

Space group (205) *Pa*-3205
*cP*4

[H ₂ S]	<i>cP</i> 4	(205) <i>Pa</i> -3 – a
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H₂S form II [2]

Structural features: Non-linear SH₂ molecules in a Cu-type (c.c.p.) arrangement, partial orientational disorder.

Cockcroft J.K., Fitch A.N. (1990) [1]

S

$a = 0.57647$ nm, $V = 0.1916$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	4 <i>a</i>	.-3.	0	0	0		cuboctahedron S ₁₂

Experimental: powder, diffractometer, neutrons, $R_B = 0.019$, $T = 120$ K

Remarks: Phase stable at $108 < T < 133$ K. Partial orientational disorder is described by a refinement considering symmetry-adapted (-3) spherical-harmonic functions for deuterium. Complete orientational disorder corresponds to space group (225) *Fm*-3*m*. A model considering 6-fold orientational disorder is proposed in [2] (Pearson symbol *cP*52). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Cockcroft J.K., Fitch A.N. (1990), *Z. Kristallogr.* 193, 1-19. [2] Sandor E., Ogunade S.O. (1969), *Nature (London)* 224, 905-907.

205
*cP*4

HBr	<i>cP</i> 4	(205) <i>Pa</i> -3 – a
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HBr form Ib [1]

Structural features: HBr molecules in a Cu-type (c.c.p.) arrangement, partial orientational disorder.

Cockcroft J.K. et al. (1988) [1]

Br

$a = 0.57907$ nm, $V = 0.1942$ nm³, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Br1	4 <i>a</i>	.-3.	0	0	0		cuboctahedron Br ₁₂

Experimental: powder, diffractometer, neutrons, $R_B = 0.094$, $T = 116$ K

Remarks: Phase stable at $114 < T < 117$ K; this intermediate structure type was not observed for deuterized samples. Partial orientational disorder is described by a refinement considering symmetry-adapted (-3) spherical-harmonic functions for hydrogen. Complete orientational disorder corresponds to space group (225) *Fm*-3*m*, which was excluded based on the existence of weak additional reflections. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Cockcroft J.K., Simon A., Ziebeck K.R.A. (1988), *Z. Kristallogr.* 184, 229-246.

205
cP8

[N ₂]	cP8	(205) <i>Pa</i> -3 – c
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N₂ α [1]Structural features: N₂ molecules in a Cu-type (c.c.p.) arrangement.

Venables J.A., English C.A. (1974) [1]

N₂ $a = 0.565 \text{ nm}$, $V = 0.1804 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	8c	.3.	0.056	0.056	0.056		single atom N

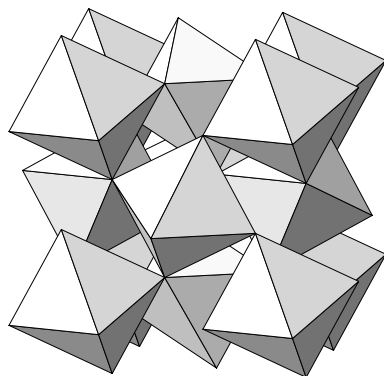
Experimental: single crystal, electron diffraction, T = 25 K

Remarks: Space group (198) *P*2₁3 was tested and rejected; controversy remains, however, in the literature concerning the correct symmetry.

References: [1] Venables J.A., English C.A. (1974), Acta Crystallogr. B 30, 929-935.

205
cP12

FeS ₂	cP12	(205) <i>Pa</i> -3 – ca
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FeS₂ pyrite [2], pyrite, Strukturbericht notation C2Structural features: Distorted FeS₆ octahedra share vertices to form a 3D-framework. Fe atoms and S₂ dumbbells in a NaCl-type arrangement. See Fig. II.38.Fig. II.38. **FeS₂ pyrite**Arrangement of FeS₆ octahedra.

Finklea S.L. III et al. (1976) [1]

FeS₂ $a = 0.54281 \text{ nm}$, $V = 0.1599 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	8c	.3.	0.38504	0.38504	0.38504		tetrahedron SFe ₃
Fe2	4a	.-3.	0	0	0		octahedron S ₆

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

Remarks: Natural specimen from York, South Carolina. S/Fe ratio 2.05 from atomic absorption. Strukturbericht notation C2 also refers to the CO₂ type.

References: [1] Finklea S.L. III, Cathey L., Amma E.L. (1976), Acta Crystallogr. A 32, 529-537. [2] (1931), Strukturberichte 1, 150.

205
cP12

CO ₂	cP12	(205) Pa-3 – ca
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CO₂ [2]; N₂O [2]

Structural features: O=C=O linear molecules in a Cu-type (c.c.p.) arrangement.

Simon A., Peters K. (1980) [1]

CO₂

$a = 0.5624$ nm, $V = 0.1779$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	8c	.3.	0.1185	0.1185	0.1185		single atom C
C2	4a	-.3.	0	0	0		colinear O ₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.040, T = 150 K

Remarks: Sometimes referred to as C2 type (Strukturbericht notation for pyrite). The structure at 1.0 GPa is studied in [3].

References: [1] Simon A., Peters K. (1980), Acta Crystallogr. B 36, 2750-2751. [2] (1931), Strukturberichte 1, 150. [3] Downs R.T., Somayazulu M.S. (1998), Acta Crystallogr. C 54, 897-898.

205
cP16

CuCl	cP16	(205) Pa-3 – c ²
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CuCl form IV [1]; CuBr form V [1], SC16 (simple cubic, 16 atoms)

Structural features: CuCl₄ tetrahedra share vertices to form a 3D-framework (Cu displaced towards a face).

Hull S., Keen D.A. (1994) [1]

ClCu

$a = 0.64162$ nm, $V = 0.2641$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	8c	.3.	0.1297	0.1297	0.1297		trigonal bipyramid Cl ₄ Cu
Cl2	8c	.3.	0.3473	0.3473	0.3473		tetrahedron Cu ₄

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

Experimental: powder, diffractometer, neutrons, time-of-flight, wR_p = 0.040, p = 5.52 GPa

Remarks: Phase stable at 5.1 < p < 10.6 GPa. Supersedes reports on CuCl-IV with different tetragonal cells ([2], [3]).

References: [1] Hull S., Keen D.A. (1994), Phys. Rev. B: Condens. Matter 50, 5868-5885. [2] Meisalo V., Kalliomäki M. (1973), High Temp. High Pressures 5, 663-673. [3] Serebryanaya N.R., Popova S.V., Rusakov A.P. (1976), Sov. Phys. Solid State (Engl. Transl.) 17, 1843.

205
cP16

[N ₂ H ₆]Cl ₂	cP16	(205) Pa-3 – c ²
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N₂H₆Cl₂ [2]

Structural features: H₃N-NH₃ units and Cl atoms in a CaF₂-type arrangement.

Donohue J., Lipscomb W.N. (1947) [1]

Cl₂H₆N₂

$a = 0.787 \text{ nm}$, $V = 0.4874 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	8c	.3.	0.052	0.052	0.052		single atom N
Cl2	8c	.3.	0.279	0.279	0.279		tetrahedron N ₄
H3	24d	1	0.126	0.392	0.461		

Experimental: single crystal, oscillation photographs, X-rays

Remarks: Hydrazinium dichloride. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In [1] the y -coordinate of the H site is misprinted as 0.039 instead of -0.039 (checked on interatomic distances).

References: [1] Donohue J., Lipscomb W.N. (1947), J. Chem. Phys. 15, 115-119. [2] Wyckoff R.W.G. (1923), Am. J. Sci. 5, 15-22.

205
cP32

NaSbF ₆	<i>cP32</i>	(205) <i>Pa-3</i> – dba
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NaSbF₆ [1]

Structural features: Na atoms and SbF₆ octahedra in a NaCl-type arrangement.

Schrewelius N. (1938) [1]

F₆NaSb

$a = 0.818 \text{ nm}$, $V = 0.5473 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	24d	1	0.05	0.45	0.225		single atom Sb
Sb2	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron F ₆
Na3	4a	-.3.	0	0	0		octahedron F ₆

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

Experimental: powder, film, X-rays

Remarks: The structure was later redetermined in space group (225) *Fm-3m* [2].

References: [1] Schrewelius N. (1938), Z. Anorg. Allg. Chem. 238, 241-254. [2] Teufer G. (1956), Acta Crystallogr. 9, 539-540.

205
cP36

Pb[NO ₃] ₂	<i>cP36</i>	(205) <i>Pa-3</i> – dca
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Pb(NO₃)₂ [2], Strukturbericht notation G2₁; Ni(NO₃)₂ [4]

Structural features: Pb atoms and planar NO₃ trigonal units in a distorted CaF₂-type arrangement (Pb cuboctahedrally coordinated to twelve O belonging to six NO₃ units). See Fig. II.39.

Nowotny H., Heger G. (1986) [1]

N₂O₆Pb

$a = 0.78586 \text{ nm}$, $V = 0.4853 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.27772	0.28869	0.4773		single atom N
N2	8c	.3.	0.34865	0.34865	0.34865		non-coplanar triangle O ₃
Pb3	4a	.-3.	0	0	0		pseudo Frank-Kasper O ₁₂ N ₆

Experimental: single crystal, diffractometer, neutrons, wR = 0.015

Remarks: An isopointal structure proposal with significantly different atom coordinates [3] is superseded (see [2]). Strukturbericht notation G2₁ was originally defined on the superseded structure proposal.

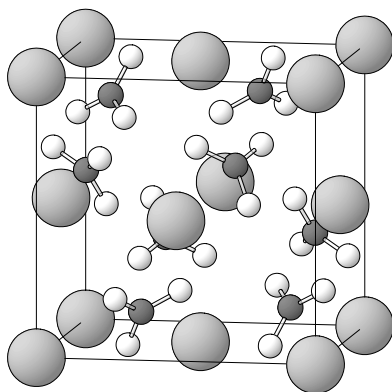


Fig. II.39. **Pb(NO₃)₂**

Arrangement of NO₃ units (N atoms dark, O atoms light) and Pb atoms.

References: [1] Nowotny H., Heger G. (1986), Acta Crystallogr. C 42, 133-135. [2] (1937), Strukturberichte 2, 73. [3] (1931), Strukturberichte 1, 304. [4] Weigel D., Imelik B., Laffitte P. (1962), Bull. Soc. Chim. Fr. 1962, 544-549.

205
cP40

SnI ₄	cP40	(205) Pa-3 – dc ²
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SnI₄ [2], Strukturbericht notation D1₁

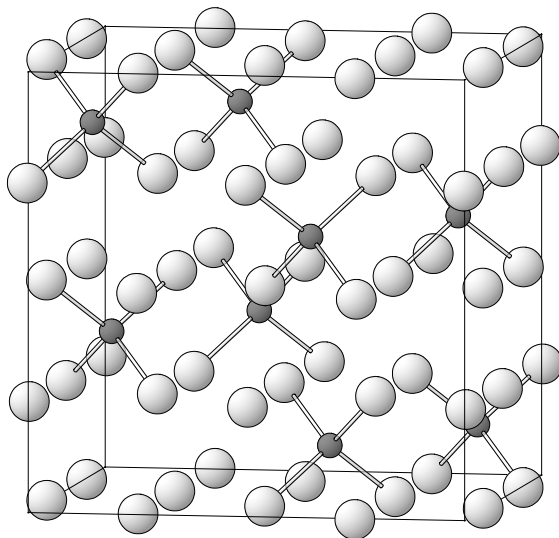


Fig. II.40. **SnI₄**

Arrangement of SnI₄ tetrahedra (Sn atoms dark, I atoms light).

Structural features: Close-packed I layers in c stacking, Sn in tetrahedral voids. Single SnI₄ tetrahedra. See Fig. II.40.

Meller F., Fankuchen I. (1955) [1]

I₄Sn

$a = 1.226 \text{ nm}$, $V = 1.8428 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
I1	24 <i>d</i>	1	0.002	0.498	0.248		single atom Sn
Sn2	8 <i>c</i>	.3.	0.125	0.125	0.125		tetrahedron I ₄
I3	8 <i>c</i>	.3.	0.252	0.252	0.252		single atom Sn

Experimental: single crystal, Weissenberg and precession photographs, X-rays, $R = 0.108$

References: [1] Meller F., Fankuchen I. (1955), Acta Crystallogr. 8, 343-344. [2] Dickinson R.G. (1923), J. Am. Chem. Soc. 45, 958-962.

205
*cP*40

NaAu ₃ Si	<i>cP</i> 40	(205) <i>Pa</i> -3 – <i>dc</i> ²
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NaAu₃Si [1]; NaAu₃Ge [1]

Structural features: SiAu₆ trigonal prisms share vertices to form a 3D-framework with approximately linear Si-Au-Si sections.

Döring W., Schuster H.U. (1980) [1]

Au₃NaSi

$a = 0.8916 \text{ nm}$, $V = 0.7088 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Au1	24 <i>d</i>	1	0.1335	0.4072	0.2265		pseudo Frank-Kasper Si ₃ Au ₆ Na ₄
Na2	8 <i>c</i>	.3.	0.097	0.097	0.097		16-vertex Frank-Kasper NaAu ₁₂ Si ₃
Si3	8 <i>c</i>	.3.	0.381	0.381	0.381		pseudo Frank-Kasper Au ₉ Na ₃ Si

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

References: [1] Döring W., Schuster H.U. (1980), Z. Naturforsch. B 35, 1482-1483.

205
*cP*40

Cs[NO ₃]	<i>cP</i> 40	(205) <i>Pa</i> -3 – <i>dcba</i>
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CsNO₃ ht [1]

Structural features: Cs atoms and planar NO₃ trigonal units in a CsCl-type arrangement.

Korhonen U. (1953) [1]

CsNO₃

$a = 0.898 \text{ nm}$, $V = 0.7242 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24 <i>d</i>	1	0.114	0.281	0.281		single atom N
N2	8 <i>c</i>	.3.	0.225	0.225	0.225		coplanar triangle O ₃
Cs3	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron O ₁₂

Cs4 4a .-3. 0 0 0 octahedron O₆

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

Experimental: powder, film, X-rays, T = 440 K

Remarks: Phase stable at T > 434 K.

References: [1] Korhonen U. (1953), Ann. Acad. Sci. Fenn., Ser. A2 150, 1-16.

205
cP40

Zr[P₂O₇]

cP40

(205) Pa-3 – dcba

ZrP₂O₇ form II [2], Strukturbericht notation K6₁

Structural features: Zr atoms and P₂O₇ units (two vertex-linked PO₄ tetrahedra) in a NaCl-type arrangement. See Fig. II.41.

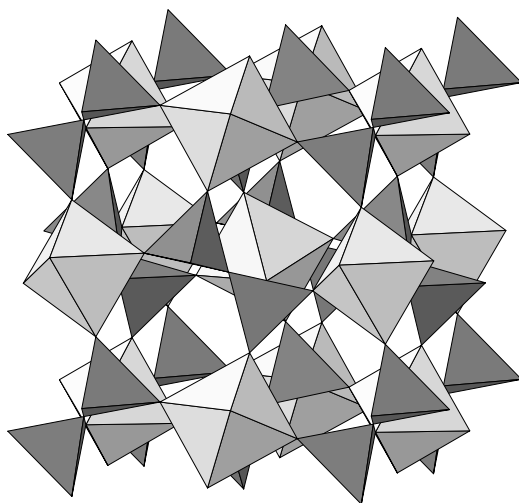


Fig. II.41. **ZrP₂O₇ form II**

Arrangement of PO₄ tetrahedra (dark) and ZrO₆ octahedra (light).

Khosrovani N. et al. (1996) [1]

O₇P₂Zr

$a = 0.82899 \text{ nm}$, $V = 0.5697 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.055	0.2733	0.076		single atom P
P2	8c	.3.	0.1054	0.1054	0.1054		tetrahedron O ₄
Zr3	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
O4	4a	.-3.	0	0	0		colinear P ₂

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.056$, T = 563 K

Remarks: Phase stable at T > 563 K. Three modifications are considered in [3], I: statistical disorder, II: superstructure with 27-fold cell volume, III: true symmetry (205) Pa-3.

References: [1] Khosrovani N., Korthuis V., Sleight A.W., Vogt T. (1996), Inorg. Chem. 35, 485-489. [2] Levi G.R., Peyronel G. (1935), Z. Kristallogr. 92, 190-209. [3] Huang C.H., Knop O., Othen D.A., Woodhams F.W.D., Howie R.A. (1975), Can. J. Chem. 53, 79-91.

205
cP40

$\text{K}[\text{H}_3\text{O}]_2\text{AlF}_6$	<i>cP40</i>	(205) <i>Pa</i> -3 – dcba
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K(H₃O)₂AlF₆ [1]

Structural features: K atoms and AlF₆ octahedra in a NaCl-type arrangement; :OH₃ ψ-tetrahedra in cubic voids.

Frenzen G., Massa W. (1990) [1]

AlF₆H₆KO₂

$a = 0.86464 \text{ nm}$, $V = 0.6464 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24 <i>d</i>	1	0.0488	0.4399	0.1946		single atom Al
O2	8 <i>c</i>	.3.	0.1971	0.1971	0.1971		non-coplanar triangle F ₃
Al3	4 <i>b</i>	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron F ₆
K4	4 <i>a</i>	.-3.	0	0	0		square prism (cube) F ₆ O ₂
H5	24 <i>d</i>	1	0.151	0.292	0.205		

Experimental: single crystal, diffractometer, X-rays, $wR = 0.019$, $T = 293 \text{ K}$

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

References: [1] Frenzen G., Massa W. (1990), Acta Crystallogr. C 46, 190-192.

205
cP52

[H ₂ S]	<i>cP52</i>	(205) <i>Pa</i> -3 – d ² a
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H₂S form II [1]

Structural features: Non-linear SH₂ molecules in a Cu-type (c.c.p.) arrangement, partial orientational disorder.

Sandor E., Ogunade S.O. (1969) [1]

D₂S

$a = 0.5739 \text{ nm}$, $V = 0.1890 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
D1	24 <i>d</i>	1	0.021	0.167	0.164	0.167	octahedron D ₅ S
D2	24 <i>d</i>	1	0.021	0.333	0.336	0.167	octahedron SD ₅
S3	4 <i>a</i>	.-3.	0	0	0		cuboctahedron D ₁₂

Experimental: powder, diffractometer, neutrons, $R_B = 0.079$, $T = 112 \text{ K}$

Remarks: Phase stable at $108 < T < 133 \text{ K}$. A refinement considering symmetry-adapted spherical-harmonic functions for deuterium is reported in [2].

References: [1] Sandor E., Ogunade S.O. (1969), Nature (London) 224, 905-907. [2] Cockcroft J.K., Fitch A.N. (1990), Z. Kristallogr. 193, 1-19.

205
cP56

TlCoCl ₆ [NH ₃] ₆	<i>cP56</i>	(205) <i>Pa</i> -3 – d ² ba
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Tl[Co(NH₃)₆]Cl₆ [1]

Structural features: $\text{Co}(\text{NH}_3)_6$ and TlCl_6 octahedra in a NaCl-type arrangement. See Fig. II.42.

Watanabe T. et al. (1950) [1]

$\text{Cl}_6\text{CoH}_{18}\text{N}_6\text{Tl}$

$a = 1.142 \text{ nm}$, $V = 1.4894 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24d	1	0.075	0.361	0.15		single atom Tl
(NH_3)2	24d	1	0.1	0.36	0.45		single atom Co
Tl3	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Cl_6
Co4	4a	.-3.	0	0	0		octahedron $(\text{NH}_3)_6$

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

Experimental: single crystal, oscillation photographs, X-rays

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

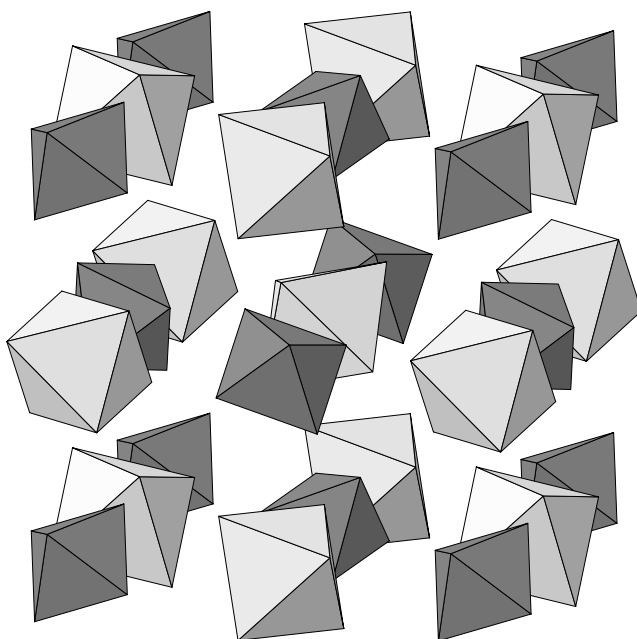


Fig. II.42. $\text{Tl}[\text{Co}(\text{NH}_3)_6]\text{Cl}_6$

Arrangement of TlCl_6 (light) and $\text{Co}(\text{NH}_3)_6$ (dark) octahedra.

References: [1] Watanabe T., Atoji M., Okazaki C. (1950), Acta Crystallogr. 3, 405-408.

205
cP60

$\text{U}[\text{P}_2\text{O}_7]$

cP60

(205) $Pa-3 - d^2ca$

UP_2O_7 [1]

Structural features: U atoms and P_2O_7 units (two vertex-linked PO_4 tetrahedra) in a NaCl-type arrangement; splitting of the bridging O site allows for non-linear P-O-P segments.

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

$\text{O}_7\text{P}_2\text{U}$

$a = 0.86311 \text{ nm}$, $V = 0.6430 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0	0.048	0.452	0.167	
O2	24d	1	0.2455	0.4321	0.4487		single atom P
P3	8c	.3.	0.4014	0.4014	0.4014		
U4	4a	.-3.	0	0	0		octahedron O ₆

Experimental: powder, diffractometer, X-rays, $R_p = 0.086$

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

References: [1] Cabeza A., Aranda M.A.G., Cantero F.M., Lozano D., Martinez Lara M., Bruque S. (1996), J. Solid State Chem. 121, 181-189.

205
cP60

Zn[BrO ₃] ₂ [H ₂ O] ₆	cP60	(205) Pa-3 – d ² ca
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Zn(BrO₃)₂·6H₂O [1], Strukturbericht notation J1₁₀

Structural features: Zn(OH₂)₆ octahedra and :BrO₃ ψ-tetrahedra in a CaF₂-type arrangement.

Yü S.H., Beevers C.A. (1936) [1]

Br₂H₁₂O₁₂Zn

$a = 1.0316$ nm, $V = 1.0978$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.145	0.33	0.19		single atom Br
(OH ₂)2	24d	1	0.195	0.45	0.465		single atom Zn
Br3	8c	.3.	0.259	0.259	0.259		non-coplanar triangle O ₃
Zn4	4a	.-3.	0	0	0		octahedron (OH ₂) ₆

Experimental: single crystal, oscillation photographs, X-rays

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

References: [1] Yü S.H., Beevers C.A. (1936), Z. Kristallogr. 95, 426-434.

205
cP60

Zr[WO ₄] ₂	cP60	(205) Pa-3 – dc ⁴ b
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ZrW₂O₈ ht [1]

Structural features: ZrO₆ octahedra and WO₄ tetrahedra (disorder between two O₄ tetrahedra with common basis) share vertices to form a 3D-framework.

Evans J.S.O. et al. (1996) [1]

O₈W₂Zr

$a = 0.9137$ nm, $V = 0.7628$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0549	0.2911	0.0671		
O2	8c	.3.	0.0055	0.0055	0.0055	0.5	
W3	8c	.3.	0.1035	0.1035	0.1035	0.5	
W4	8c	.3.	0.1606	0.1606	0.1606	0.5	
O5	8c	.3.	0.2678	0.2678	0.2678	0.5	single atom W

Zr6 4b .-3. $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ octahedron O₆

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

Experimental: powder, diffractometer, neutrons, $R_B = 0.058$, $T = 483$ K

Remarks: Phase stable at $T > 428$ K. Negative thermal expansion. Short interatomic distances for partly occupied site(s).

References: [1] Evans J.S.O., Mary T.A., Vogt T., Subramanian M.A., Sleight A.W. (1996), Chem. Mater. 8, 2809-2823.

205
cP64

In₇Cl₉ cP64 (205) Pa-3 – d²cba

In₇Cl₉ [1]

Structural features: Distorted close-packed Cl layers in c stacking; In⁺ and In³⁺ in octahedral voids, the former being displaced from the octahedron centers to form In₃ trigonal clusters ($d(\text{In-In}) = 0.388$ nm).

Beck H.P., Wilhelm D. (1991) [1]

Cl₉In₇

$a = 1.2218$ nm, $V = 1.8239$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24d	1	0.0433	0.4486	0.1955		single atom In
(In ⁺)2	24d	1	0.1716	0.3164	0.4299		bicapped square prism Cl ₈ In ₂
Cl3	8c	.3.	0.1677	0.1677	0.1677		non-coplanar triangle In ₃
(In ³⁺)4	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Cl ₆
Cl5	4a	.-3.	0	0	0		octahedron In ₆

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

References: [1] Beck H.P., Wilhelm D. (1991), Angew. Chem. 103, 897-898 (Angew. Chem. Int. Ed. Engl. 30, 824-825).

205
cP64

(Pb_{0.66}Sb_{0.34})₆SnS₉ cP64 (205) Pa-3 – d²cba

(Pb_{0.66}Sb_{0.34})₆SnS₉ [1]

Structural features: Distorted close-packed S layers in c stacking; Sn and (Pb,Sb) in octahedral voids (the latter being displaced from the octahedron center). SnS₆ octahedra and (Pb,Sb)S₆S₂ bicapped trigonal prisms share atoms to form a 3D-framework. Ordering variant of In₇Cl₉.

Kaplunnik L.N. et al. (1977) [1]

Pb_{3.96}S₉Sb_{2.04}Sn

$a = 1.1549$ nm, $V = 1.5404$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24d	1	0.0479	0.4465	0.2127		non-colinear SnPb
M2	24d	1	0.1585	0.2999	0.4346		8-vertex polyhedron S ₈
S3	8c	.3.	0.1691	0.1691	0.1691		non-coplanar triangle Pb ₃
Sn4	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron S ₆

S5 4a .-3. 0 0 0 octahedron Pb₆

M2 = 0.66Pb + 0.34Sb

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

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

References: [1] Kaplunnik L.N., Pobedinskaya E.A., Belov N.V. (1977), Dokl. Akad. Nauk SSSR 237, 1086-1089.

205
cP64

Rb₇NaGe₈ cP64 (205) Pa-3 – d²cba

Rb₇NaGe₈ [1]; K₇LiSi₈ [2]

Structural features: Single Ge₄ tetrahedra.

Llanos J. et al. (1983) [1]

Ge₈NaRb₇

$a = 1.3165$ nm, $V = 2.2817$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24d	1	0.0574	0.2061	0.0753		4-vertex polyhedron Ge ₃ Na
Rb2	24d	1	0.1849	0.4572	0.274		tricapped trigonal prism Ge ₆ NaRb ₂
Ge3	8c	.3.	0.2018	0.2018	0.2018		non-coplanar triangle Ge ₃
Rb4	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron Ge ₆ Rb ₆
Na5	4a	.-3.	0	0	0		octahedron Ge ₆

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

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

References: [1] Llanos J., Nesper R., Von Schnering H.G. (1983), Angew. Chem. 95, 1026-1027. [2] Charbonnel M., Belin C. (1985), Acta Crystallogr. C 41, 1398-1400.

205
cP64

CsFe₂[CN]₆ cP64 (205) Pa-3 – d²cba

CsFe[Fe(CN)₆] [1]

Structural features: Fe²⁺(CN)₆ octahedral units (non-linear Fe-C-N segments) in a Cu-type (c.c.p.) arrangement; Cs in "tetrahedral" (disorder), Fe³⁺ in "octahedral" voids.

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

C₆CsFe₂N₆

$a = 1.025$ nm, $V = 1.0769$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24d	1	0.0	0.193	0.02		single atom N
N2	24d	1	0.0	0.202	0.485		single atom C
Cs3	8c	.3.	0.25	0.25	0.25	0.5	cuboctahedron C ₆ N ₆
Fe4	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N ₆
Fe5	4a	.-3.	0	0	0		octahedron C ₆

Experimental: powder, diffractometer, X-rays

Remarks: The description in space group (198) $P2_13$ in [1] does not take into consideration all symmetry elements of the proposed structure.

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

205
cP68

$\text{Cd}_7\text{P}_4\text{Cl}_6$	cP68	(205) $Pa-3 - d^2c^2a$
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$\text{Cd}_7\text{P}_4\text{Cl}_6$ [2]

Structural features: $\text{Cd}_3\text{P}-\text{PCd}_3$ units (a P_2 dumbbell in a Cd_6 octahedron) share vertices to form a 3D-framework; CdCl_6 octahedra in voids.

Shevelkov A.V. et al. (1998) [1]

$\text{Cd}_7\text{Cl}_6\text{P}_4$

$a = 1.1936 \text{ nm}$, $V = 1.7005 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	24d	1	0.01488	0.27415	0.23101		octahedron P_2Cl_4
Cl2	24d	1	0.0216	0.2812	0.4623		non-collinear Cd_2
P3	8c	.3.	0.2125	0.2125	0.2125		tetrahedron PCd_3
P4	8c	.3.	0.3183	0.3183	0.3183		tetrahedron PCd_3
Cd5	4a	-.3.	0	0	0		octahedron Cl_6

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

References: [1] Shevelkov A.V., Reshetova L.N., Popivkin B.A. (1998), J. Solid State Chem. 137, 138-142. [2] Rebbah A., Yazbeck J., Deschamps A. (1980), Rev. Chim. Miner. 17, 96-101.

205
cP72

$\text{BaNb}([\text{OH}]_{0.21}\text{F}_{0.79})_7$	cP72	(205) $Pa-3 - d^2c^2ba$
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$\text{BaNbF}_{7-x}(\text{OH})_x$ [1]; CsMoF_7 [2]

Structural features: Ba atoms and $\text{Nb}(\text{F},\text{OH})_6(\text{F},\text{OH})$ monocapped trigonal prisms in a CsCl-type arrangement.

Crosnier Lopez M.P. et al. (1993) [1]

$\text{BaF}_{5.50}\text{H}_{1.50}\text{NbO}_{1.50}$

$a = 0.99259 \text{ nm}$, $V = 0.9779 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24d	1	0.0557	0.1162	0.257		single atom Nb
M2	24d	1	0.1028	0.3627	0.278		single atom Nb
Nb3	8c	.3.	0.2234	0.2234	0.2234		monocapped trigonal prism F_7
M4	8c	.3.	0.3351	0.3351	0.3351		single atom Nb
Ba5	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron F_{14}
Ba6	4a	-.3.	0	0	0		icosahedron F_{12}

$\text{M1} = 0.786\text{F} + 0.214\text{OH}$; $\text{M2} = 0.786\text{F} + 0.214\text{OH}$; $\text{M4} = 0.786\text{F} + 0.214\text{OH}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.019$, $T = 293 \text{ K}$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In [2] the cell parameter is misprinted as 0.1028 nm instead of 1.0528 nm (from cell volume).

References: [1] Crosnier Lopez M.P., Duroy H., Fourquet J.L. (1993), Eur. J. Solid State Inorg. Chem. 30, 549-556. [2] Giese S., Seppelt K. (1994), Angew. Chem. Int. Ed. Engl. 33, 461-463.

205
cP72

$\text{H}_2(\text{NH}_4)_6\text{BiBr}_7\text{F}_4$	<i>cP72</i>	(205) <i>Pa</i> -3 – d ² c ² ba
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(NH₄)₆H₂BiBr₇F₄ [1]

Structural features: BiBr₆ octahedra and single Br atoms, F₂ dumbbells.

Gerasimenko A.V. et al. (1991) [1]

BiBr₇F₄H₂₄N₆

a = 1.3109 nm, *V* = 2.2527 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Br1	24 <i>d</i>	1	0.0522	0.4294	0.2		single atom Bi
(NH ₄) ₂	24 <i>d</i>	1	0.175	0.315	0.441		single atom F
F3	8 <i>c</i>	.3.	0.173	0.173	0.173		single atom F
F4	8 <i>c</i>	.3.	0.269	0.269	0.269		tetrahedron F(NH ₄) ₃
Bi5	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Br ₆
Br6	4 <i>a</i>	-.3.	0	0	0		14-vertex Frank-Kasper (NH ₄) ₆ F ₂ Br ₆

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.041

Remarks: H not belonging to NH₄ was not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gerasimenko A.V., Bukvetskii B.V., Udovenko A.A., Davidovich R.L. (1991), Koord. Khim. 17, 322-324.

205
cP72

$\text{Hg}_7\text{Sb}_4\text{Br}_6$	<i>cP72</i>	(205) <i>Pa</i> -3 – d ² c ² ba
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Hg₇Sb₄Br₆ [1]

Structural features: Hg₃Sb-SbHg₃ units (a Sb₂ dumbbell in a Hg₆ octahedron) share vertices to form a 3D-framework; HgBr₆ octahedra and single Hg atoms in voids (partial Hg vacancies). Partly disordered variant of Cd₇P₄Cl₆.

Shevelkov A.V. et al. (1992) [1]

Br₆Hg₇Sb₄

a = 1.2994 nm, *V* = 2.1940 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Br1	24 <i>d</i>	1	0.0455	0.4491	0.2058		single atom Hg
Hg2	24 <i>d</i>	1	0.1859	0.3033	0.4532		non-colinear Sb ₂
Sb3	8 <i>c</i>	.3.	0.1474	0.1474	0.1474		tetrahedron Hg ₃ Sb
Sb4	8 <i>c</i>	.3.	0.2704	0.2704	0.2704		tetrahedron Hg ₃ Sb
Hg5	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.7	octahedron Br ₆
Hg6	4 <i>a</i>	-.3.	0	0	0	0.3	rhombic dodecahedron Sb ₂ Hg ₆ Br ₆

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.073, *T* = 293 K

Remarks: Identical to so-called HgSbBr in [2].

References: [1] Shevelkov A.V., Dikarev E.V., Popovkin B.A. (1992), J. Solid State Chem. 98, 133-136. [2] Puff H., Gotta H. (1965), Z. Anorg. Allg. Chem. 337, 157-163.

205
cP72

Hg ₆ BiAs ₄ Cl ₇	cP72	(205) <i>Pa</i> -3 – d ² c ² ba
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Hg₆BiAs₄Cl₇ [1]; Hg₆MoAs₄Cl₇ [2]

Structural features: Hg₃As-AsHg₃ units (an As₂ dumbbell in a Hg₆ octahedron) share vertices to form a 3D-framework; BiCl₆ octahedra and single Cl atoms in voids.

Beck J. et al. (2000) [1]

As₄BiCl₇Hg₆

$a = 1.2178 \text{ nm}$, $V = 1.8060 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24 <i>d</i>	1	0.0454	0.4491	0.2114		single atom Bi
Hg2	24 <i>d</i>	1	0.18707	0.30488	0.45466		non-collinear As ₂
As3	8 <i>c</i>	.3.	0.1541	0.1541	0.1541		tetrahedron AsHg ₃
As4	8 <i>c</i>	.3.	0.2693	0.2693	0.2693		tetrahedron AsHg ₃
Bi5	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Cl ₆
Cl6	4 <i>a</i>	-.3.	0	0	0		rhombic dodecahedron As ₂ Hg ₆ Cl ₆

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

References: [1] Beck J., Hedderich S., Neisel U. (2000), J. Solid State Chem. 154, 350-355. [2] Beck J., Neisel U. (2000), Z. Anorg. Allg. Chem. 626, 1620-1626.

205
cP72

Ni[CO] ₄	cP72	(205) <i>Pa</i> -3 – d ² c ³
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Ni(CO)₄ [2]

Structural features: Single Ni(CO)₄ tetrahedral units (linear Ni-C-O segments).

Braga D. et al. (1993) [1]

C₄NiO₄

$a = 1.0832 \text{ nm}$, $V = 1.2709 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24 <i>d</i>	1	0.0231	0.02757	0.219		single atom O
O2	24 <i>d</i>	1	0.0387	0.46898	0.22105		single atom C
Ni3	8 <i>c</i>	.3.	0.12184	0.12184	0.12184		tetrahedron C ₄
C4	8 <i>c</i>	.3.	0.21878	0.21878	0.21878		single atom O
O5	8 <i>c</i>	.3.	0.27872	0.27872	0.27872		single atom C

Experimental: single crystal, diffractometer, X-rays, $wR = 0.090$, $T = 198 \text{ K}$

References: [1] Braga D., Grepioni F., Orpen G. (1993), Organometallics 12, 1481-1483. [2] Ladell J., Post B., Fankuchen I. (1952), Acta Crystallogr. 5, 795-800.

205
cP72

In ₅ S ₄	cP72	(205) Pa-3 – d ² c ³
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"In₅S₄" [1]Structural features: In(InS₃) tetrahedra share vertices to form a 3D-framework.

Wadsten T. et al. (1980) [1]

In₅S₄ $a = 1.234 \text{ nm}$, $V = 1.8791 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	24d	1	0.02646	0.06670	0.26925		tetrahedron S ₃ In
S2	24d	1	0.07265	0.25849	0.32323		non-coplanar triangle In ₃
S3	8c	.3.	0.07443	0.07443	0.07443		non-coplanar triangle In ₃
In4	8c	.3.	0.27108	0.27108	0.27108		tetrahedron S ₃ In
In5	8c	.3.	0.40018	0.40018	0.40018		tetrahedron In ₄

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

Remarks: The structure was later redetermined and the composition corrected to In₄SnS₄ [2].

References: [1] Wadsten T., Arnberg L., Berg J.E. (1980), Acta Crystallogr. B 36, 2220-2223. [2] Deiseroth H.J., Pfeifer H. (1991), Z. Kristallogr. 196, 197-205.

205
cP72

In ₄ SnS ₄	cP72	(205) Pa-3 – d ² c ³
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SnIn₄S₄ [1]Structural features: In(SnS₃) tetrahedra share vertices to form a 3D-framework.

Deiseroth H.J., Pfeifer H. (1991) [1]

In₄S₄Sn $a = 1.23475 \text{ nm}$, $V = 1.8825 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
In1	24d	1	0.02634	0.0666	0.26915		tetrahedron S ₃ Sn
S2	24d	1	0.0724	0.25878	0.32346		non-coplanar triangle In ₃
S3	8c	.3.	0.07453	0.07453	0.07453		non-coplanar triangle In ₃
In4	8c	.3.	0.27108	0.27108	0.27108		tetrahedron S ₃ Sn
Sn5	8c	.3.	0.40024	0.40024	0.40024		tetrahedron In ₄

Experimental: single crystal, X-rays, R = 0.014, T = 293 K

Remarks: Supersedes a refinement for so-called In₅S₄ in [2].

References: [1] Deiseroth H.J., Pfeifer H. (1991), Z. Kristallogr. 196, 197-205. [2] Wadsten T., Arnberg L., Berg J.E. (1980), Acta Crystallogr. B 36, 2220-2223.

205
cP72

Cd ₄ As ₂ I ₃	cP72	(205) Pa-3 – d ² c ³
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Cd₄As₂I₃ [1]

Structural features: Distorted close-packed Cd layers in c stacking; I atoms and As₂ dumbbells in octahedral, remaining As in tetrahedral voids. Cd₃As-AsCd₃ units and AsCd₄ tetrahedra (one As₂ dumbbell for two single As). See Fig. II.43.

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

As₂Cd₄I₃

$a = 1.2993 \text{ nm}$, $V = 2.1935 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	24d	1	0.0048	0.2583	0.0341		non-colinear As ₂
I2	24d	1	0.1862	0.4369	0.2567		non-colinear Cd ₂
As3	8c	.3.	0.1033	0.1033	0.1033		tetrahedron Cd ₄
Cd4	8c	.3.	0.2176	0.2176	0.2176		tetrahedron AsI ₃
As5	8c	.3.	0.4467	0.4467	0.4467		tetrahedron AsCd ₃

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

Remarks: Preliminary data in [2].

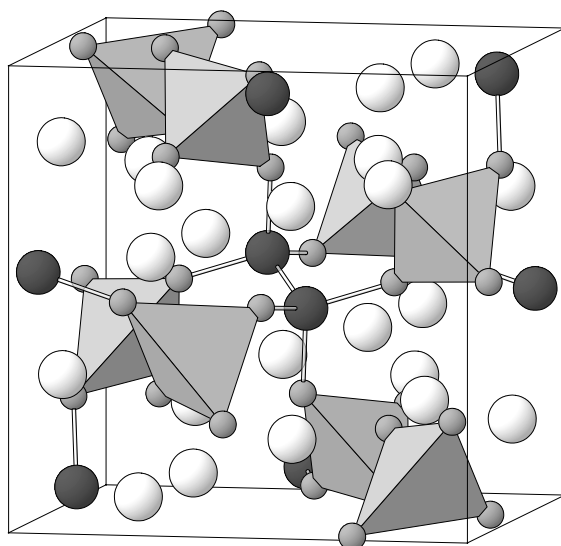


Fig. II.43. **Cd₄As₂I₃**

Arrangement of AsCd₄ tetrahedra (Cd atoms small), I (light) and additional As (dark) atoms.

References: [1] Gallay J., Allais G., Deschanvres A. (1975), Acta Crystallogr. B 31, 2274-2276. [2] Suchow L., Stemple N.R. (1963), J. Electrochem. Soc. 110, 766-769.

205
cP72

C₂N

cP72

(205) $Pa-3 - d^3$

C₁₂N₆ [2], benzenehexacarbonitrile, hexacyanobenzene

Structural features: Planar C₆(CN)₆ molecules (a C₆ hexagon with a CN unit bonded to each C) perpendicular to $\langle 111 \rangle$.

Drück U., Kutoglu A. (1984) [1]

C₂N

$a = 1.0781 \text{ nm}$, $V = 1.2531 \text{ nm}^3$, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24d	1	0.0045	0.0938	0.4107		coplanar triangle C ₃
C2	24d	1	0.0095	0.1903	0.3191		non-colinear NC
N3	24d	1	0.0142	0.2677	0.2460		single atom C

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

Experimental: single crystal, diffractometer, X-rays, R = 0.035, T = 120 K

Remarks: Refinement on diffraction data from [2]. Electron density study.

References: [1] Drück U., Kutoglu A. (1984), Z. Kristallogr. 166, 233-244. [2] Drück U., Kutoglu A. (1983), Acta Crystallogr. C 39, 638-640.

205
cP80

Cu ₃ WO ₆	cP80	(205) <i>Pa</i> -3 – d ³ c
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Cu₃WO₆ [1]

Structural features: WO₆ octahedra and CuO₅ trigonal bipyramids share edges and vertices to form a 3D-framework.

Gebert E., Kihlberg L. (1969) [1]

Cu₃O₆W

$a = 0.97989$ nm, $V = 0.9409$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0891	0.2193	0.3016		tetrahedron Cu ₃ W
Cu2	24d	1	0.13762	0.40443	0.24568		trigonal bipyramid O ₅
O3	24d	1	0.1953	0.4446	0.4636		non-coplanar triangle WCu ₂
W4	8c	.3.	0.11703	0.11703	0.11703		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.065

References: [1] Gebert E., Kihlberg L. (1969), Acta Chem. Scand. 23, 221-231.

205
cP80

Nb ₃ ICl ₆	cP80	(205) <i>Pa</i> -3 – d ³ c
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Nb₆Cl₁₂I₂ [1]

Structural features: Nb₆Cl₁₂I₆ clusters (a Nb₆ octahedron surrounded by a Cl₁₂ cuboctahedron and a I₆ octahedron) in a Cu-type (c.c.p.) arrangement share I atoms to form a 3D-framework.

Sägebarth M., Simon A. (1990) [1]

Cl₆INb₃

$a = 1.2578$ nm, $V = 1.9899$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Nb1	24d	1	0.04374	0.35394	0.06042		monocapped square prism Cl ₄ Nb ₄ I
Cl2	24d	1	0.12407	0.2208	0.39933		non-colinear Nb ₂
Cl3	24d	1	0.25462	0.47898	0.37988		non-colinear Nb ₂
I4	8c	.3.	0.12864	0.12864	0.12864		non-coplanar triangle Nb ₃

Experimental: single crystal, diffractometer, X-rays, wR = 0.026, T = 296 K

References: [1] Sägebarth M., Simon A. (1990), Z. Anorg. Allg. Chem. 587, 119-128.

205
cP84

CaB_2O_4	<i>cP84</i>	(205) <i>Pa</i> -3 – d ³ ca
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CaB₂O₄ form IV [1]; BaAl₂S₄ [2]; BaGa₂S₄ [2]

Structural features: BO₄ tetrahedra share vertices to form a 3D-framework. See Fig. II.44.

Marezio M. et al. (1969) [1]

B₂CaO₄

$a = 0.9008 \text{ nm}$, $V = 0.7309 \text{ nm}^3$, $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.0064	0.0906	0.2823		non-colinear B ₂
B2	24 <i>d</i>	1	0.1189	0.1901	0.3457		tetrahedron O ₄
O3	24 <i>d</i>	1	0.1208	0.3336	0.2692		non-colinear B ₂
Ca4	8 <i>c</i>	.3.	0.37305	0.37305	0.37305		tricapped trigonal prism O ₉
Ca5	4 <i>a</i>	-.3.	0	0	0		cuboctahedron O ₁₂

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

Remarks: Phase stable at $2.5 < p < 4.0 \text{ GPa}$ at 1173 K.

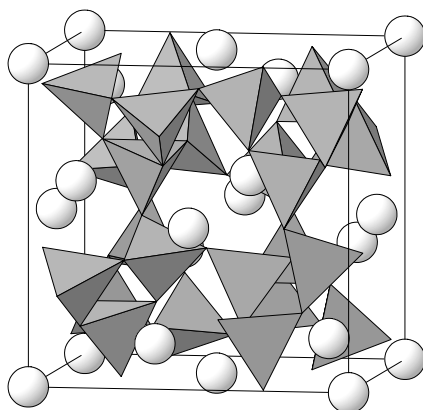


Fig. II.44. **CaB₂O₄ form IV**

Arrangement of BO₄ tetrahedra and Ca atoms.

References: [1] Marezio M., Remeika J.P., Dernier P.D. (1969), Acta Crystallogr. B 25, 965-970. [2] Eisenmann B., Schäfer M.J.H. (1982), Mater. Res. Bull. 17, 1169-1175.

205
cP88

$\text{KGaTe}_6\text{O}_{14}$	<i>cP88</i>	(205) <i>Pa</i> -3 – d ³ cba
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KGaTe₆O₁₄ [1]

Structural features: :TeO₄ trigonal ψ-bipyramids and GaO₆ octahedra share vertices to form a 3D-framework.

Ok K.M., Halasyamani P.S. (2001) [1]

GaKO₁₄Te₆

$a = 1.09267 \text{ nm}$, $V = 1.3046 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Te1	24d	1	0.00895	0.26507	0.22841		4-vertex polyhedron O ₄
O2	24d	1	0.0666	0.3866	0.1256		non-colinear TeGa
O3	24d	1	0.1936	0.3753	0.3892		non-colinear Te ₂
O4	8c	.3.	0.1472	0.1472	0.1472		non-coplanar triangle Te ₃
Ga5	4b	-.3.	1/2	1/2	1/2		octahedron O ₆
K6	4a	-.3.	0	0	0		square prism (cube) O ₈

Experimental: single crystal, diffractometer, X-rays, R = 0.017

References: [1] Ok K.M., Halasyamani P.S. (2001), Chem. Mater. 13, 4278-4284.

205
cP96

KAl[SO ₄] ₂ [H ₂ O] ₁₂	cP96	(205) Pa-3 – d ³ c ² ba
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KAl(SO₄)₂·12H₂O (see remark), kalinite, alum α, Strukturbericht notation H4₁₃

Structural features: Al(OH₂)₆ octahedra and SO₄ tetrahedra in a CaF₂-type arrangement; K and additional H₂O between the units (K(OH₂)₆O₆ polyhedra).

Beevers C.A., Lipson H. (1934) [1]

AlH₂₄KO₂₀S₂

a = 1.2181 nm, V = 1.8074 nm³, Z = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24d	1	0.02	0.02	0.34		single atom Al
O2	24d	1	0.07	0.2	0.23		single atom S
(OH ₂)3	24d	1	0.2	0.46	0.37		non-colinear (OH ₂)O
S4	8c	.3.	0.19	0.19	0.19		tetrahedron O ₄
O5	8c	.3.	0.26	0.26	0.26		single atom S
Al6	4b	-.3.	1/2	1/2	1/2		octahedron (OH ₂) ₆
K7	4a	-.3.	0	0	0		octahedron (OH ₂) ₆

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

Experimental: single crystal, rotation photographs, X-rays

Remarks: Strukturbericht notation H4₂ was defined on a model where the water molecules were not located [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Partly disordered models are proposed in [3] and [4]. Criteria for distinguishing isopointal α- and β-alums are discussed in [5] and [6].

References: [1] Beevers C.A., Lipson H. (1934), Nature (London) 134, 327. [2] (1931), Strukturberichte 1, 369. [3] Larson A.C., Cromer D.T. (1967), Acta Crystallogr. 22, 793-800. [4] Lipson H. (1935), Proc. R. Soc. London, Ser. A 151, 347-356. [5] Nyburg S.C., Steed J.W., Aleksovska S., Petrusevski V.M. (2000), Acta Crystallogr. B 56, 204-209. [6] Beattie J.K., Best S.P., Skelton B.W., White A.H. (1981), J. Chem. Soc., Dalton Trans. 1981, 2105-2111.

205
cP96

CsAl[SO ₄] ₂ [H ₂ O] ₁₂	cP96	(205) Pa-3 – d ³ c ² ba
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CsAl(SO₄)₂·12H₂O (see remark), alum β; NH₃CH₃Al(SO₄)₂·12H₂O (see remark), Strukturbericht notation H4₁₄

Structural features: $\text{Al}(\text{OH}_2)_6$ octahedra and SO_4 tetrahedra in a CaF_2 -type arrangement; Cs and additional H_2O between the units ($\text{Cs}(\text{OH}_2)_6\text{O}_6$ polyhedra). See Fig. II.45.

Beattie J.K. et al. (1981) [1]

$\text{AlCsH}_{24}\text{O}_{20}\text{S}_2$

$a = 1.2357 \text{ nm}$, $V = 1.8869 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0002	0.1518	0.4978		single atom Al
O2	24d	1	0.0638	0.221	0.1597		single atom S
O3	24d	1	0.1574	0.4497	0.2848		non-coplanar triangle O_3
S4	8c	.3.	0.17159	0.17159	0.17159		tetrahedron O_4
O5	8c	.3.	0.2407	0.2407	0.2407		single atom S
Al6	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O_6
Cs7	4a	-.3.	0	0	0		14-vertex polyhedron O_{12}S_2
H8	24d	1	0.018	0.313	0.045		
H9	24d	1	0.051	0.483	0.198		
H10	24d	1	0.177	0.391	0.275		
H11	24d	1	0.223	0.49	0.268		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.043$, $T = 295 \text{ K}$

Remarks: Strukturbericht notation $\text{H}4_{14}$ was defined on $\text{NH}_3\text{CH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$, for which the positions of the centers of the NH_3CH_3 units were determined [2]. $\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ was stated to be isotypic in [3], and was refined in [4]. Criteria for distinguishing isopointal α - and β -alums are discussed in [1] and [3]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

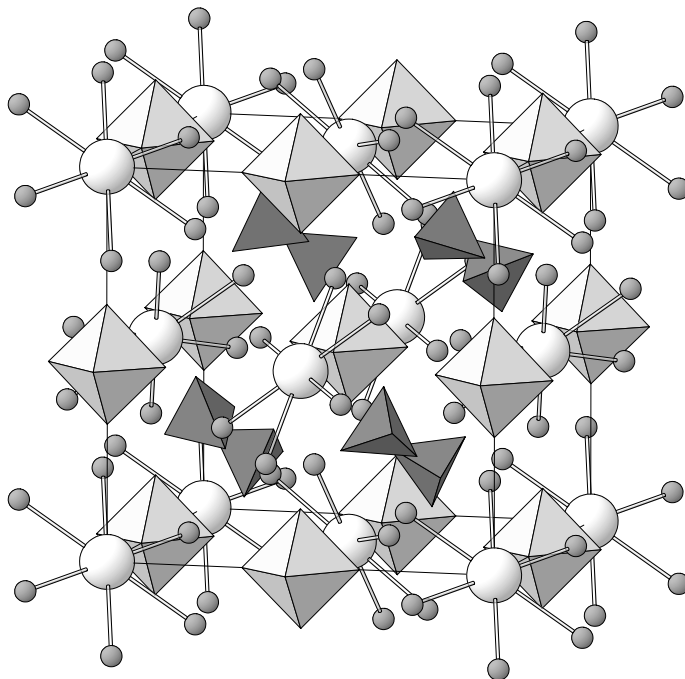


Fig. II.45. $\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$

Arrangement of SO_4 tetrahedra (dark), $\text{Al}(\text{OH}_2)_6$ octahedra (light), Cs (large) and additional H_2O molecules (O atoms small).

References: [1] Beattie J.K., Best S.P., Skelton B.W., White A.H. (1981), J. Chem. Soc., Dalton Trans. 1981, 2105-2111. [2] (1937), Strukturberichte 2, 111. [3] Lipson H. (1935), Proc. R. Soc. London, Ser. A 151, 347-356. [4] Cromer D.T., Kay M.I., Larson A.C. (1966), Acta Crystallogr. 21, 383-389.

205
cP96

NaAl[SO ₄] ₂ [H ₂ O] ₁₂	cP96	(205) <i>Pa</i> -3 – d ³ c ² ba
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NaAl(SO₄)₂·12H₂O [2], Strukturbericht notation H4₁₅, alum γ

Structural features: Al(OH₂)₆ octahedra and SO₄ tetrahedra in a CaF₂-type arrangement; Na(OH₂)₆ octahedra in "cubic" voids.

Kay M.I., Cromer D.T. (1970) [1]

AlH₂₄NaO₂₀S₂

a = 1.2213 nm, *V* = 1.8217 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.0404	0.4427	0.1371		single atom Al
O2	24 <i>d</i>	1	0.1812	0.4233	0.4597		tetrahedron NaO ₃
O3	24 <i>d</i>	1	0.2029	0.2212	0.3518		single atom S
O4	8 <i>c</i>	.3.	0.165	0.165	0.165		single atom S
S5	8 <i>c</i>	.3.	0.2347	0.2347	0.2347		tetrahedron O ₄
Al6	4 <i>b</i>	-.3.	¹ / ₂	¹ / ₂	¹ / ₂		octahedron O ₆
Na7	4 <i>a</i>	-.3.	0	0	0		octahedron O ₆
H8	24 <i>d</i>	1	0.002	0.445	0.202		
H9	24 <i>d</i>	1	0.014	0.192	0.117		
H10	24 <i>d</i>	1	0.113	0.412	0.161		
H11	24 <i>d</i>	1	0.181	0.378	0.415		

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

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

Remarks: Diffraction data from [3]; we took all atom coordinates except those of the sulfate group from this reference. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kay M.I., Cromer D.T. (1970), Acta Crystallogr. B 26, 1349-1355. [2] Lipson H. (1935), Proc. R. Soc. London, Ser. A 151, 347-356. [3] Cromer D.T., Kay M.I., Larson A.C. (1967), Acta Crystallogr. 22, 182-187.

205
cP96

Ag ₄ Te[NO ₃] ₂	cP96	(205) <i>Pa</i> -3 – d ³ c ² ba
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Ag₄Te(NO₃)₂ α [1]

Structural features: Ignoring vacancies, Ag and Te form a Cu-type (c.c.p.) sublattice; NO₃ trigonal units in voids (partial disorder).

Schultze Rhonhof E. (1975) [1]

Ag₄N₂O₆Te

a = 0.8173 nm, *V* = 0.5459 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	24 <i>d</i>	1	0.0	0.25	0.25	0.5	tetrahedron O ₄
O2	24 <i>d</i>	1	0.125	0.125	0.31	0.5	single atom N

O3	24d	1	0.19	0.375	0.375	0.5	single atom N
N4	8c	.3.	0.19	0.19	0.19	0.5	non-coplanar triangle O ₃
N5	8c	.3.	0.31	0.31	0.31	0.5	non-coplanar triangle O ₃
Ag6	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Te7	4a	-.3.	0	0	0		octahedron O ₆

Experimental: powder, film, X-rays, R = 0.105

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

References: [1] Schultze Rhonhof E. (1975), Acta Crystallogr. B 31, 2837-2840.

205
cP96

Li ₇ NbN ₄	cP96	(205) Pa-3 – d ³ c ³
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Li₇NbN₄ [1]; Li₇TaN₄ [2]

Structural features: Close-packed N layers in c stacking; Li and Nb in tetrahedral voids. Single NbN₄ tetrahedra. Substitution derivative of CaF₂ (fluorite) antitype.

Vennos D.A., DiSalvo F.J. (1992) [1]

Li₇N₄Nb

a = 0.9829 nm, *V* = 0.9496 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24d	1	0.0117	0.2439	0.0143		square prism (cube) NbLi ₇
Li2	24d	1	0.1151	0.368	0.3603		fourcapped trigonal prism N ₄ Li ₅ Nb
Li3	24d	1	0.119	0.4012	0.1348		fourcapped trigonal prism N ₄ Li ₅ Nb
Nb4	8c	.3.	0.1278	0.1278	0.1278		tetrahedron N ₄
N5	8c	.3.	0.2411	0.2411	0.2411		square prism (cube) NbLi ₇
Li6	8c	.3.	0.3679	0.3679	0.3679		fourcapped trigonal prism N ₄ Li ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.031, T = 298 K

References: [1] Vennos D.A., DiSalvo F.J. (1992), Acta Crystallogr. C 48, 610-612. [2] Wachsmann C., Jacobs H. (1992), J. Alloys Compd. 190, 113-116.

205
cP104

[UO ₂]Te ₃ O ₇	cP104	(205) Pa-3 – d ³ c ³ ba
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UTe₃O₉ [1], cliffordite

Structural features: :TeO₄ trigonal ψ-bipyramids share vertices to form a 3D-framework; U in voids (hexagonal bipyramid).

Galy J., Meunier G. (1971) [1]

O₉Te₃U

a = 1.137 nm, *V* = 1.4699 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Te1	24d	1	0.0474	0.2636	0.2845		8-vertex polyhedron O ₈
O2	24d	1	0.092	0.178	0.408		single atom Te
O3	24d	1	0.106	0.419	0.348		non-colinear Te ₂
O4	8c	.3.	0.104	0.104	0.104		colinear UO

O5	8c	.3.	0.221	0.221	0.221	non-coplanar triangle Te ₃
O6	8c	.3.	0.4	0.4	0.4	single atom U
U7	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	8-vertex polyhedron O ₈
U8	4a	-.3.	0	0	0	8-vertex polyhedron O ₈

Experimental: powder, X-rays, R = 0.064

Remarks: Off-stoichiometric cliffordite is studied in [2].

References: [1] Galy J., Meunier G. (1971), Acta Crystallogr. B 27, 608-616. [2] Brandstaetter F. (1981), TPM, Tschermaks Mineral. Petrogr. Mitt. 29, 1-8.

205
cP104

Nb ₃ I(I _{0.2} Cl _{0.8}) ₃ Cl ₃	cP104	(205) Pa-3 – d ⁴ c
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Nb₆Cl_{10.8}I_{3.2} [1]

Structural features: Nb₆Cl₆(Cl,I)₆I₆ clusters (a Nb₆ octahedron surrounded by a Cl₆(Cl,I)₆ cuboctahedron (distinct positions for Cl and I) and a I₆ octahedron) in a Cu-type (c.c.p.) arrangement share I atoms to form a 3D-framework.

Sägebarth M., Simon A. (1990) [1]

Cl_{5.38}I_{1.62}Nb₃

$a = 1.272$ nm, $V = 2.0581$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24d	1	0.0177	0.1191	0.2436	0.792	
I2	24d	1	0.0257	0.1192	0.2653	0.208	
Cl3	24d	1	0.0974	0.3752	0.28		non-collinear Nb ₂
Nb4	24d	1	0.14364	0.43864	0.45584		
I5	8c	.3.	0.36665	0.36665	0.36665		

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.026, T = 296 K

Remarks: Homogeneity range Nb₆Cl_{12-x}I_{2+x}, $0 < x < 2$. Short interatomic distances for partly occupied site(s).

References: [1] Sägebarth M., Simon A. (1990), Z. Anorg. Allg. Chem. 587, 119-128.

205
cP108

[NH ₃ OH]Al[SO ₄] ₂ [H ₂ O] ₁₂	cP108	(205) Pa-3 – d ³ c ⁴ b
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(NH₃OH)Al(SO₄)₂·12H₂O [1], alum NH₃OH

Structural features: Al(OH₂)₆ octahedra and SO₄ tetrahedra in a CaF₂-type arrangement; N(H₃[OH]) tetrahedra and additional H₂O between the units (partial disorder for the former).

Abdeen A.M. et al. (1981) [1]

AlH₂₈NO₂₁S₂

$a = 1.2328$ nm, $V = 1.8736$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0186	0.3509	0.0204		single atom Al
O2	24d	1	0.0911	0.1913	0.2474		single atom S
O3	24d	1	0.2016	0.4581	0.3627		non-coplanar triangle O ₃

N4	8c	.3.	0.013	0.013	0.013	0.5	
O5	8c	.3.	0.0433	0.0433	0.0433	0.5	
S6	8c	.3.	0.1978	0.1978	0.1978		tetrahedron O ₄
O7	8c	.3.	0.2672	0.2672	0.2672		single atom S
Al8	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
H9	24d	1	0.0067	0.3042	0.2862		
H10	24d	1	0.0475	0.0863	0.3163		
H11	24d	1	0.0815	0.4713	0.4764	0.5	
H12	24d	1	0.1032	0.4226	0.4831	0.167	
H13	24d	1	0.2127	0.3908	0.3305		
H14	24d	1	0.2989	0.4732	0.4583		

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

Experimental: single crystal, diffractometer, neutrons, wR = 0.019

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] Abdeen A.M., Will G., Weiss A. (1981), Z. Kristallogr. 154, 45-57.

205
cP116

NaZr ₆ BI _{3.06} Cl _{10.94}	cP116	(205) Pa-3 – d ⁴ c ² a
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NaZr₆Cl_{12-x}I_{2+x}B [2]

Structural features: BZr₆Cl₆(Cl,I)₆I₆ clusters (a central B atom surrounded by a Zr₆ octahedron, a Cl₆(Cl,I)₆ cuboctahedron (distinct positions for Cl and I) and a I₆ octahedron) in a Cu-type (c.c.p.) arrangement share I atoms to form a 3D-framework.

Köckerling M. (1999) [1]

BCl_{10.94}I_{3.06}NaZr₆

$a = 1.3313 \text{ nm}$, $V = 2.3595 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24d	1	0.021	0.1192	0.2416	0.823	
I2	24d	1	0.0211	0.1224	0.2677	0.177	
Cl3	24d	1	0.09867	0.37679	0.27948		non-coplanar triangle Zr ₂ Na
Zr4	24d	1	0.1538	0.43523	0.45318		square pyramid BCl ₄
Na5	8c	.3.	0.2182	0.2182	0.2182	0.5	
I6	8c	.3.	0.36717	0.36717	0.36717		
B7	4a	-.3.	0	0	0		octahedron Zr ₆

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

Remarks: Homogeneity range NaZr₆BCl_{12-x}I_{2+x}, $0 < x < 6.0$. Short interatomic distances for partly occupied site(s). The same data are reported in [2].

References: [1] Köckerling M. (1999), Z. Anorg. Allg. Chem. 625, 24-30. [2] Köckerling M. (1998), Inorg. Chem. 37, 380-381.

205
cP116

Cs ₃ Mg ₂ P ₆ (N _{0.17} O _{0.83}) ₆ O ₁₂	cP116	(205) Pa-3 – d ⁴ c ² a
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Cs₃Mg₂P₆O₁₇N [1]

Structural features: Rings formed by six vertex-linked $P(O_3(O,N))$ tetrahedra share vertices with MgO_6 octahedra to form a 3D-framework.

Feldmann W. et al. (2000) [1]

$Cs_3Mg_2NO_{17}P_6$

$a = 1.2239 \text{ nm}$, $V = 1.8333 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24d	1	0.0266	0.1736	0.4257		non-colinear P_2
O2	24d	1	0.0269	0.1649	0.2203		single atom P
P3	24d	1	0.15157	0.18144	0.45759		tetrahedron O_4
O4	24d	1	0.1717	0.3582	0.2202		single atom P
Mg5	8c	.3.	0.1921	0.1921	0.1921		octahedron O_6
Cs6	8c	.3.	0.37263	0.37263	0.37263		tricapped trigonal prism O_9
Cs7	4a	-.3.	0	0	0		octahedron O_6

$M1 = 0.833O + 0.167N$

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.029$, $T = 293 \text{ K}$

References: [1] Feldmann W., L'Haridon P., Marchand R. (2000), J. Solid State Chem. 153, 185-191.

205
cP124

$H_3CdCu_2[CN]_7[H_2O]_{14}$	cP124	(205) $Pa-3 - d^4c^3b$
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$[H_{31}O_{14}][CdCu_2(CN)_7]$ [1]

Structural features: $Cu_2[CN]_7$ units (two vertex-linked $Cu(CN)_4$ tetrahedral units with approximately linear Cu-C-N segments, orientational disorder CN/NC for the bridging cyanide unit) and Cd atoms in a NaCl-type arrangement (Cd and Cu form a pyrite-type sublattice), embedded in a framework of hydrogen-bonded H_2O/H_3O with 12-membered rings.

Nishikiori S., Iwamoto T. (1993) [1]

$C_7CdCu_2H_{28}N_7O_{14}$

$a = 1.29401 \text{ nm}$, $V = 2.1668 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24d	1	0.0488	0.3409	0.0681		single atom C
C2	24d	1	0.0742	0.2594	0.0882		single atom N
(OH ₂)3	24d	1	0.084	0.318	0.3426		non-colinear (OH ₂) ₂
(OH ₂)4	24d	1	0.1359	0.455	0.2842		non-colinear (OH ₂) ₂
M5	8c	.3.	0.0262	0.0262	0.0262		single atom C
Cu6	8c	.3.	0.11652	0.11652	0.11652		tetrahedron C_4
(OH ₂)7	8c	.3.	0.3138	0.3138	0.3138		6-vertex polyhedron (OH ₂) ₆
Cd8	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron N_6

$M5 = 0.5C + 0.5N$

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

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

Remarks: H not belonging to H_2O was not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nishikiori S., Iwamoto T. (1993), J. Chem. Soc., Chem. Commun. 1993, 1555-1556.

205
cP128

$[\text{NH}_4]\text{Al}[\text{SO}_4]_2[\text{H}_2\text{O}]_{12}$	<i>cP128</i>	(205) <i>Pa-3</i> – d^4c^3ba
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 $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [1], alum α

Structural features: $\text{Al}(\text{OH}_2)_6$ octahedra and SO_4 tetrahedra (orientational disorder) in a CaF_2 -type arrangement; NH_4 (orientational disorder) and additional H_2O between the units.

Cromer D.T., Kay M.I. (1967) [1]

 $\text{AlD}_{28}\text{NO}_{20}\text{S}_2$ $a = 1.2243 \text{ nm}$, $V = 1.8351 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.017	0.0171	0.3495		single atom Al
O2	24 <i>d</i>	1	0.0806	0.1861	0.2351	0.5	
O3	24 <i>d</i>	1	0.1225	0.2058	0.2823	0.5	
O4	24 <i>d</i>	1	0.2007	0.4533	0.3626		
O5	8 <i>c</i>	.3.	0.1243	0.1243	0.1243	0.5	4-vertex polyhedron SO_3
S6	8 <i>c</i>	.3.	0.1899	0.1899	0.1899		
O7	8 <i>c</i>	.3.	0.2603	0.2603	0.2603	0.5	4-vertex polyhedron SO_3
Al8	4 <i>b</i>	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
N9	4 <i>a</i>	.-3.	0	0	0		square prism (cube) O_8
D10	24 <i>d</i>	1	0.0041	0.3048	0.2848		
D11	24 <i>d</i>	1	0.0428	0.0847	0.3144		0.5
D12	24 <i>d</i>	1	0.0655	0.4866	0.4505		
D13	24 <i>d</i>	1	0.2074	0.3837	0.3319		
D14	24 <i>d</i>	1	0.2973	0.4727	0.4559		
D15	8 <i>c</i>	.3.	0.0521	0.0521	0.0521	0.5	

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, neutrons, $R = 0.084$

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] Cromer D.T., Kay M.I. (1967), *Acta Crystallogr.* 22, 800-805.205
cP128

$\text{MgCe}[\text{NO}_3]_6[\text{H}_2\text{O}]_6$	<i>cP128</i>	(205) <i>Pa-3</i> – d^5ba
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 $\text{MgCe}(\text{NO}_3)_6 \cdot 6\text{H}_2\text{O}$ [1]

Structural features: $\text{Ce}(\text{NO}_3)_6$ icosahedral units (a central CeO_{12} icosahedron sharing edges with six NO_3 trigonal units) and $\text{Mg}(\text{OH}_2)_6$ octahedra.

Guillou N. et al. (1995) [1]

 $\text{CeH}_{12}\text{MgN}_6\text{O}_{24}$ $a = 1.25702 \text{ nm}$, $V = 1.9862 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.0005	0.1837	0.0851		single atom N
(OH ₂)2	24 <i>d</i>	1	0.0506	0.3933	0.1102		single atom Mg
O3	24 <i>d</i>	1	0.0508	0.3475	0.3886		single atom N
N4	24 <i>d</i>	1	0.1462	0.3433	0.4328		non-coplanar triangle O_3
O5	24 <i>d</i>	1	0.205	0.2684	0.407		single atom N

Mg6	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	octahedron (OH ₂) ₆
Ce7	4a	.-3.	0	0	0	icosahedron O ₁₂

Experimental: powder, diffractometer, X-rays, $R_p = 0.064$, $T = 295$ K

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

References: [1] Guillou N., Louer M., Auffredic J.P., Louer D. (1995), Eur. J. Solid State Inorg. Chem. 32, 35-47.

205
cP132

[NH ₄]Al[SO ₄] ₂ [H ₂ O] ₁₂	cP132	(205) <i>Pa</i> -3 – d ⁴ c ⁴ b
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NH₄Al(SO₄)₂·12H₂O [1], alum α

Structural features: Al(OH₂)₆ octahedra and SO₄ tetrahedra (orientational disorder) in a CaF₂-type arrangement; NH₄ (orientational disorder) and additional H₂O between the units.

Abdeen A.M. et al. (1981) [1]

AlH₂₈NO₂₀S₂

$a = 1.2248$ nm, $V = 1.8374$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0171	0.347	0.0177		single atom Al
O2	24d	1	0.0801	0.1863	0.236	0.831	
O3	24d	1	0.1444	0.2177	0.2895	0.169	
O4	24d	1	0.201	0.4558	0.3633		single atom O
N5	8c	.-3.	0.007	0.007	0.007	0.5	
O6	8c	.-3.	0.1169	0.1169	0.1169	0.169	4-vertex polyhedron SO ₃
S7	8c	.-3.	0.1889	0.1889	0.1889		
O8	8c	.-3.	0.2615	0.2615	0.2615	0.831	tetrahedron SO ₃
Al9	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
H10	24d	1	0.0042	0.3035	0.2834		
H11	24d	1	0.0429	0.0829	0.3126		
H12	24d	1	0.0625	0.4969	0.4686	0.5	
H13	24d	1	0.2063	0.3818	0.3324		
H14	24d	1	0.2941	0.4725	0.4568		
H15	8c	.-3.	0.0611	0.0611	0.0611	0.5	

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

Experimental: single crystal, diffractometer, neutrons, $wR = 0.014$

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] Abdeen A.M., Will G., Schäfer W., Kirfel A., Bargouth M.O., Recker K., Weiss A. (1981), Z. Kristallogr. 157, 147-166.

205
cP136

KAl[SO ₄] ₂ [H ₂ O] ₁₂	cP136	(205) <i>Pa</i> -3 – d ⁴ c ⁴ ba
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KAl(SO₄)₂·12H₂O [1], alum α

Structural features: Al(OH₂)₆ octahedra and SO₄ tetrahedra (orientational disorder) in a CaF₂-type arrangement; K (disorder) and additional H₂O between the units.

Larson A.C., Cromer D.T. (1967) [1]

$\text{AlH}_{24}\text{KO}_{20}\text{S}_2$

$a = 1.2157 \text{ nm}$, $V = 1.7967 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24 <i>d</i>	1	0.019	0.3456	0.0206		single atom Al
O2	24 <i>d</i>	1	0.0772	0.1895	0.2352	0.699	
O3	24 <i>d</i>	1	0.1264	0.2099	0.2962	0.301	
(OH ₂)4	24 <i>d</i>	1	0.1993	0.4535	0.3647		single atom (OH ₂)
K5	8 <i>c</i>	.3.	0.015	0.015	0.015	0.15	
O6	8 <i>c</i>	.3.	0.1271	0.1271	0.1271	0.301	4-vertex polyhedron SO ₃
S7	8 <i>c</i>	.3.	0.1925	0.1925	0.1925		
O8	8 <i>c</i>	.3.	0.2612	0.2612	0.2612	0.699	4-vertex polyhedron SO ₃
Al9	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron (OH ₂) ₆
K10	4 <i>a</i>	-.3.	0	0	0	0.699	

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

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

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] Larson A.C., Cromer D.T. (1967), Acta Crystallogr. 22, 793-800.

205
cP144

$\text{B}_{11}\text{SeH}_{11}$	<i>cP144</i>	(205) <i>Pa</i> -3 – d ⁶
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SeB₁₁H₁₁ [1]

Structural features: B₁₁SeH₁₁ icosahedral units (an empty (B₁₁Se) icosahedron with one H bonded to each B, substitutional disorder with distinct positions for Se and B) in a Cu-type (c.c.p.) arrangement.

Ferguson G. et al. (1987) [1]

$\text{B}_{11}\text{H}_{11}\text{Se}$

$a = 0.9847 \text{ nm}$, $V = 0.9548 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
B1	24 <i>d</i>	1	0.0359	0.043	0.174	0.871	
Se2	24 <i>d</i>	1	0.0416	0.0513	0.2081	0.088	
H3	24 <i>d</i>	1	0.0595	0.069	0.2779	0.871	
B4	24 <i>d</i>	1	0.1017	0.4148	0.3743	0.962	
Se5	24 <i>d</i>	1	0.1172	0.3971	0.3472	0.079	
H6	24 <i>d</i>	1	0.1546	0.3598	0.295	0.962	

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

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

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

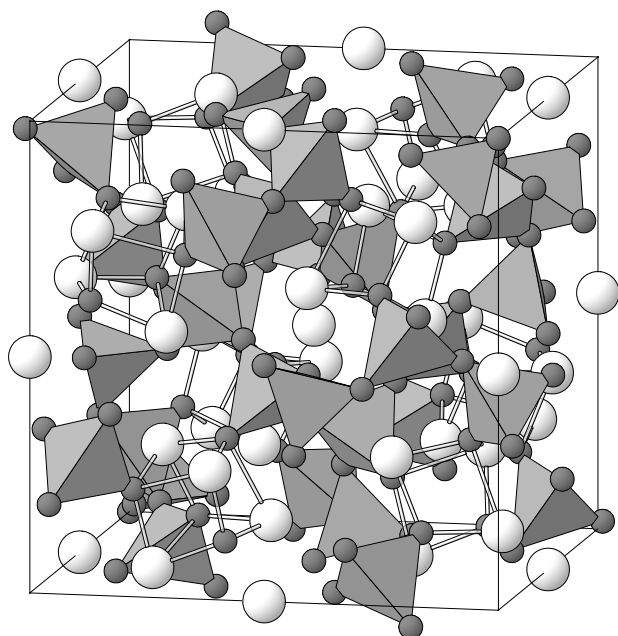
References: [1] Ferguson G., Parvez M., MacCurtain J.A., Dhubghaill O.N., Spalding T.R. (1987), J. Chem. Soc., Dalton Trans. 1987, 699-704.

$\text{Al}_8\text{Pb}_9\text{O}_{21}$

cP152

(205) $Pa-3 - d^5c^3ba$ **$\text{Pb}_9\text{Al}_8\text{O}_{21}$ [1]**

Structural features: AlO_4 tetrahedra share vertices to form a 3D-framework; Pb and additional O in large voids. Pb_9O_8 units consisting of two Pb_4O_4 cubane-like clusters interconnected via a bridging Pb. See Fig. II.46.

Fig. II.46. **$\text{Pb}_9\text{Al}_8\text{O}_{21}$**

Arrangement of AlO_4 tetrahedra, Pb_4O_4 units and additional Pb atoms (Pb atoms large, O atoms small).

Plötz K.B., Müller Buschbaum H. (1981) [1]

 $\text{Al}_8\text{O}_{21}\text{Pb}_9$ $a = 1.326 \text{ nm}$, $V = 2.3315 \text{ nm}^3$, $Z = 4$

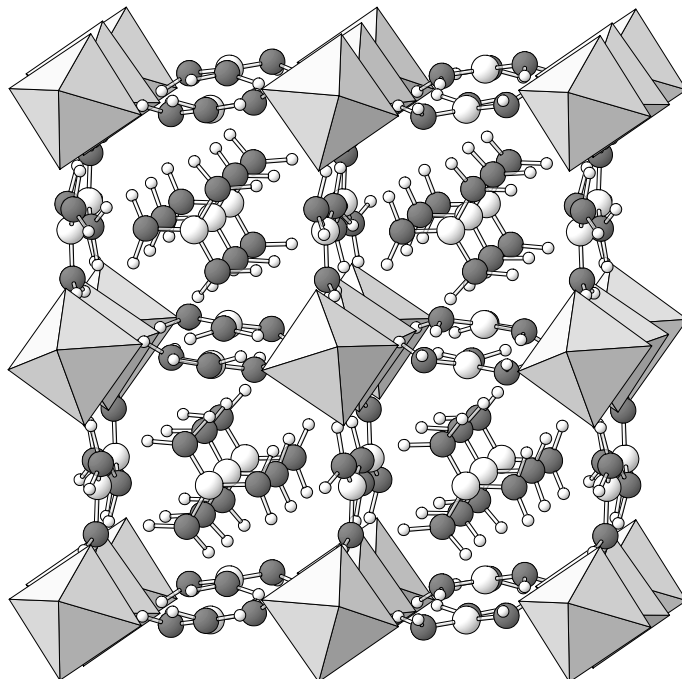
site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.006	0.172	0.386		non-colinear Al_2
O2	24d	1	0.052	0.052	0.198		non-colinear Al_2
Al3	24d	1	0.107	0.218	0.453		tetrahedron O_4
O4	24d	1	0.194	0.294	0.377		non-coplanar triangle AlPb_2
Pb5	24d	1	0.2353	0.4587	0.3751		non-coplanar triangle O_3
Al6	8c	.3.	0.075	0.075	0.075		tetrahedron O_4
Pb7	8c	.3.	0.2246	0.2246	0.2246		non-coplanar triangle O_3
O8	8c	.3.	0.394	0.394	0.394		tetrahedron Pb_4
Pb9	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		square prism (cube) O_8
O10	4a	.-3.	0	0	0		colinear Al_2

Experimental: single crystal, diffractometer, X-rays, $R = 0.079$

References: [1] Plötz K.B., Müller Buschbaum H. (1981), Z. Anorg. Allg. Chem. 480, 149-152.

205
cP152 $[\text{CN}_3\text{H}_6]_3\text{FeF}_6$

cP152

(205) $Pa-3 - d^6ba$ $[\text{C}(\text{NH}_2)_3]_3\text{FeF}_6$ [1]Structural features: Planar $\text{C}(\text{NH}_2)_3$ (guanidinium) trigonal units and FeF_6 octahedra. See Fig. II.47.Fig. II.47. $[\text{C}(\text{NH}_2)_3]_3\text{FeF}_6$ Arrangement of FeF_6 octahedra and $\text{C}(\text{NH}_2)_3$ units (C atoms light, N atoms dark, H atoms small).

Fourquet J.L. et al. (1987) [1]

 $\text{C}_3\text{F}_6\text{FeH}_{18}\text{N}_9$ $a = 1.413 \text{ nm}$, $V = 2.8212 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24d	1	0.0153	0.2199	0.1692		single atom C
F2	24d	1	0.0205	0.367	0.0267		single atom Fe
N3	24d	1	0.0231	0.36	0.2532		single atom C
C4	24d	1	0.0263	0.2648	0.2511		non-colinear N_2
F5	24d	1	0.0286	0.3683	0.4763		single atom Fe
N6	24d	1	0.0385	0.2179	0.3319		single atom C
Fe7	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron F_6
Fe8	4a	.-3.	0	0	0		octahedron F_6
H9	24d	1	0.0028	0.1451	0.1705		
H10	24d	1	0.0041	0.3883	0.317		
H11	24d	1	0.0107	0.3852	0.1848		
H12	24d	1	0.0194	0.1433	0.337		
H13	24d	1	0.0199	0.2649	0.3847		
H14	24d	1	0.2604	0.3822	0.4822		

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

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

References: [1] Fourquet J.L., Plet F., Calage Y., De Pape R. (1987), J. Solid State Chem. 69, 76-80.

205
cP160

CsXe ₃ O ₃ F ₁₃	cP160	(205) <i>Pa</i> -3 – d ⁶ cba
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Cs[(XeOF₄)₃F] [1]

Structural features: Xe₃O₃F₁₃ units consisting of three distorted Xe(F₅O) octahedra having a common F vertex.

Holloway J.H. et al. (1985) [1]

CsF₁₃O₃Xe₃

$a = 1.3933$ nm, $V = 2.7048$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	24d	1	0.0095	0.3752	0.1818		single atom Xe
Xe2	24d	1	0.0232	0.254	0.2452		square pyramid OF ₄
F3	24d	1	0.0407	0.1397	0.3198		single atom Xe
F4	24d	1	0.0426	0.3252	0.3632		single atom Xe
F5	24d	1	0.1876	0.37	0.4979		single atom Xe
O6	24d	1	0.2118	0.4092	0.2607		single atom Xe
F7	8c	.3.	0.1946	0.1946	0.1946		non-coplanar triangle Xe ₃
Cs8	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron F ₁₂
Cs9	4a	-.3.	0	0	0		icosahedron F ₁₂

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.096, T = 293 K

References: [1] Holloway J.H., Kaucic V., Martin Rovet D., Russell D.R., Schrobilgen G.J., Selig H. (1985), Inorg. Chem. 24, 678-683.

205
cP168

BaMn ₉ [(V _{0.9} As _{0.1})O ₄] ₆ [OH] ₂	cP168	(205) <i>Pa</i> -3 – d ⁶ c ² ba
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BaMn₉[(V,As)O₄]₆(OH)₂ [1], nabisite

Structural features: Close-packed O₉ and BaO₈ layers in c stacking; Mn in octahedral, (V,As) in tetrahedral voids. MnO₆ and Mn(O₅OH) octahedra share edges to form a 3D-framework; Ba in voids surrounded by six (V,As)O₄ tetrahedra.

Brugger J. et al. (1999) [1]

As_{0.62}BaH₂Mn₉O₂₆V_{5.38}

$a = 1.2832$ nm, $V = 2.1129$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.003	0.0074	0.3308		single atom V
Mn2	24d	1	0.0054	0.341	0.1949		octahedron O ₆
O3	24d	1	0.0088	0.1701	0.1798		non-coplanar triangle VMn ₂
O4	24d	1	0.0207	0.3299	0.3586		non-colinear VMn
M5	24d	1	0.093	0.2458	0.4274		tetrahedron O ₄
O6	24d	1	0.1678	0.1728	0.3439		non-coplanar triangle VMn ₂
Mn7	8c	.3.	0.1758	0.1758	0.1758		octahedron O ₆

O8	8c	.3.	0.3456	0.3456	0.3456	non-coplanar triangle Mn ₃ octahedron O ₆ cuboctahedron O ₁₂
Mn9	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	
Ba10	4a	-.3.	0	0	0	
H11	8c	.3.	0.3138	0.3138	0.3138	

M5 = 0.897V + 0.103As

Experimental: single crystal, diffractometer, X-rays, R = 0.026, T = 293 K

Remarks: Natural specimen from Pla de Labasse, central Pyrenees, France. Composition Ba_{1.03}(Mn_{9.02}Sr_{0.01})(V_{5.27}As_{0.70})O₂₄(OH)₂ from electron microprobe analysis. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Brugger J., Bonin M., Schenk K.J., Meisser N., Berlepsch P., Ragu A. (1999), Eur. J. Mineral. 11, 879-890.

205
cP168

Na_{1.03}Li_{0.52}Ca_{1.42}Mg_{0.06}Mn_{3.56}Fe_{0.78}Al_{1.92}[PO₄]₆F₂ *cP168* (205) *Pa*-3 – d⁶c²ba

(Mn,Na,Li,Ca,Mg)₁₉Ca₄(Fe,Al)₄Al₈(PO₄)₂₄F₈ [1], griphite

Structural features: (Al,Fe)O₆ and FeO₆ octahedra, Ca(O₆F₂) cubes and PO₄ tetrahedra share vertices to form a 3D-framework; additional atoms in voids.

Rinaldi R. (1978) [1]

Al_{1.92}Ca_{1.42}F₂Fe_{1.19}Li_{0.54}Mg_{0.06}Mn_{3.60}Na_{1.02}O₂₄P₆

a = 1.2205 nm, *V* = 1.8181 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24 <i>d</i>	1	0.0057	0.1208	0.2608		tetrahedron O ₃ F
O2	24 <i>d</i>	1	0.0171	0.4604	0.3036		single atom P
P3	24 <i>d</i>	1	0.0403	0.3597	0.2352		tetrahedron O ₄
O4	24 <i>d</i>	1	0.0782	0.3959	0.1194		single atom P
O5	24 <i>d</i>	1	0.1276	0.2848	0.2876		non-collinear PAI
O6	24 <i>d</i>	1	0.2785	0.4403	0.2828		single atom P
F7	8 <i>c</i>	.3.	0.1145	0.1145	0.1145		non-coplanar triangle Mn ₃
M8	8 <i>c</i>	.3.	0.2846	0.2846	0.2846		octahedron O ₆
Fe9	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.75	octahedron O ₆
Ca10	4 <i>a</i>	-.3.	0	0	0		square prism (cube) F ₂ O ₆

M1 = 0.6Mn + 0.17Na + 0.09Li + 0.07Ca + 0.06Fe + 0.01Mg; M8 = 0.96Al + 0.04Fe

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

Remarks: Natural specimen from Albères, eastern Pyrenees, France. Composition (Mn_{14.24}Na_{4.13}Li_{2.08}Ca_{1.66}Fe²⁺_{1.29}Mg_{0.24}Fe³⁺_{0.05})Ca₄(Fe_{0.7}Al_{0.13}□_{0.17})₄(Al_{0.96}Fe³⁺_{0.04})₈[(PO₄)_{0.93}(H₄O₄)_{0.03}]₂₄[F_{0.8}(OH)_{0.2}]₈ from chemical analysis.

References: [1] Rinaldi R. (1978), Bull. Mineral. 101, 543-547.

205
cP208

KMo₃CoAs₃O₁₅[H₂O]₃ *cP208* (205) *Pa*-3 – d⁸cba

K₂[Co(H₂O)₆][As₆CoMo₆O₃₀] [1]

Structural features: CoMo₆As₆O₃₀ units (a central CoO₆ octahedron sharing edges with a ring formed by six edge-linked MoO₆ octahedra, and vertices with two units formed by three vertex-linked :AsO₃ ψ-tetrahedra) and Co(OH₂)₆ octahedra.

Martin Frère J. et al. (1991) [1]



$$a = 1.489 \text{ nm}, V = 3.3013 \text{ nm}^3, Z = 8$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
As1	24d	1	0.00862	0.15788	0.17053		non-coplanar triangle O ₃
(OH ₂)2	24d	1	0.0521	0.4142	0.098		single atom Co
O3	24d	1	0.0529	0.443	0.2861		non-colinear Mo ₂
O4	24d	1	0.0758	0.2602	0.3228		single atom Mo
O5	24d	1	0.0797	0.215	0.0907		non-colinear As ₂
O6	24d	1	0.0881	0.407	0.4481		single atom As
Mo7	24d	1	0.1571	0.497	0.34105		octahedron O ₆
O8	24d	1	0.2356	0.4156	0.3246		single atom Mo
K9	8c	.3.	0.2473	0.2473	0.2473		octahedron O ₆
Co10	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron (OH ₂) ₆
Co11	4a	.-3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 298 K

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

References: [1] Martin Frère J., Jeannin Y., Robert F., Vaissermann J. (1991), Inorg. Chem. 30, 3635-3639.

205
cP216

CsVP ₄ O ₁₂	cP216	(205) Pa-3 – d ⁸ c ² ba
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CsV(PO₃)₄ [1]

Structural features: Rings formed by twelve vertex-linked PO₄ tetrahedra share vertices with VO₆ octahedra to form a 3D-framework (V at the centers of the rings and between rings). See Fig. II.48.

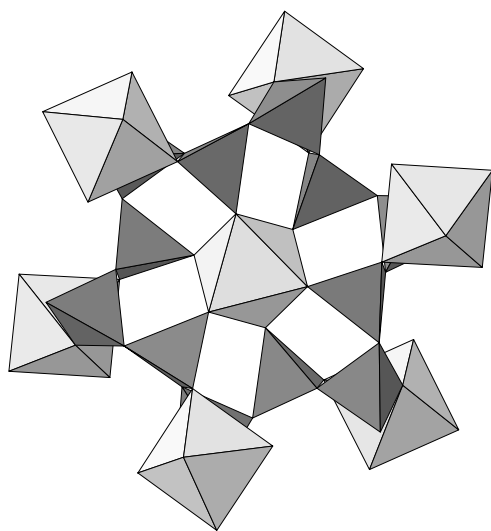
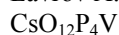


Fig. II.48. CsV(PO₃)₄

Arrangement of PO₄ tetrahedra (dark) and VO₆ octahedra (light) around a central VO₆ octahedra.

Lavrov A.V. et al. (1981) [1]



$$a = 1.4543 \text{ nm}, V = 3.0758 \text{ nm}^3, Z = 12$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0185	0.3659	0.0211		single atom P
P2	24d	1	0.0228	0.0842	0.2866		tetrahedron O ₄
P3	24d	1	0.0493	0.2793	0.334		tetrahedron O ₄
O4	24d	1	0.0615	0.2838	0.4435		non-colinear P ₂
O5	24d	1	0.0859	0.2334	0.1106		single atom P
O6	24d	1	0.1438	0.2651	0.2941		single atom P
O7	24d	1	0.179	0.4943	0.1838		non-colinear P ₂
O8	24d	1	0.1938	0.492	0.3565		single atom P
V9	8c	.3.	0.19015	0.19015	0.19015		octahedron O ₆
Cs10	8c	.3.	0.34321	0.34321	0.34321		tricapped trigonal prism O ₉
V11	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Cs12	4a	-.3.	0	0	0		icosahedron O ₁₂

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

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

References: [1] Lavrov A.V., Nikolaev V.P., Sadikov G.G., Voitenkov M.J. (1981), Dokl. Akad. Nauk SSSR 259, 103-106.

205
cP224

NaMgP ₃ O ₉	cP224	(205) Pa-3 – d ⁸ c ³ ba
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NaMg(PO₃)₃ [1]

Structural features: Rings formed by twelve vertex-linked PO₄ tetrahedra share vertices with MgO₆ octahedra to form a 3D-framework.

Abrahams I. et al. (2000) [1]

MgNaO₉P₃

$a = 1.42502$ nm, $V = 2.8938$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	24d	1	0.0014	0.2692	0.2801		tetrahedron O ₄
P2	24d	1	0.015	0.4753	0.2614		tetrahedron O ₄
O3	24d	1	0.0168	0.2324	0.3849		non-colinear P ₂
O4	24d	1	0.0271	0.1614	0.0319		non-colinear PMg
O5	24d	1	0.0309	0.3741	0.3078		non-colinear P ₂
O6	24d	1	0.0814	0.2157	0.2409		single atom P
O7	24d	1	0.2797	0.2865	0.4222		single atom P
O8	24d	1	0.3395	0.4898	0.4727		single atom P
Mg9	8c	.3.	0.1154	0.1154	0.1154		octahedron O ₆
Na10	8c	.3.	0.2555	0.2555	0.2555		octahedron O ₆
Mg11	8c	.3.	0.3731	0.3731	0.3731		octahedron O ₆
Na12	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Na13	4a	-.3.	0	0	0		octahedron O ₆

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

Experimental: powder, diffractometer, X-rays, R_p = 0.098

Remarks: In [1] the structure is erroneously stated to contain polyphosphate chains.

References: [1] Abrahams I., Ahmed A., Groombridge C.J., Hawkes G.E., Nunes T.G. (2000), J. Chem. Soc., Dalton Trans. 2000, 155-160.

205
cP232

$\text{Be}_4[\text{NO}_3]_6\text{O}$	<i>cP232</i>	$(205) Pa-3 - d^9 c^2$
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Be₄O(NO₃)₆ [1]

Structural features: Be₄(NO₃)₆O units formed by four vertex-linked BeO₄ tetrahedra (central O common to all four tetrahedra) sharing vertices with NO₃ trigonal units (one NO₃ unit shares vertices with two BeO₄ tetrahedra).

Haley M.J. et al. (1997) [1]

Be₄N₆O₁₉ $a = 1.4025 \text{ nm}$, $V = 2.7587 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.0101	0.0461	0.3356		single atom N
O2	24 <i>d</i>	1	0.0519	0.1692	0.2525		non-colinear NBe
N3	24 <i>d</i>	1	0.0717	0.0967	0.3062		coplanar triangle O ₃
O4	24 <i>d</i>	1	0.0813	0.3266	0.1596		non-colinear NBe
O5	24 <i>d</i>	1	0.0994	0.3191	0.3444		non-colinear NBe
Be6	24 <i>d</i>	1	0.122	0.2617	0.2466		tetrahedron O ₄
O7	24 <i>d</i>	1	0.1311	0.4266	0.4502		single atom N
N8	24 <i>d</i>	1	0.1566	0.3789	0.3842		coplanar triangle O ₃
O9	24 <i>d</i>	1	0.2419	0.3857	0.3512		non-colinear NBe
O10	8 <i>c</i>	.3.	0.2332	0.2332	0.2332		tetrahedron Be ₄
Be11	8 <i>c</i>	.3.	0.3003	0.3003	0.3003		tetrahedron O ₄

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

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

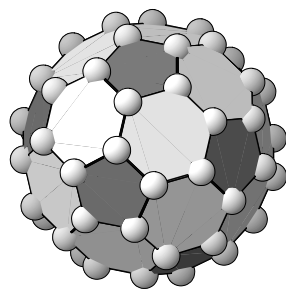
References: [1] Haley M.J., Wallwork S.C., Duffin B., Logan N., Addison C.C. (1997), Acta Crystallogr. C 53, 829-830.

205
cP240

[C ₆₀]	<i>cP240</i>	$(205) Pa-3 - d^{10}$
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C₆₀ It [1], fullerene, buckminsterfullerene

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement. See Fig. II.49.

Fig. II.49. C₆₀ It

C₆₀ cage with pentagonal (dark) and hexagonal (light) faces.

David W.I.F. et al. (1991) [1]

C₆₀ $a = 1.40478 \text{ nm}$, $V = 2.7722 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24d	1	0.0192	0.0636	0.2561		non-coplanar triangle C ₃
C2	24d	1	0.0325	0.399	0.2294		non-coplanar triangle C ₃
C3	24d	1	0.036	0.2066	0.3599		non-coplanar triangle C ₃
C4	24d	1	0.0371	0.2764	0.1122		non-coplanar triangle C ₃
C5	24d	1	0.054	0.4939	0.2467		non-coplanar triangle C ₃
C6	24d	1	0.0963	0.341	0.171		non-coplanar triangle C ₃
C7	24d	1	0.1323	0.1793	0.3814		non-coplanar triangle C ₃
C8	24d	1	0.1503	0.2017	0.4798		non-coplanar triangle C ₃
C9	24d	1	0.2919	0.4354	0.3711		non-coplanar triangle C ₃
C10	24d	1	0.2947	0.3651	0.4384		non-coplanar triangle C ₃

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

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.023$, $T = 5$ K

Remarks: Phase stable at $T < 249$ K. Preliminary data in [2].

References: [1] David W.I.F., Ibberson R.M., Matthewman J.C., Prassides K., Dennis T.J.S., Hare J.P., Kroto H.W., Taylor R., Walton D.R.M. (1991), *Nature* (London) 353, 147-149. [2] Heiney P.A., Fischer J.E., McGhie A.R., Romanow W.J., Denenstein A.M. McCauley J.P. Jr., Smith A.B., Cox D.E. (1991), *Phys. Rev. Lett.* 66, 2911-2914.

205
cP240

KPO ₃	cP240	(205) $Pa-3 - d^9 c^2 ba$
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K₆P₆O₁₈ [2]

Structural features: Rings formed by six vertex-linked PO₄ tetrahedra.

Averbuch Pouchot M.T. (1989) [1]

KO₃P

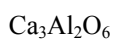
$a = 1.5753$ nm, $V = 3.9092$ nm³, $Z = 48$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24d	1	0.0033	0.3271	0.0241		single atom P
O2	24d	1	0.0116	0.1851	0.09398		non-colinear P ₂
O3	24d	1	0.0236	0.13882	0.2443		non-colinear P ₂
P4	24d	1	0.05892	0.27471	0.07798		tetrahedron O ₄
O5	24d	1	0.0748	0.3556	0.4129		single atom P
O6	24d	1	0.0923	0.3088	0.1587		single atom P
K7	24d	1	0.12017	0.44141	0.25612		octahedron O ₆
P8	24d	1	0.15484	0.32806	0.45358		tetrahedron O ₄
O9	24d	1	0.2251	0.2959	0.4003		single atom P
K10	8c	.3.	0.23249	0.23249	0.23249		octahedron O ₆
K11	8c	.3.	0.37173	0.37173	0.37173		octahedron O ₆
K12	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
K13	4a	-.3.	0	0	0		icosahedron O ₁₂

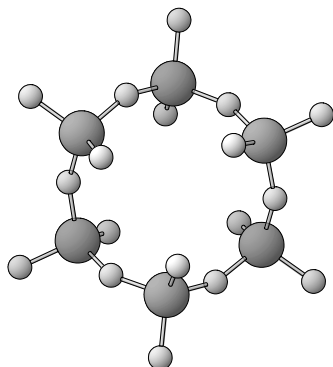
Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.023$, $T = 293$ K

References: [1] Averbuch Pouchot M.T. (1989), *Acta Crystallogr. C* 45, 1273-1275. [2] Kholodkovskaya L.N., Borodina L.A., Trunov V.K., Chudinova N.N. (1989), *Inorg. Mater.* 25, 405-408.



cP264

(205) $Pa-3 - d^{10}c^2ba$ **Ca₃Al₂O₆** [1], Strukturbericht notation E9₁, cement C₃AStructural features: Rings formed by six vertex-linked AlO₄ tetrahedra. See Fig. II.50.Fig. II.50. **Ca₃Al₂O₆**6-ring of AlO₄ tetrahedra (Al atoms large, O atoms small).

Mondal P., Jeffery J.W. (1975) [1]

 $a = 1.5263 \text{ nm}$, $V = 3.5557 \text{ nm}^3$, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24d	1	0.0046	0.2444	0.2335		tetrahedron O ₄
O2	24d	1	0.0103	0.2777	0.1241		non-colinear Al ₂
O3	24d	1	0.0104	0.4758	0.3491		single atom Al
Al4	24d	1	0.0133	0.0197	0.2526		tetrahedron O ₄
O5	24d	1	0.0385	0.4826	0.1509		single atom Al
O6	24d	1	0.1049	0.2664	0.2841		single atom Al
Ca7	24d	1	0.1209	0.38	0.3838		trigonal bipyramid O ₅
Ca8	24d	1	0.1272	0.1386	0.3763		square pyramid O ₅
O9	24d	1	0.1315	0.2536	0.4835		non-colinear Al ₂
O10	24d	1	0.235	0.4047	0.2921		single atom Al
Ca11	8c	.3.	0.2561	0.2561	0.2561		octahedron O ₆
Ca12	8c	.3.	0.375	0.375	0.375		octahedron O ₆
Ca13	4b	.-3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Ca14	4a	.-3.	0	0	0		octahedron O ₆

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.051$ Remarks: Supersedes a structure proposal in space group (221) $Pm-3m$ [2] and a partly correct structure proposal in (205) $Pa-3$ [3]. Strukturbericht notation E9₁ was defined on the superseded structure proposal.

References: [1] Mondal P., Jeffery J.W. (1975), Acta Crystallogr. B 31, 689-697. [2] Steele A.F., Davey W.P. (1929), Z. Kristallogr. 73, 17-30. [3] Moore A.E. (1966), Mag. Concr. Res. 18(55), 59-64.



cP268

(205) $Pa-3 - d^{10}c^3a$ **Ba₃Al₂O₆** [1]Structural features: Rings formed by twelve vertex-linked AlO₄ tetrahedra.

Antipov E.V. et al. (1987) [1]

 $\text{Al}_2\text{Ba}_3\text{O}_6$ $a = 1.6494 \text{ nm}$, $V = 4.4872 \text{ nm}^3$, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24d	1	0.0018	0.232	0.2697		tetrahedron O ₄
O2	24d	1	0.005	0.127	0.247		non-colinear Al ₂
O3	24d	1	0.011	0.25	0.372		non-colinear Al ₂
Al4	24d	1	0.0191	0.253	0.4806		tetrahedron O ₄
O5	24d	1	0.087	0.274	0.221		single atom Al
Ba6	24d	1	0.1008	0.3866	0.1149		non-coplanar triangle O ₃
Ba7	24d	1	0.1373	0.3705	0.3616		8-vertex polyhedron O ₈
O8	24d	1	0.157	0.484	0.478		single atom Al
O9	24d	1	0.262	0.405	0.265		single atom Al
O10	24d	1	0.337	0.484	0.483		single atom Al
Ba11	8c	.3.	0.1319	0.1319	0.1319	0.8	octahedron O ₆
Ba12	8c	.3.	0.2449	0.2449	0.2449	0.7	octahedron O ₆
Ba13	8c	.3.	0.3736	0.3736	0.3736		octahedron O ₆
Ba14	4a	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.078

Remarks: In table 1 of [1] the Wyckoff position of former Ba(1) is misprinted as 4b instead of 4a.

References: [1] Antipov E.V., Lykova L.N., Paromova M.V., Rozanova O.N., Kovba L.M. (1987), Koord. Khim. 13, 1119-1122.

205
cP272

$\text{K}_4\text{SrGe}_3\text{O}_9$	cP272	(205) $Pa-3 - d^{10}c^3ba$
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 $\text{K}_4\text{SrGe}_3\text{O}_9$ [1]Structural features: Rings formed by twelve vertex-linked GeO_4 tetrahedra.

Baumgartner O., Völlenkle H. (1977) [1]

 $\text{Ge}_3\text{K}_4\text{O}_9\text{Sr}$ $a = 1.6625 \text{ nm}$, $V = 4.5950 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24d	1	0.0107	0.2811	0.2789		tetrahedron O ₄
O2	24d	1	0.0175	0.2377	0.3767		non-colinear Ge ₂
O3	24d	1	0.0194	0.0295	0.1683		single atom Ge
Ge4	24d	1	0.0271	0.4769	0.2582		tetrahedron O ₄
O5	24d	1	0.0464	0.3805	0.2962		non-colinear Ge ₂
O6	24d	1	0.0801	0.229	0.2249		single atom Ge
K7	24d	1	0.1068	0.3531	0.1103		square pyramid O ₅
K8	24d	1	0.1546	0.3556	0.4149		octahedron O ₆
O9	24d	1	0.2574	0.4133	0.2871		single atom Ge
O10	24d	1	0.3361	0.479	0.4721		single atom Ge
Sr11	8c	.3.	0.1271	0.1271	0.1271		octahedron O ₆
K12	8c	.3.	0.2502	0.2502	0.2502		octahedron O ₆
Sr13	8c	.3.	0.3748	0.3748	0.3748		octahedron O ₆
K14	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆

K15 4a .-3. 0 0 0 octahedron O₆

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

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

References: [1] Baumgartner O., Völlenkle H. (1977), Z. Kristallogr. 146, 261-268.

205
cP272

Ba ₃ Ga ₂ O ₆	cP272	(205) <i>Pa</i> -3 – d ¹⁰ c ⁴
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Ba₃Ga₂O₆ [1]

Structural features: Rings formed by twelve vertex-linked GaO₄ tetrahedra.

Kahlenberg V. (2001) [1]

Ba₃Ga₂O₆

a = 1.6746 nm, *V* = 4.6961 nm³, *Z* = 24

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	24 <i>d</i>	1	0.00297	0.23457	0.26281		tetrahedron O ₄
O2	24 <i>d</i>	1	0.011	0.2493	0.3741		non-colinear Ga ₂
O3	24 <i>d</i>	1	0.013	0.1255	0.2437		non-colinear Ga ₂
Ga4	24 <i>d</i>	1	0.01679	0.25477	0.48626		tetrahedron O ₄
O5	24 <i>d</i>	1	0.0911	0.2815	0.2198		single atom Ga
Ba6	24 <i>d</i>	1	0.10368	0.38858	0.11359		non-coplanar triangle O ₃
Ba7	24 <i>d</i>	1	0.13579	0.36926	0.35919		8-vertex polyhedron O ₈
O8	24 <i>d</i>	1	0.1533	0.4797	0.4708		single atom Ga
O9	24 <i>d</i>	1	0.2622	0.2639	0.4028		single atom Ga
O10	24 <i>d</i>	1	0.3457	0.4839	0.4862		single atom Ga
Ba11	8 <i>c</i>	.3.	0.0079	0.0079	0.0079	0.5	
Ba12	8 <i>c</i>	.3.	0.1205	0.1205	0.1205		non-coplanar triangle O ₃
Ba13	8 <i>c</i>	.3.	0.24409	0.24409	0.24409	0.5	octahedron O ₆
Ba14	8 <i>c</i>	.3.	0.37476	0.37476	0.37476		octahedron O ₆

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

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

References: [1] Kahlenberg V. (2001), Cryst. Res. Technol. 36, 319-326.

205
cP276

Ce ₁₆ Si ₁₅ N ₃₂ O ₆	cP276	(205) <i>Pa</i> -3 – d ¹⁰ c ⁴
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Ce₁₆Si₁₅O₆N₃₂ [1]

Structural features: SiN₄, Si(N₃O) and Si(NO₃) tetrahedra share vertices with SiN₆ octahedra to form a 3D-framework.

Köllich K., Schnick W. (1999) [1]

Ce₁₆N₃₂O₆Si₁₅

a = 1.54036 nm, *V* = 3.6548 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24 <i>d</i>	1	0.0002	0.2671	0.1238		non-colinear Si ₂
N2	24 <i>d</i>	1	0.0037	0.1338	0.2492		non-colinear Si ₂

N3	24d	1	0.0049	0.4972	0.3635	non-colinear Si ₂
Si4	24d	1	0.01288	0.02033	0.24552	tetrahedron N ₄
N5	24d	1	0.0409	0.3001	0.3	single atom Si
N6	24d	1	0.0408	0.476	0.168	single atom Si
Ce7	24d	1	0.12038	0.14563	0.36788	8-vertex polyhedron N ₇ O
Ce8	24d	1	0.12905	0.39694	0.37433	4-vertex polyhedron N ₃ O
Si9	24d	1	0.24135	0.269	0.48353	tetrahedron N ₃ O
O10	24d	1	0.2417	0.3756	0.2553	non-colinear Si ₂
Ce11	8c	.3.	0.11974	0.11974	0.11974	single atom N
N12	8c	.3.	0.2072	0.2072	0.2072	single atom Si
Si13	8c	.3.	0.26984	0.26984	0.26984	tetrahedron NO ₃
Ce14	8c	.3.	0.40417	0.40417	0.40417	octahedron N ₆
Si15	4a	-.3.	0	0	0	octahedron N ₆

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

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

References: [1] Köllich K., Schnick W. (1999), Angew. Chem. Int. Ed. 38, 357-359.

205
cP320

Rb₃Sc₂[AsO₄]₃ cP320 (205) Pa-3 – d¹²c³ba

Rb₃Sc₂(AsO₄)₃ [1]

Structural features: ScO₆ octahedra and AsO₄ tetrahedra share vertices to form a 3D-framework; Rb in voids.

Harrison W.T.A. et al. (1998) [1]

As₃O₁₂Rb₃Sc₂

$a = 1.68749 \text{ nm}$, $V = 4.8053 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Rb1	24d	1	0.00215	0.4944	0.24511		tetrahedron O ₄
Sc2	24d	1	0.00318	0.24902	0.28303		octahedron O ₆
O3	24d	1	0.0353	0.399	0.0661		non-colinear AsSc
O4	24d	1	0.0538	0.3304	0.2087		non-colinear AsSc
O5	24d	1	0.0678	0.3073	0.371		non-colinear AsSc
O6	24d	1	0.0956	0.1595	0.2893		non-colinear AsSc
O7	24d	1	0.1008	0.4387	0.4613		non-colinear AsSc
As8	24d	1	0.10416	0.36538	0.13065		tetrahedron O ₄
As9	24d	1	0.13892	0.36901	0.40057		tetrahedron O ₄
O10	24d	1	0.1574	0.443	0.1607		non-colinear AsSc
O11	24d	1	0.1923	0.4071	0.3253		non-colinear AsSc
O12	24d	1	0.2068	0.3229	0.4575		non-colinear AsSc
Rb13	8c	.3.	0.12474	0.12474	0.12474		octahedron O ₆
Rb14	8c	.3.	0.24816	0.24816	0.24816		octahedron O ₆
Rb15	8c	.3.	0.36946	0.36946	0.36946		9-vertex polyhedron O ₉
Sc16	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Sc17	4a	-.3.	0	0	0		octahedron O ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.035, T = 160 K

References: [1] Harrison W.T.A., Phillips M.L.F., Clegg W., Teat S.J. (1998), J. Solid State Chem. 139, 299-303.

Eu _{2.82} [C ₆₀]	cP344	(205) <i>Pa</i> -3 – d ¹³ c ³ ba
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Eu_{2.82}C₆₀ [1], fulleride-Eu_{2.82}

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement; Eu in octahedral and tetrahedral voids (partial order, displaced from the centers).

Claves D. et al. (1998) [1]

C₆₀Eu_{2.82}

$a = 2.821$ nm, $V = 22.4496$ nm³, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(C ₆₀)1	24 <i>d</i>	1	0.0	0.25	0.25		
Eu2	24 <i>d</i>	1	0.0471	0.0471	0.2029	0.019	
Eu3	24 <i>d</i>	1	0.0471	0.0471	0.2971	0.019	
Eu4	24 <i>d</i>	1	0.0471	0.2029	0.4529	0.019	
Eu5	24 <i>d</i>	1	0.0471	0.2971	0.4529	0.019	
Eu6	24 <i>d</i>	1	0.0471	0.4529	0.2029	0.019	
Eu7	24 <i>d</i>	1	0.0471	0.4529	0.2971	0.019	
Eu8	24 <i>d</i>	1	0.1154	0.3877	0.3568		
Eu9	24 <i>d</i>	1	0.122	0.1337	0.369		
Eu10	24 <i>d</i>	1	0.2029	0.2029	0.2971	0.019	
Eu11	24 <i>d</i>	1	0.2029	0.2971	0.2971	0.019	
Eu12	24 <i>d</i>	1	0.2029	0.4529	0.4529	0.019	
Eu13	24 <i>d</i>	1	0.2971	0.4529	0.4529	0.936	
Eu14	8 <i>c</i>	.3.	0.1217	0.1217	0.1217		
Eu15	8 <i>c</i>	.3.	0.2029	0.2029	0.2029	0.019	
Eu16	8 <i>c</i>	.3.	0.2971	0.2971	0.2971	0.936	
(C ₆₀)17	4 <i>b</i>	-.3.	¹ / ₂	¹ / ₂	¹ / ₂		
(C ₆₀)18	4 <i>a</i>	-.3.	0	0	0		

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

Experimental: powder, diffractometer, X-rays, R_B = 0.103

Remarks: The atom coordinates correspond to the positions of Eu atoms and the centers of C₆₀ units. Short interatomic distances for partly occupied site(s). In table 1 of [1] the Wyckoff position of the third C₆₀ site is misprinted as 24*b* instead of 24*d*.

References: [1] Claves D., Ksari Habiles Y., Chouteau G., Touzain P. (1998), Solid State Commun. 106, 431-435.

Ba ₁₇ Sm ₁₀ Cl ₆₄	cP364	(205) <i>Pa</i> -3 – d ¹⁴ c ³ a
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Ba₁₇Sm₁₀Cl₆₄ [1]

Structural features: (Sm,Ba)₆Cl₃₇ clusters consisting of six vertex-linked distorted (Sm,Ba)Cl₈ square antiprisms around a capping Cl atom (an off-centered Cl atom surrounded by a (Sm,Ba)₆ octahedron, a Cl₁₂ cuboctahedron and a Cl₂₄ polyhedron).

Liu G., Eick H.A. (1999) [1]

Ba_{16.98}Cl₆₄Sm_{10.02}

$a = 2.1366$ nm, $V = 9.7537$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	24d	1	0.0092	0.3257	0.0168		10-vertex polyhedron Cl ₁₀
Ba2	24d	1	0.0123	0.3277	0.3219		10-vertex polyhedron Cl ₁₀
Cl3	24d	1	0.0329	0.0333	0.1673		non-collinear Sm ₂
Cl4	24d	1	0.0456	0.2893	0.1668		non-collinear Sm ₂
Cl5	24d	1	0.0528	0.1613	0.2867		non-collinear Sm ₂
Cl6	24d	1	0.0878	0.4274	0.0914		single atom Sm
Cl7	24d	1	0.0881	0.4154	0.4092		non-collinear SmBa
Cl8	24d	1	0.0894	0.425	0.2449		single atom Sm
Cl9	24d	1	0.0898	0.2481	0.4158		single atom Sm
M10	24d	1	0.1619	0.339	0.4982		tricapped trigonal prism Cl ₉
Sm11	24d	1	0.1638	0.3486	0.1662		square antiprism Cl ₈
Cl12	24d	1	0.1651	0.2826	0.2795		non-collinear Sm ₂
Cl13	24d	1	0.2402	0.2484	0.4183		single atom Sm
Cl14	24d	1	0.2468	0.4097	0.4082		tetrahedron SmBa ₃
Cl15	8c	.3.	0.1425	0.1425	0.1425		non-coplanar triangle Sm ₃
Ba16	8c	.3.	0.3195	0.3195	0.3195		10-vertex polyhedron Cl ₁₀
Cl17	8c	.3.	0.4148	0.4148	0.4148		non-coplanar triangle Ba ₃
Ba18	4a	-.3.	0	0	0		icosahedron Cl ₁₂

M10 = 0.67Sm + 0.33Ba

Experimental: single crystal, diffractometer, X-rays, R = 0.093

References: [1] Liu G., Eick H.A. (1999), J. Solid State Chem. 146, 124-128.

205
cP372

Ca₁₅(Ca_{0.17}Yb_{0.83})₁₂F₆₄

cP372

(205) *Pa*-3 – d¹⁴c⁴a

Ca₁₅(Ca₂Yb₁₀)F₆₄ [1]

Structural features: Derivative of fluorite with the cations forming pairs of (Yb,Ca)₆Ca₈ clusters (an (Yb,Ca)₆ octahedron surrounded by a Ca₈ cube) sharing a Ca vertex; F₈ cubes are replaced by FF₁₂ cuboctahedra in the cluster regions (one split F site).

Golubev A.M., Simonov V.I. (1986) [1]

Ca₁₇F₆₄Yb₁₀

a = 1.652 nm, *V* = 4.5085 nm³, *Z* = 4

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ca1	24d	1	0.0	0.0	0.333		10-vertex polyhedron F ₁₀
M2	24d	1	0.0	0.167	0.167		tricapped trigonal prism F ₉
Ca3	24d	1	0.0	0.333	0.333		10-vertex polyhedron F ₁₀
F4	24d	1	0.04	0.04	0.167		non-collinear Yb ₂
F5	24d	1	0.04	0.167	0.293		non-collinear Yb ₂
F6	24d	1	0.04	0.293	0.167		non-collinear Yb ₂
F7	24d	1	0.083	0.083	0.417		tetrahedron Ca ₃ Yb
F8	24d	1	0.083	0.25	0.417		tetrahedron Ca ₂ Yb ₂
F9	24d	1	0.083	0.417	0.25		tetrahedron Ca ₃ Yb
F10	24d	1	0.083	0.417	0.417		tetrahedron Ca ₃ Yb
M11	24d	1	0.167	0.167	0.333		tricapped trigonal prism F ₉
F12	24d	1	0.167	0.293	0.293		non-collinear Yb ₂
F13	24d	1	0.25	0.25	0.417		tetrahedron Yb ₂ Ca ₂
F14	24d	1	0.25	0.417	0.417		tetrahedron Ca ₃ Yb

F15	8c	.3.	0.157	0.157	0.157	0.5	
F16	8c	.3.	0.177	0.177	0.177	0.5	
Ca17	8c	.3.	0.333	0.333	0.333		10-vertex polyhedron F ₁₀
F18	8c	.3.	0.417	0.417	0.417		tetrahedron Ca ₄
Ca19	4a	-.3.	0	0	0		icosahedron F ₁₂

M2 = 0.833Yb + 0.167Ca; M11 = 0.833Yb + 0.167Ca

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

Remarks: Cell parameter from [2]. Idealized coordinates proposed based on crystal-chemical considerations. Short interatomic distances for partly occupied site(s).

References: [1] Golubev A.M., Simonov V.I. (1986), Sov. Phys. Crystallogr. (Engl. Transl.) 31, 281-287.
[2] Greis O., Haschke J.M. (1982), in Handbook on the Physics and Chemistry of the Rare Earths, Eds. Gschneider K.A. Jr., Eyring L.R., North-Holland, Vol. 5, Ch. 45.

205
cP492

CsNa ₂ [C ₆₀]	cP492	(205) <i>Pa</i> -3 – d ²⁰ ca
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CsNa₂C₆₀ rt [1], fulleride-CsNa₂

Structural features: Pseudo-spherical C₆₀ fullerene units (twelve 5- and twenty 6-membered rings) in a Cu-type (c.c.p.) arrangement; Cs in "octahedral", Na in "tetrahedral" voids. The fullerene units are rotated by 98° (occ.= 0.88) or 38° (occ.= 0.12) on <111>.

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

C₆₀CsNa₂

a = 1.40458 nm, *V* = 2.7710 nm³, *Z* = 4

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	24 <i>d</i>	1	0.0103	0.2524	0.4935	0.117	
C2	24 <i>d</i>	1	0.014	0.062	0.2559	0.883	
C3	24 <i>d</i>	1	0.025	0.4117	0.2352	0.117	
C4	24 <i>d</i>	1	0.0273	0.2666	0.0927	0.117	
C5	24 <i>d</i>	1	0.0314	0.2051	0.3571	0.883	
C6	24 <i>d</i>	1	0.0342	0.3935	0.2265	0.883	
C7	24 <i>d</i>	1	0.0362	0.276	0.1107	0.883	
C8	24 <i>d</i>	1	0.0519	0.1845	0.3365	0.117	
C9	24 <i>d</i>	1	0.0581	0.491	0.2455	0.883	
C10	24 <i>d</i>	1	0.0806	0.2269	0.4239	0.117	
C11	24 <i>d</i>	1	0.0953	0.3365	0.1673	0.883	
C12	24 <i>d</i>	1	0.1134	0.3832	0.1928	0.117	
C13	24 <i>d</i>	1	0.1145	0.311	0.1219	0.117	
C14	24 <i>d</i>	1	0.1273	0.1801	0.3771	0.883	
C15	24 <i>d</i>	1	0.1462	0.2039	0.4739	0.883	
C16	24 <i>d</i>	1	0.1673	0.1828	0.4528	0.117	
C17	24 <i>d</i>	1	0.2937	0.438	0.3678	0.883	
C18	24 <i>d</i>	1	0.2939	0.4381	0.3675	0.117	
C19	24 <i>d</i>	1	0.295	0.3652	0.4393	0.117	
C20	24 <i>d</i>	1	0.2949	0.3655	0.4391	0.883	
Na21	8c	.3.	0.259	0.259	0.259		
Cs22	4a	-.3.	0	0	0		octahedron C ₆

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

Experimental: powder, diffractometer, neutrons, R_p = 0.013, T = 1.6 K

Remarks: Phase stable at $T < 299$ K. Short interatomic distances for partly occupied site(s).

References: [1] Prassides K., Christides C., Thomas I.M., Mizuki J., Tanigaki K., Hirose I., Ebbesen T.W. (1994), *Science* (Washington D.C.) 263, 950-954.

205
cP536

$\text{Na}_{0.87}\text{Sr}_{1.40}\text{Mg}_{0.17}[\text{UO}_2][\text{CO}_3]_3[\text{H}_2\text{O}]_{4.66}$

cP536

(205) $Pa-3 - d^{21}c^3ba$

$\text{Na}_{0.87}\text{Sr}_{1.40}\text{Mg}_{0.17}[\text{UO}_2(\text{CO}_3)_3] \cdot 4.66\text{H}_2\text{O}$ [1]

Structural features: $\text{UO}_2(\text{CO}_3)_3$ units (UO_8 hexagonal bipyramid sharing edges with three CO_3 trigonal units in the equatorial plane); Na, Sr, Mg and H_2O between the units.

Effenberg H., Mereiter K. (1988) [1]

$\text{C}_3\text{H}_{9.33}\text{Mg}_{0.17}\text{Na}_{0.79}\text{O}_{15.67}\text{Sr}_{1.40}\text{U}$

$a = 2.029$ nm, $V = 8.3531$ nm³, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	24d	1	0.001	0.3553	0.1888		non-coplanar triangle O ₃
M2	24d	1	0.00207	0.3666	0.37055	0.75	square antiprism (OH ₂) ₄ O ₄
O3	24d	1	0.0024	0.3357	0.2491		single atom C
O4	24d	1	0.0036	0.3088	0.1455		single atom C
U5	24d	1	0.00805	0.21854	0.22309		non-coplanar O ₂
O6	24d	1	0.0149	0.2429	0.3412		single atom C
Sr7	24d	1	0.02281	0.2763	0.02608		8-vertex polyhedron O ₆ (OH ₂) ₂
C8	24d	1	0.0276	0.1832	0.3581		coplanar triangle O ₃
O9	24d	1	0.0289	0.1407	0.3096		single atom C
(OH ₂)10	24d	1	0.0344	0.4155	0.0488		single atom Mg
(OH ₂)11	24d	1	0.0362	0.4629	0.3212		non-coplanar Sr ₂
O12	24d	1	0.0389	0.1669	0.4168		single atom C
O13	24d	1	0.0799	0.419	0.4629		single atom C
O14	24d	1	0.0944	0.2193	0.2139		single atom U
O15	24d	1	0.1065	0.3165	0.497		single atom C
C16	24d	1	0.1211	0.3775	0.4837		non-coplanar triangle O ₃
(OH ₂)17	24d	1	0.1372	0.3591	0.329		trigonal bipyramid Sr ₂ (OH ₂) ₂ O
(OH ₂)18	24d	1	0.1629	0.3386	0.189		4-vertex polyhedron O ₂ Na(OH ₂)
O19	24d	1	0.1833	0.3902	0.4918		single atom C
O20	24d	1	0.2169	0.2688	0.4204		single atom U
O21	24d	1	0.3267	0.4949	0.4136		single atom C
Na22	8c	.3.	0.2111	0.2111	0.2111	0.82	monocapped trigonal prism (OH ₂) ₄ O ₃
(OH ₂)23	8c	.3.	0.2728	0.2728	0.2728		single atom Na
(OH ₂)24	8c	.3.	0.3489	0.3489	0.3489		single atom (OH ₂)
Mg25	4b	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron (OH ₂) ₆
Na26	4a	-.3.	0	0	0		octahedron O ₆

$\text{M2} = 0.533\text{Sr} + 0.467\text{Na}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.036$, $T = 295$ K

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

References: [1] Effenberg H., Mereiter K. (1988), *Acta Crystallogr. C* 44, 1172-1175.

Si[P ₂ O ₇]	cP1080	(205) <i>Pa</i> -3 – d ⁴³ c ⁵ ba
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SiP₂O₇ form X [1]

Structural features: P₂O₇ units (two vertex-linked PO₄ tetrahedra) share vertices with SiO₆ octahedra to form a 3D-framework.

Tillmanns E. et al. (1973) [1]

O₇P₂Si

$a = 2.2418 \text{ nm}$, $V = 11.2665 \text{ nm}^3$, $Z = 108$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>d</i>	1	0.0004	0.1099	0.3797		non-colinear PSi
O2	24 <i>d</i>	1	0.002	0.2638	0.1187		non-colinear PSi
Si3	24 <i>d</i>	1	0.0032	0.1779	0.3393		octahedron O ₆
O4	24 <i>d</i>	1	0.0048	0.2457	0.2997		non-colinear PSi
Si5	24 <i>d</i>	1	0.0054	0.3372	0.4981		octahedron O ₆
O6	24 <i>d</i>	1	0.0063	0.4235	0.008		non-colinear PSi
O7	24 <i>d</i>	1	0.007	0.3546	0.3114		non-colinear P ₂
O8	24 <i>d</i>	1	0.0077	0.0463	0.0979		non-colinear PSi
O9	24 <i>d</i>	1	0.0077	0.0692	0.2067		non-colinear PSi
Si10	24 <i>d</i>	1	0.008	0.3355	0.1519		octahedron O ₆
O11	24 <i>d</i>	1	0.0103	0.463	0.2746		non-colinear PSi
O12	24 <i>d</i>	1	0.0111	0.4086	0.1783		non-colinear PSi
O13	24 <i>d</i>	1	0.0133	0.4403	0.3804		non-colinear PSi
O14	24 <i>d</i>	1	0.0213	0.3373	0.4201		non-colinear PSi
O15	24 <i>d</i>	1	0.0214	0.1829	0.4893		non-colinear P ₂
P16	24 <i>d</i>	1	0.0241	0.0472	0.3719		tetrahedron O ₄
P17	24 <i>d</i>	1	0.0347	0.4618	0.2117		tetrahedron O ₄
P18	24 <i>d</i>	1	0.0381	0.3789	0.3708		tetrahedron O ₄
P19	24 <i>d</i>	1	0.0396	0.128	0.2149		tetrahedron O ₄
O20	24 <i>d</i>	1	0.0418	0.1436	0.2805		non-colinear PSi
O21	24 <i>d</i>	1	0.048	0.3592	0.0894		non-colinear PSi
O22	24 <i>d</i>	1	0.0719	0.1942	0.3726		non-colinear PSi
O23	24 <i>d</i>	1	0.0769	0.3185	0.1838		non-colinear PSi
O24	24 <i>d</i>	1	0.1009	0.1279	0.1879		non-colinear PSi
O25	24 <i>d</i>	1	0.1024	0.4659	0.2125		non-colinear PSi
O26	24 <i>d</i>	1	0.1048	0.3829	0.3575		non-colinear PSi
P27	24 <i>d</i>	1	0.1337	0.2965	0.209		tetrahedron O ₄
P28	24 <i>d</i>	1	0.1354	0.2141	0.377		tetrahedron O ₄
O29	24 <i>d</i>	1	0.1386	0.3185	0.2707		non-colinear PSi
O30	24 <i>d</i>	1	0.1418	0.281	0.3728		non-colinear PSi
O31	24 <i>d</i>	1	0.142	0.2289	0.2054		non-colinear PSi
O32	24 <i>d</i>	1	0.1629	0.1925	0.4345		non-colinear PSi
O33	24 <i>d</i>	1	0.1636	0.4247	0.4924		non-colinear PSi
Si34	24 <i>d</i>	1	0.1705	0.3432	0.3388		octahedron O ₆
O35	24 <i>d</i>	1	0.1714	0.187	0.323		non-colinear P ₂
O36	24 <i>d</i>	1	0.1779	0.3148	0.4997		non-colinear P ₂
O37	24 <i>d</i>	1	0.1938	0.4065	0.3003		non-colinear PSi
P38	24 <i>d</i>	1	0.2035	0.3741	0.4728		tetrahedron O ₄
O39	24 <i>d</i>	1	0.2054	0.3674	0.4063		non-colinear PSi
P40	24 <i>d</i>	1	0.2166	0.4709	0.301		tetrahedron O ₄
O41	24 <i>d</i>	1	0.2361	0.3041	0.3217		non-colinear PSi

O42	24 <i>d</i>	1	0.2825	0.4702	0.3125	non-colinear PSi
O43	24 <i>d</i>	1	0.3524	0.3833	0.4409	non-colinear PSi
P44	8 <i>c</i>	.3.	0.0398	0.0398	0.0398	tetrahedron O ₄
Si45	8 <i>c</i>	.3.	0.166	0.166	0.166	octahedron O ₆
P46	8 <i>c</i>	.3.	0.2997	0.2997	0.2997	tetrahedron O ₄
O47	8 <i>c</i>	.3.	0.3408	0.3408	0.3408	colinear P ₂
P48	8 <i>c</i>	.3.	0.3804	0.3804	0.3804	tetrahedron O ₄
Si49	4 <i>b</i>	-.3.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	octahedron O ₆
O50	4 <i>a</i>	-.3.	0	0	0	colinear P ₂

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

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

References: [1] Tillmanns E., Gebert W., Baur W.H. (1973), J. Solid State Chem. 7, 69-84.