si ₂
Ba6	4a	.3.	0.0319	0.0319	0.0319	0.5	
Eu7	4a	.3.	0.0389	0.0389	0.0389	0.5	
N8	4a	.3.	0.1998	0.1998	0.1998		non-coplanar triangle Si ₃
Ba9	4a	.3.	0.36051	0.36051	0.36051		trigonal bipyramid N ₅
N10	4a	.3.	0.516	0.516	0.516		non-coplanar triangle Si ₃
Yb11	4a	.3.	0.66335	0.66335	0.66335		octahedron N ₆
Eu12	4a	.3.	0.83175	0.83175	0.83175		6-vertex polyhedron N ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.041$, $T = 293$ K

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

References: [1] Huppertz H., Schnick W. (1998), Z. Anorg. Allg. Chem. 624, 371-374.

198
cP88

NaSr[PO ₄](H ₂ O) ₉	cP88	(198) $P2_13 - b^6a^4$
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NaSrPO₄·9H₂O [1], nastrophite

Structural features: Na(OH₂)₆ octahedra and Sr(OH₂)₆(OH)₃ tricapped trigonal prisms share edges to form a 3D-framework; single PO₄ tetrahedra in voids (orientational disorder).

Takagi S. et al. (1982) [1]

H₁₈NaO₁₃PSr

$a = 1.0544$ nm, $V = 1.1722$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0691	0.2686	0.1471	0.21	single atom O
O2	12b	1	0.1015	0.5419	0.1504		single atom Na
O3	12b	1	0.1128	0.191	0.3035	0.5	4-vertex polyhedron O ₃ P
O4	12b	1	0.1313	0.3001	0.2203	0.29	4-vertex polyhedron O ₃ P
O5	12b	1	0.1692	0.6488	0.4017		tricapped trigonal prism SrO ₈
O6	12b	1	0.2044	0.3826	0.4588		single atom Na
O7	4a	.3.	0.0926	0.0926	0.0926		single atom P
P8	4a	.3.	0.1743	0.1743	0.1743		bicapped square prism O ₁₀
Na9	4a	.3.	0.4267	0.4267	0.4267		octahedron O ₆
Sr10	4a	.3.	0.8032	0.8032	0.8032		tricapped trigonal prism O ₉
H11	12b	1	0.034	0.553	0.179		
H12	12b	1	0.045	0.803	0.194		
H13	12b	1	0.087	0.66	0.425		
H14	12b	1	0.121	0.456	0.153		
H15	12b	1	0.181	0.432	0.437		
H16	12b	1	0.193	0.336	0.41		

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

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

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 1 of [1] the x-coordinate of former O1 is misprinted as 0.9426 instead of 0.8426 (checked on interatomic distances).

References: [1] Takagi S., Mathew M., Brown W.E. (1982), Acta Crystallogr. B 38, 1408-1413.

198
cP92

NaBa[PO ₄][H ₂ O] ₉	cP92	(198) P2 ₁ 3 – b ⁶ a ⁵
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NaBaPO₄·9H₂O [1], nabaphite

Structural features: Na(OH₂)₆ octahedra and Ba(OH₂)₆(OH)₃ tricapped trigonal prisms share edges to form a 3D-framework; single PO₄ tetrahedra in voids (orientational disorder).

Baturin S.V. et al. (1982) [1]

BaH₁₈NaO₁₃P

$a = 1.07116$ nm, $V = 1.2290$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.057	0.251	0.138	0.39	single atom O
(OH ₂)2	12b	1	0.091	0.5379	0.1539		single atom Na
O3	12b	1	0.113	0.305	0.205	0.33	non-colinear O ₂
O4	12b	1	0.1163	0.1879	0.3105	0.28	single atom O
(OH ₂)5	12b	1	0.1615	0.6517	0.4117		non-colinear O ₂
(OH ₂)6	12b	1	0.209	0.3934	0.4511		non-colinear NaO
O7	4a	.3.	0.095	0.095	0.095	0.86	4-vertex polyhedron PO ₃
P8	4a	.3.	0.178	0.178	0.178		11-vertex polyhedron O ₁₁
O9	4a	.3.	0.261	0.261	0.261	0.14	single atom P
Na10	4a	.3.	0.4308	0.4308	0.4308		octahedron (OH ₂) ₆
Ba11	4a	.3.	0.802	0.802	0.802		tricapped trigonal prism (OH ₂) ₉

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

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

Remarks: Natural specimen from Kola Peninsula. Composition $\text{Na}(\text{Ba}_{0.96}\text{Sr}_{0.04})\text{PO}_4 \cdot 9\text{H}_2\text{O}$ from chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Baturin S.V., Malinovskii I.A., Belov N.V. (1982), Dokl. Akad. Nauk SSSR 266, 624-627.

198
cP92

$\text{K}_{1.83}\text{V}_{2.5}[\text{PO}_4]_3\text{O}_{0.17}$	cP92	(198) $P2_13 - b^6a^5$
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$\text{K}_{11}\text{V}_{15}\text{P}_{18}\text{O}_{73}$ [1]; $\text{K}_{11}\text{Fe}_{15}(\text{PO}_4)_{18}\text{O}$ [2]

Structural features: VO_6 octahedra and PO_4 tetrahedra share vertices to form a langbeinite-type 3D-framework; K atoms and additional O surrounded by three V (centering new O_6 octahedra) in voids (partial disorder).

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

$\text{K}_{1.83}\text{O}_{12.17}\text{P}_3\text{V}_{2.50}$

$a = 0.9896 \text{ nm}$, $V = 0.9691 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0095	0.0632	0.3288		single atom P
P2	12b	1	0.0196	0.2101	0.3753		tetrahedron O_4
O3	12b	1	0.0448	0.8018	0.23		single atom P
V4	12b	1	0.0895	0.4674	0.3258	0.167	
O5	12b	1	0.1663	0.2506	0.4007		single atom P
O6	12b	1	0.2664	0.4939	0.4401		single atom P
O7	4a	.3.	0.016	0.016	0.016	0.167	
K8	4a	.3.	0.0438	0.0438	0.0438	0.833	
V9	4a	.3.	0.33685	0.33685	0.33685		octahedron O_6
V10	4a	.3.	0.60421	0.60421	0.60421		octahedron O_6
K11	4a	.3.	0.8188	0.8188	0.8188		icosahedron O_{12}

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.030$, $T = 294 \text{ K}$

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

References: [1] Benmoussa A., Borel M.M., Grandin A., Leclaire A., Raveau B. (1992), J. Solid State Chem. 97, 314-318. [2] Lajmi B., Hidouri M., Wattiaux A., Fournés L., Darriet J., Ben Amara M. (2003), J. Alloys Compd. 361, 77-83.

198
cP96

ReBi_3O_8	cP96	(198) $P2_13 - b^6a^6$
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Bi_3ReO_8 [1]

Structural features: BiO_3 ψ -tetrahedra and single ReO_4 tetrahedra share atoms to form a 3D-framework.

Cheetham A.K., Smith A.R.R. (1985) [1]

$\text{Bi}_3\text{O}_8\text{Re}$

$a = 1.159 \text{ nm}$, $V = 1.5569 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0019	0.2605	0.5399		non-colinear Bi_2

O2	12b	1	0.057	0.1391	0.2543	single atom Re
O3	12b	1	0.1163	0.7411	0.4326	single atom Re
Bi4	12b	1	0.1193	0.153	0.6308	non-coplanar triangle O ₃
Bi5	12b	1	0.1448	0.3513	0.389	8-vertex polyhedron O ₈
O6	12b	1	0.214	0.4935	0.2329	non-colinear Bi ₂
O7	4a	.3.	0.0323	0.0323	0.0323	single atom Re
Re8	4a	.3.	0.1192	0.1192	0.1192	tetrahedron O ₄
O9	4a	.3.	0.2911	0.2911	0.2911	non-coplanar triangle Bi ₃
O10	4a	.3.	0.5319	0.5319	0.5319	single atom Re
Re11	4a	.3.	0.6192	0.6192	0.6192	tetrahedron O ₄
O12	4a	.3.	0.7797	0.7797	0.7797	non-coplanar triangle Bi ₃

Experimental: powder, diffractometer, neutrons, $R_B = 0.053$

Remarks: Space group (195) $P23$ was tested and rejected.

References: [1] Cheetham A.K., Smith A.R.R. (1985), Acta Crystallogr. B 41, 225-230.

198
cP96

CeZrO ₄	cP96	(198) $P2_13 - b^6a^6$
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CeZrO₄ κ [1]

Structural features: Close-packed CeZr layers in c stacking, O in tetrahedral voids. Substitution derivative of CaF₂ with the cations forming large Ce₄ and Zr₄ tetrahedra.

Kishimoto H. et al. (2000) [1]

CeO₄Zr

$a = 1.0527$ nm, $V = 1.1666$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0	0.0	0.23		fourcapped trigonal prism Zr ₂ Ce ₂ O ₆
O2	12b	1	0.02	0.26	0.26		fourcapped trigonal prism Zr ₂ O ₆ Ce ₂
O3	12b	1	0.04	0.26	0.46		single atom Zr
Zr4	12b	1	0.123	0.382	0.37		square prism (cube) O ₈
Ce5	12b	1	0.125	0.62	0.127		square prism (cube) O ₈
O6	12b	1	0.25	0.48	0.26		single atom Zr
O7	4a	.3.	0.0	0.0	0.0		fourcapped trigonal prism Zr ₄ O ₆
Zr8	4a	.3.	0.12	0.12	0.12		square prism (cube) O ₈
O9	4a	.3.	0.24	0.24	0.24		fourcapped trigonal prism Zr ₄ O ₆
O10	4a	.3.	0.51	0.51	0.51		fourcapped trigonal prism Ce ₄ O ₆
Ce11	4a	.3.	0.619	0.619	0.619		square prism (cube) O ₈
O12	4a	.3.	0.75	0.75	0.75		fourcapped trigonal prism Ce ₄ O ₆

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$

Experimental: powder, diffractometer, X-rays, $R_p = 0.051$

Remarks: Metastable phase. Refinement of the enantiomorphic setting gave a slightly different arrangement of O atoms.

References: [1] Kishimoto H., Omata T., Otsuka Yao Matsuo S., Ueda K., Hosono H., Kawazoe H. (2000), J. Alloys Compd. 312, 94-103.

198
cP100

$[\text{NH}_4]_7\text{Th}_2\text{F}_{15}[\text{H}_2\text{O}]$	<i>cP100</i>	(198) $P2_13 - b^7a^4$
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(NH₄)₇Th₂F₁₅·H₂O [1]Structural features: Single Th₂F₁₅ units consisting of two face-sharing ThF₉ polyhedra.

Penneman R.A. et al. (1976) [1]

F₁₅H₃₀N₇OTh₂ $a = 1.2753 \text{ nm}$, $V = 2.0741 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(NH ₄)1	12 <i>b</i>	1	0.001	0.36	0.398		non-coplanar triangle F ₂ (OH ₂)
F2	12 <i>b</i>	1	0.001	0.759	0.34		non-coplanar triangle F ₂ Th
F3	12 <i>b</i>	1	0.038	0.134	0.301		trigonal bipyramid F ₃ Th(NH ₄)
(NH ₄)4	12 <i>b</i>	1	0.151	0.554	0.161		square pyramid F ₄ (NH ₄)
F5	12 <i>b</i>	1	0.183	0.394	0.434		4-vertex polyhedron (NH ₄)ThF ₂
F6	12 <i>b</i>	1	0.203	0.334	0.209		5-vertex polyhedron F ₃ Th ₂
F7	12 <i>b</i>	1	0.277	0.517	0.315		non-coplanar square ThF ₂ (NH ₄)
(OH ₂)8	4 <i>a</i>	.3.	0.053	0.053	0.053		tetrahedron Th(NH ₄) ₃
Th9	4 <i>a</i>	.3.	0.1613	0.1613	0.1613		10-vertex polyhedron F ₉ (OH ₂)
Th10	4 <i>a</i>	.3.	0.3432	0.3432	0.3432		bicapped square prism F ₉ (NH ₄)
(NH ₄)11	4 <i>a</i>	.3.	0.458	0.458	0.458		single atom Th

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.063$

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

References: [1] Penneman R.A., Ryan R.R., Larson A.C. (1976), J. Inorg. Nucl. Chem. 38, 265-269.

198
cP112

$\text{NaSr}[\text{PO}_4][\text{H}_2\text{O}]_9$	<i>cP112</i>	(198) $P2_13 - b^8a^4$
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Na(Sr,Ba)PO₄·9H₂O [1], nastrophiteStructural features: Na(OH₂)₆ octahedra and Sr(OH₂)₆(OH)₃ tricapped trigonal prisms share edges to form a 3D-framework; single PO₄ tetrahedra in voids (orientational disorder).

Baturin S.V. et al. (1981) [1]

H₁₈NaO₁₃PSr $a = 1.0559 \text{ nm}$, $V = 1.1772 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>b</i>	1	0.06	0.09	0.14	0.187	
O2	12 <i>b</i>	1	0.0642	0.2689	0.1482	0.25	
O3	12 <i>b</i>	1	0.1001	0.541	0.1506		non-colinear NaO
O4	12 <i>b</i>	1	0.1095	0.1972	0.3044	0.44	
O5	12 <i>b</i>	1	0.128	0.3073	0.2268	0.27	
O6	12 <i>b</i>	1	0.135	0.31	0.16	0.04	
O7	12 <i>b</i>	1	0.1665	0.6491	0.4036		single atom O
O8	12 <i>b</i>	1	0.2034	0.3832	0.4608		single atom Na
O9	4 <i>a</i>	.3.	0.0902	0.0902	0.0902	0.44	
P10	4 <i>a</i>	.3.	0.1743	0.1743	0.1743		

Na11	4a	.3.	0.4265	0.4265	0.4265	octahedron O ₆
Sr12	4a	.3.	0.8033	0.8033	0.8033	tricapped trigonal prism O ₉
H13	12b	1	0.03	0.58	0.21	
H14	12b	1	0.07	0.64	0.37	
H15	12b	1	0.11	0.46	0.18	
H16	12b	1	0.16	0.68	0.47	
H17	12b	1	0.17	0.34	0.41	
H18	12b	1	0.19	0.48	0.42	

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

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

Remarks: Natural specimen from Kola Peninsula. Composition Na(Sr_{0.77}Ba_{0.20}Ca_{0.03})[PO₄] \cdot 9H₂O from chemical analysis. Refinement of the occupancy of site Sr12 assuming partial substitution by Ba showed no significant deviation from full occupation by Sr. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the multiplicity of former O9 is misprinted as 4 instead of 12 and the corresponding occupation factor as 0.56 instead of 0.187.

References: [1] Baturin S.V., Malinovskii I.A., Belov N.V. (1981), Dokl. Akad. Nauk SSSR 261, 619-623.

198
cP124

K ₂ Mn ₂ [SO ₄] ₃	cP124	(198) P2 ₁ 3 – b ⁹ a ⁴
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K₂Mn₂(SO₄)₃ rt [2], langbeinite

Structural features: MnO₆ octahedra and SO₄ tetrahedra share vertices to form a 3D-framework; the O sublattice adopts two reorientational arrangements (split sites).

Ukeda T. et al. (1995) [1]

K₂Mn₂O₁₂S₃

$a = 1.034$ nm, $V = 1.1055$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.00381	0.40811	0.3527	0.5	
O2	12b	1	0.00495	0.20084	0.24311	0.5	
O3	12b	1	0.01312	0.05787	0.72092	0.5	
O4	12b	1	0.01806	0.17101	0.26943	0.5	
S5	12b	1	0.02877	0.26494	0.37462		
O6	12b	1	0.03892	0.06273	0.69903	0.5	
O7	12b	1	0.10788	0.66867	0.48383	0.5	
O8	12b	1	0.162	0.27416	0.43407	0.5	
O9	12b	1	0.16511	0.24482	0.4158	0.5	
Mn10	4a	.3.	0.08363	0.08363	0.08363		
Mn11	4a	.3.	0.34387	0.34387	0.34387		
K12	4a	.3.	0.56553	0.56553	0.56553		non-coplanar triangle O ₃
K13	4a	.3.	0.80076	0.80076	0.80076		non-coplanar triangle O ₃

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 296 K

Remarks: Phase stable at T > 181 K. Short interatomic distances for partly occupied site(s). Refinement of the ordered structure model gave R = 0.039.

References: [1] Ukeda T., Itoh K., Moriyoshi C. (1995), J. Phys. Soc. Jpn. 64, 504-512. [2] Yamada N., Maeda M., Adachi H. (1981), J. Phys. Soc. Jpn. 50, 907-913.

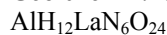
198
cP128

$\text{LaAl}[\text{NO}_3]_6[\text{H}_2\text{O}]_6$	<i>cP</i> 128	(198) $P2_13 - b^{10}a^2$
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$\text{LaAl}(\text{NO}_3)_6 \cdot 6\text{H}_2\text{O}$ [1]

Structural features: $\text{La}(\text{NO}_3)_6$ icosahedral units (a LaO_{12} icosahedron sharing edges with six NO_3 trigonal units) and $\text{Al}(\text{OH}_2)_6$ octahedra, loosely interconnected via additional H_2O .

Gobichon A.E. et al. (1998) [1]



$a = 1.2301 \text{ nm}$, $V = 1.8613 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.0123	0.1862	0.6028		single atom N
O2	12 <i>b</i>	1	0.0176	0.3096	0.1045		single atom N
(OH ₂)3	12 <i>b</i>	1	0.0501	0.6042	0.4008		single atom Al
O4	12 <i>b</i>	1	0.0622	0.6746	0.1103		single atom N
N5	12 <i>b</i>	1	0.0749	0.3443	0.1821		non-coplanar triangle O ₃
N6	12 <i>b</i>	1	0.0753	0.1568	0.6813		non-coplanar triangle O ₃
O7	12 <i>b</i>	1	0.0958	0.2797	0.2555		single atom N
(OH ₂)8	12 <i>b</i>	1	0.1092	0.4032	0.4491		single atom Al
O9	12 <i>b</i>	1	0.1093	0.439	0.1776		single atom N
O10	12 <i>b</i>	1	0.2391	0.5935	0.2869		single atom N
Al11	4 <i>a</i>	.3.	0.0	0.0	0.0		octahedron (OH ₂) ₆
La12	4 <i>a</i>	.3.	0.5	0.5	0.5		icosahedron O ₁₂

Transformation from published data: $\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z$

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

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

References: [1] Gobichon A.E., Auffrédic J.P., Louer D. (1998), J. Alloys Compd. 275/277, 130-136.

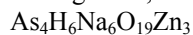
198
cP128

$\text{Na}_6\text{Zn}_3[\text{AsO}_4]_4[\text{H}_2\text{O}]_3$	<i>cP</i> 128	(198) $P2_13 - b^8a^8$
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$\text{Na}_6\text{Zn}_3(\text{AsO}_4)_4 \cdot 3\text{H}_2\text{O}$ [2]

Structural features: ZnO_4 and AsO_4 tetrahedra share vertices to form a 3D-framework; Na and H_2O in channels parallel to $\langle 111 \rangle$. See Fig. II.82.

Gesing T.M., Wartchow R. (1999) [1]



$a = 1.2245 \text{ nm}$, $V = 1.8360 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12 <i>b</i>	1	0.0023	0.2454	0.3736		non-colinear Na ₂
Na2	12 <i>b</i>	1	0.0043	0.248	0.1706		octahedron O ₆
O3	12 <i>b</i>	1	0.0208	0.556	0.3453		non-colinear AsZn
O4	12 <i>b</i>	1	0.0519	0.4237	0.1235		non-coplanar triangle AsZnNa
Zn5	12 <i>b</i>	1	0.12509	0.50286	0.24148		tetrahedron O ₄

O6	12b	1	0.1705	0.195	0.6313	non-colinear AsZn
O7	12b	1	0.2401	0.412	0.294	non-colinear AsZn
Na8	12b	1	0.2443	0.4222	0.4931	octahedron O ₆
As9	4a	.3.	0.02878	0.02878	0.02878	tetrahedron O ₄
O10	4a	.3.	0.2035	0.2035	0.2035	single atom As
As11	4a	.3.	0.28146	0.28146	0.28146	tetrahedron O ₄
O12	4a	.3.	0.4416	0.4416	0.4416	single atom As
As13	4a	.3.	0.51905	0.51905	0.51905	tetrahedron O ₄
O14	4a	.3.	0.6897	0.6897	0.6897	single atom As
As15	4a	.3.	0.76778	0.76778	0.76778	tetrahedron O ₄
O16	4a	.3.	0.9509	0.9509	0.9509	single atom As
H17	12b	1	0.049	0.182	0.361	
H18	12b	1	0.071	0.715	0.125	

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: single crystal, diffractometer, X-rays, wR = 0.036, T = 300 K

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

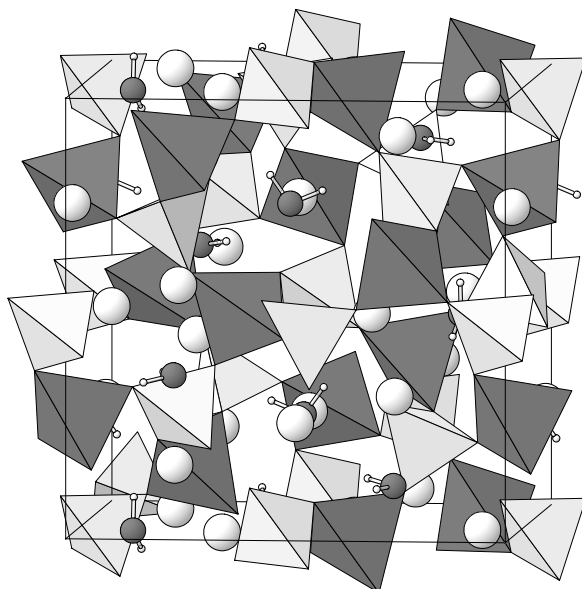


Fig. II.82. **Na₆Zn₃(AsO₄)₄·3H₂O**

Arrangement of AsO₄ (light) and ZnO₄ (dark) tetrahedra, Na atoms and H₂O molecules.

References: [1] Gesing T.M., Wartchow R. (1999), Z. Kristallogr., New Cryst. Struct. 214, 145-146. [2] Grey I.E., Madsen I.C., Jones D.J., Smith P.W. (1989), J. Solid State Chem. 82, 52-59.

198
cP128

CsMgP₃O₉

cP128

(198) P2₁3 – b⁹a⁵

Cs₂Mg₂P₆O₁₈ form II [1]

Structural features: Rings formed by six vertex-linked PO₄ tetrahedra share vertices with MgO₆ octahedra to form a 3D-framework; Cs in voids (disorder).

Chudinova N.N. et al. (2003) [1]

CsMgO₉P₃

$a = 1.20424$ nm, $V = 1.7464$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cs1	12b	1	0.0048	0.4798	0.4852	0.22	
O2	12b	1	0.0268	0.1727	0.2208		single atom P
O3	12b	1	0.0403	0.1295	0.4188		non-collinear P ₂
P4	12b	1	0.0404	0.6522	0.1826		tetrahedron O ₄
O5	12b	1	0.072	0.5219	0.2091		non-collinear P ₂
O6	12b	1	0.1371	0.722	0.159		single atom P
P7	12b	1	0.1542	0.18	0.4593		tetrahedron O ₄
O8	12b	1	0.1559	0.2779	0.5362		single atom P
O9	12b	1	0.1822	0.3571	0.2255		single atom P
Cs10	4a	.3.	0.0126	0.0126	0.0126	0.3	
Mg11	4a	.3.	0.1945	0.1945	0.1945		octahedron O ₆
Cs12	4a	.3.	0.37651	0.37651	0.37651	0.54	octahedron O ₆
Cs13	4a	.3.	0.624	0.624	0.624	0.5	icosahedron O ₁₂
Mg14	4a	.3.	0.8073	0.8073	0.8073		octahedron O ₆

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

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

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

References: [1] Chudinova N.N., Murashova E.V., Ilyukin A.B. (2003), Inorg. Mater. 39, 1298-1302.

198
cP176

Li ₃ La ₂ [NO ₃] ₉ [H ₂ O] ₃	cP176	(198) P2 ₁ 3 – b ¹⁴ a ²
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Li₃[La₂(NO₃)₉]·3H₂O [1]

Structural features: La(NO₃)₆ icosahedral units (a central LaO₁₂ icosahedron sharing edges with six trigonal NO₃ units) are interconnected to form a 3D-framework; Li and H₂O in channels.

Vigdorchik A.G. et al. (1991) [1]

H₆La₂Li₃N₉O₃₀

a = 1.3354 nm, V = 2.3814 nm³, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12b	1	0.0116	0.2609	0.123		non-coplanar triangle O ₃
O2	12b	1	0.0133	0.1628	0.5084		single atom N
O3	12b	1	0.0269	0.1823	0.168		single atom N
O4	12b	1	0.0663	0.7796	0.4222		single atom N
O5	12b	1	0.0801	0.3282	0.1231		single atom N
O6	12b	1	0.0896	0.2974	0.3461		single atom N
O7	12b	1	0.0962	0.5491	0.1543		single atom N
N8	12b	1	0.1028	0.1737	0.5411		coplanar triangle O ₃
O9	12b	1	0.1058	0.4391	0.4207		single atom N
O10	12b	1	0.1358	0.2556	0.5631		single atom N
N11	12b	1	0.1364	0.3783	0.3587		coplanar triangle O ₃
Li12	12b	1	0.206	0.55	0.468		tetrahedron O ₄
O13	12b	1	0.2127	0.3939	0.3074		single atom N
O14	12b	1	0.217	0.6318	0.3507		single atom Li
La15	4a	.3.	0.2179	0.2179	0.2179		icosahedron O ₁₂
La16	4a	.3.	0.5279	0.5279	0.5279		icosahedron O ₁₂
H17	12b	1	0.17	0.68	0.35		

H18 12*b* 1 0.225 0.6 0.295

Transformation from published data: $1/4+y, 1/4+x, 1/4+z$; origin shift $1/2 \ 1/2 \ 1/2$

Experimental: single crystal, diffractometer, X-rays, $R = 0.037$, $T = 258 \text{ K}$

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

References: [1] Vigdorichik A.G., Malinovskii Y.A., Dryuchko A.G., Verin I.A. (1991), Sov. Phys. Crystallogr. (Engl. Transl.) 36, 789-793.

198
cP248

$\text{Na}_{1.45}(\text{Al}_{0.725}\text{Si}_{0.275})_2\text{O}_4$

cP248

(198) $P2_13 - b^{18}a^8$

$\text{Na}_{1.45}\text{Al}_{2.45}\text{Si}_{0.55}\text{O}_4$ [1]

Structural features: (Al,Si) O_4 tetrahedra share vertices to form a 3D-framework where the (Al,Si) atoms form a diamond-type sublattice; Na in voids (disorder).

Withers R.L. et al. (1998) [1]

$\text{Al}_{1.45}\text{Na}_{1.37}\text{O}_4\text{Si}_{0.55}$

$a = 1.4553 \text{ nm}$, $V = 3.0822 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	12 <i>b</i>	1	0.0	0.0	0.25	0.24	single atom O
O2	12 <i>b</i>	1	0.0055	0.3315	0.3315		non-colinear Al_2
M3	12 <i>b</i>	1	0.0143	0.7476	0.2578		tetrahedron O_4
O4	12 <i>b</i>	1	0.0435	0.0435	0.6195		non-colinear Al_2
O5	12 <i>b</i>	1	0.0435	0.7935	0.3695		non-coplanar triangle Al_2Na
O6	12 <i>b</i>	1	0.0815	0.1685	0.2445		non-coplanar triangle Al_2Na
O7	12 <i>b</i>	1	0.0815	0.4945	0.4185		non-colinear Al_2
Na8	12 <i>b</i>	1	0.097	0.121	0.371	0.967	single atom O
M9	12 <i>b</i>	1	0.1002	0.3998	0.3502		tetrahedron O_4
M10	12 <i>b</i>	1	0.1118	0.1382	0.6382		tetrahedron O_4
O11	12 <i>b</i>	1	0.1195	0.7065	0.2065		non-coplanar triangle Al_2Na
O12	12 <i>b</i>	1	0.1305	0.2065	0.5435		non-colinear Al_2
Na13	12 <i>b</i>	1	0.144	0.633	0.361	0.967	single atom O
O14	12 <i>b</i>	1	0.1685	0.3315	0.4185		non-colinear Al_2
O15	12 <i>b</i>	1	0.1685	0.4185	0.2555		non-colinear Al_2
M16	12 <i>b</i>	1	0.212	0.25	0.481		tetrahedron O_4
Na17	12 <i>b</i>	1	0.231	0.488	0.484		non-coplanar triangle O_3
O18	12 <i>b</i>	1	0.2935	0.2935	0.5435		non-colinear Al_2
M19	4 <i>a</i>	.3.	0.0132	0.0132	0.0132		tetrahedron O_4
O20	4 <i>a</i>	.3.	0.0815	0.0815	0.0815		colinear Al_2
M21	4 <i>a</i>	.3.	0.1498	0.1498	0.1498		tetrahedron O_4
Na22	4 <i>a</i>	.3.	0.264	0.264	0.264	0.725	non-coplanar triangle O_3
M23	4 <i>a</i>	.3.	0.4572	0.4572	0.4572		non-coplanar triangle O_3
O24	4 <i>a</i>	.3.	0.5435	0.5435	0.5435		colinear Al_2
M25	4 <i>a</i>	.3.	0.6118	0.6118	0.6118		tetrahedron O_4
Na26	4 <i>a</i>	.3.	0.736	0.736	0.736	0.725	non-coplanar triangle O_3

$\text{M3} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M9} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M10} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M16} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M19} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M21} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M23} = 0.725\text{Al} + 0.275\text{Si}$; $\text{M25} = 0.725\text{Al} + 0.275\text{Si}$

Experimental: powder, diffractometer, X-rays, $R_B = 0.138$, $T = 293 \text{ K}$

Remarks: General formula $\text{Na}_{2-x}\text{Al}_{2-x}\text{Si}_x\text{O}_4$. Refinement of a commensurately modulated model considering a modulation wave $q_1 = \frac{1}{4}(0\ 2\ 0)$ for the framework, and a modulation wave $q_2 = \frac{1}{4}(2\ 2\ 0)$ for the Na/vacancy ordering.

References: [1] Withers R.L., Thompson J.G., Melnitchenko A., Palethorpe S.R. (1998), Acta Crystallogr. B 54, 547-557.

198
cP296

$\text{Na}_{0.62}\text{Ca}_{8.69}\text{Al}_6\text{O}_{18}$	cP296	(198) $P2_13 - b^{22}a^8$
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$\text{Na}_{0.625}\text{Ca}_{8.688}\text{Al}_6\text{O}_{18}$ [1]

Structural features: Rings formed by six vertex-linked AlO_4 tetrahedra.

Takéuchi Y. et al. (1980) [1]

$\text{Al}_6\text{Ca}_{8.43}\text{Na}_{0.63}\text{O}_{18}$

$a = 1.5248\text{ nm}$, $V = 3.5452\text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12b	1	0.0029	0.263	0.1264		non-colinear Al_2
O2	12b	1	0.0048	0.631	0.2368		non-colinear Al_2
Al3	12b	1	0.0053	0.2434	0.2371		tetrahedron O_4
Al4	12b	1	0.0134	0.0167	0.2539		tetrahedron O_4
O5	12b	1	0.0173	0.4829	0.3503		single atom Al
O6	12b	1	0.023	0.2342	0.6258		non-colinear Al_2
O7	12b	1	0.0233	0.0234	0.6495		single atom Al
Al8	12b	1	0.0232	0.2466	0.5129		tetrahedron O_4
O9	12b	1	0.0321	0.4726	0.1498		single atom Al
O10	12b	1	0.0938	0.7878	0.2281		single atom Al
O11	12b	1	0.1082	0.2729	0.2765		single atom Al
Ca12	12b	1	0.1119	0.6201	0.38		non-coplanar triangle O_3
Ca13	12b	1	0.118	0.6232	0.1376	0.5	octahedron O_6
Ca14	12b	1	0.1213	0.3821	0.3863	0.5	
Ca15	12b	1	0.1262	0.1345	0.3678	0.5	
Ca16	12b	1	0.1287	0.6431	0.1363	0.5	non-colinear Al_2
O17	12b	1	0.1327	0.2475	0.4759		
Ca18	12b	1	0.1361	0.372	0.14	0.5	
O19	12b	1	0.1515	0.515	0.4837		single atom Al
O20	12b	1	0.2094	0.6058	0.2629		single atom Al
O21	12b	1	0.2406	0.4114	0.304		single atom Al
Al22	12b	1	0.2445	0.2623	0.5063		tetrahedron O_4
Ca23	4a	.3.	0.0	0.0	0.0	0.5	single atom Na
Na24	4a	.3.	0.0121	0.0121	0.0121	0.26	
Na25	4a	.3.	0.0875	0.0875	0.0875	0.37	
M26	4a	.3.	0.263	0.263	0.263		octahedron O_6
M27	4a	.3.	0.3814	0.3814	0.3814		tricapped trigonal prism O_9
Ca28	4a	.3.	0.5018	0.5018	0.5018		octahedron O_6
M29	4a	.3.	0.6237	0.6237	0.6237		tricapped trigonal prism O_9
M30	4a	.3.	0.7438	0.7438	0.7438		octahedron O_6

$\text{M26} = 0.91\text{Ca} + 0.09\text{Na}$; $\text{M27} = 0.97\text{Ca} + 0.03\text{Na}$; $\text{M29} = 0.76\text{Ca} + 0.24\text{Na}$; $\text{M30} = 0.73\text{Ca} + 0.27\text{Na}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.046$

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

References: [1] Takéuchi Y., Nishi F., Maki I. (1980), *Z. Kristallogr.* 152, 259-307.

198
cP564

Mn ₈ Al ₃₉			cP564			(198) P2 ₁ 3 – b ⁴⁷	
Mn ₈ Al ₃₉ [1]							
Structural features: Commensurate approximant of icosahedral quasicrystals.							
Hansen V., Gjonnes J. (1996) [1]							
Al ₃₉ Mn ₈							
a = 2.0516 nm, V = 8.6353 nm ³ , Z = 12							
site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	12b	1	0.0	0.1	0.03		11-vertex polyhedron Al ₁₀ Mn
Al2	12b	1	0.01	0.09	0.66		11-vertex polyhedron MnAl ₁₀
Al3	12b	1	0.01	0.1	0.53		11-vertex polyhedron MnAl ₁₀
Al4	12b	1	0.01	0.59	0.34		11-vertex polyhedron Al ₁₀ Mn
Al5	12b	1	0.02	0.03	0.41		13-vertex polyhedron Mn ₃ Al ₁₀
Al6	12b	1	0.02	0.17	0.41		14-vertex polyhedron Mn ₃ Al ₁₁
Mn7	12b	1	0.02	0.29	0.6		bicapped square prism Al ₁₀
Al8	12b	1	0.02	0.4	0.17		13-vertex polyhedron Al ₁₀ Mn ₃
Al9	12b	1	0.02	0.53	0.22		tricapped pentagonal prism Al ₁₀ Mn ₃
Al10	12b	1	0.02	0.66	0.22		tricapped pentagonal prism Al ₁₀ Mn ₃
Al11	12b	1	0.02	0.79	0.17		pseudo Frank-Kasper Mn ₃ Al ₁₀
Al12	12b	1	0.03	0.2	0.1		11-vertex polyhedron MnAl ₁₀
Al13	12b	1	0.03	0.28	0.21		tricapped pentagonal prism Mn ₂ Al ₁₁
Mn14	12b	1	0.03	0.39	0.4		icosahedron Al ₁₂
Mn15	12b	1	0.03	0.8	0.4		11-vertex polyhedron Al ₁₁
Al16	12b	1	0.09	0.1	0.33		tricapped pentagonal prism Mn ₃ Al ₁₀
Al17	12b	1	0.09	0.21	0.52		14-vertex polyhedron Mn ₂ Al ₁₂
Al18	12b	1	0.09	0.21	0.67		12-vertex polyhedron Al ₁₀ Mn ₂
Al19	12b	1	0.09	0.29	0.39		icosahedron Mn ₂ Al ₁₀
Al20	12b	1	0.09	0.48	0.33		tricapped pentagonal prism Mn ₃ Al ₁₀
Al21	12b	1	0.09	0.48	0.48		tricapped pentagonal prism Al ₁₀ Mn ₃
Al22	12b	1	0.09	0.59	0.14		tricapped pentagonal prism Al ₁₀ Mn ₃
Al23	12b	1	0.09	0.71	0.34		12-vertex polyhedron Al ₁₀ Mn ₂
Al24	12b	1	0.09	0.71	0.47		tricapped pentagonal prism Mn ₂ Al ₁₁
Mn25	12b	1	0.09	0.72	0.1		11-vertex polyhedron Al ₁₁
Mn26	12b	1	0.1	0.1	0.47		11-vertex polyhedron Al ₁₁
Al27	12b	1	0.1	0.16	0.2		11-vertex polyhedron MnAl ₁₀
Mn28	12b	1	0.1	0.22	0.3		icosahedron Al ₁₂
Al29	12b	1	0.1	0.36	0.29		14-vertex polyhedron Mn ₃ Al ₁₁
Al30	12b	1	0.11	0.36	0.49		bicapped square prism Mn ₃ Al ₇
Mn31	12b	1	0.11	0.59	0.28		11-vertex polyhedron Al ₁₁
Al32	12b	1	0.12	0.81	0.29		pseudo Frank-Kasper Al ₁₁ Mn ₂
Al33	12b	1	0.13	0.6	0.41		tricapped pentagonal prism Mn ₃ Al ₁₀
Al34	12b	1	0.15	0.5	0.22		14-vertex Frank-Kasper Mn ₃ Al ₁₁
Al35	12b	1	0.16	0.18	0.4		pseudo Frank-Kasper Al ₁₀ Mn ₃
Al36	12b	1	0.16	0.68	0.21		pseudo Frank-Kasper Al ₁₁ Mn ₂
Al37	12b	1	0.17	0.28	0.21		tricapped pentagonal prism Mn ₃ Al ₁₀
Al38	12b	1	0.17	0.4	0.4		14-vertex polyhedron Al ₁₁ Mn ₃
Al39	12b	1	0.2	0.67	0.32		icosahedron Al ₁₀ Mn ₂
Al40	12b	1	0.21	0.27	0.63		pseudo Frank-Kasper Al ₁₁ Mn ₂

Mn41	12b	1	0.21	0.41	0.28	11-vertex polyhedron Al ₁₁
Al42	12b	1	0.22	0.29	0.33	14-vertex polyhedron Mn ₃ Al ₁₁
Al43	12b	1	0.22	0.29	0.48	14-vertex Frank-Kasper Mn ₂ Al ₁₂
Al44	12b	1	0.22	0.52	0.33	14-vertex polyhedron Mn ₃ Al ₁₁
Al45	12b	1	0.22	0.52	0.48	14-vertex polyhedron Mn ₃ Al ₁₁
Al46	12b	1	0.3	0.4	0.47	11-vertex polyhedron MnAl ₁₀
Al47	12b	1	0.3	0.41	0.34	11-vertex polyhedron MnAl ₁₀

Transformation from published data: $\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}+z$

Experimental: polycrystalline sample, electron diffraction

Remarks: Model tested on diffraction data from [2].

References: [1] Hansen V., Gjonnes J. (1996), Acta Crystallogr. A 52, 125-132. [2] Gratias D., Cahn J.W., Mozer B. (1988), Phys. Rev. B: Condens. Matter 38, 1643-1646.