

Space group (217) *I*-43*m*217
*cI*10

SiF ₄	<i>cI</i> 10	(217) <i>I</i> -43 <i>m</i> – ca
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SiF₄ [2], Strukturbericht notation D1₂Structural features: Single SiF₄ tetrahedra in a W-type (b.c.c.) arrangement.

Mootz D., Korte L. (1984) [1]

F₄Si $a = 0.5476 \text{ nm}$, $V = 0.1642 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	8 <i>c</i>	.3 <i>m</i>	0.1624	0.1624	0.1624		single atom Si
Si2	2 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron F ₄

Experimental: single crystal, diffractometer, X-rays, $R = 0.029$, $T = 156 \text{ K}$

References: [1] Mootz D., Korte L. (1984), Z. Naturforsch. B 39, 1295-1299. [2] Natta G. (1930), Gazz. Chim. Ital. 60, 911-922.

217
*cI*16

(Li _{0.62} B _{0.38}) ₄ B _{0.5}	<i>cI</i> 16	(217) <i>I</i> -43 <i>m</i> – c ²
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Li₅B₄ [1]Structural features: BB₃ triangles and (Li,B)₅ trigonal bipyramids (high degree of disorder).

Wang F.E. et al. (1978) [1]

B₂Li_{2.50} $a = 0.493 \text{ nm}$, $V = 0.1198 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
B1	8 <i>c</i>	.3 <i>m</i>	0.075	0.075	0.075	0.125	
M2	8 <i>c</i>	.3 <i>m</i>	0.325	0.325	0.325		

 $M2 = 0.625\text{Li} + 0.375\text{B}$ Transformation from published data: -*x*, -*y*, -*z*

Experimental: bulk sample, diffractometer, neutrons

Remarks: The structure was analyzed jointly on X-ray and neutron diffraction data; ¹¹B isotope was used for the neutron diffraction. Average structure; two different Li and two different B non-cubic environments were identified by NMR. A model for short-range order is proposed in space group (160) *R*3*m*. Short interatomic distances for partly occupied site(s). In table 2 of [1] the space group is misprinted as *I*23 instead of *I*-43*m* (given elsewhere). According to [2] several peaks in the powder pattern are misinterpreted and a better agreement is observed for a structure proposal in space group (194) *P*6₃/*mmc*.

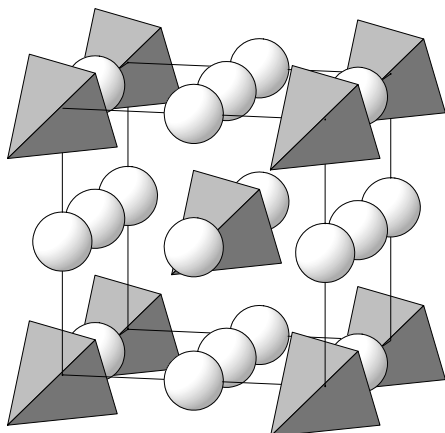
References: [1] Wang F.E., Mitchell M.A., Sutula R.A., Holden J.R., Bennett L.H. (1978), J. Less-Common Met. 61, 237-251. [2] Wörle M., Nesper R. (2000), Angew. Chem. Int. Ed. 39, 2349-2353.

217
*cI*16

Tl ₃ VS ₄	<i>cI</i> 16	(217) <i>I</i> -43 <i>m</i> – cba
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Tl₃VS₄ [2]; (NH₄)₃SbS₄ [3]

Structural features: Single VS₄ tetrahedra in a W-type (b.c.c.) arrangement. See Fig. II.5.

Fig. II.5. **Tl₃VS₄**

Arrangement of VS₄ tetrahedra and Tl atoms.

Vlasse M., Fournes L. (1978) [1]

S₄Tl₃V

$a = 0.7504 \text{ nm}$, $V = 0.4226 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	8c	.3m	0.167	0.167	0.167		single atom V
Tl2	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron S ₄
V3	2a	-43m	0	0	0		tetrahedron S ₄

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

References: [1] Vlasse M., Fournes L. (1978), C. R. Seances Acad. Sci., Ser. C 287, 47-49. [2] Crevecoeur C. (1964), Acta Crystallogr. 17, 757. [3] Graf H., Schäfer H., Weiss A. (1969), Z. Naturforsch. B 24, 1345-1346.

217
c/16

ZrFe_{5.5}SiB_{0.5}

$c/16$

(217) $I-43m - cba$

Zr₂Fe₁₂Si₂B [1]

Structural features: Distorted substitution derivative of W (prototype for a b.c.c. atom arrangement).

Khan Y. (1992) [1]

B_{0.48}Fe_{5.58}Si_{0.94}Zr

$a = 0.5852 \text{ nm}$, $V = 0.2004 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	8c	.3m	0.19	0.19	0.19		single atom Fe
M2	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Fe ₄
M3	2a	-43m	0	0	0		tetrahedron Fe ₄

M1 = 0.77Fe + 0.12B + 0.11Si; M2 = 0.667Fe + 0.333Zr; M3 = 0.5Fe + 0.5Si

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

Experimental: powder, film, X-rays

Remarks: Phase observed in melt-spun ribbons. Short interatomic distances: $d(\text{M1-M3}) = 0.193 \text{ nm}$. We adjusted the number of Fe atoms in the chemical formula in agreement with the proposed structure.

References: [1] Khan Y. (1992), Phys. Status Solidi A 130, K7-K12.

217
cI22

$\text{Na}_3\text{Pt}_4\text{Ge}_4$	<i>cI22</i>	(217) $I-43m - c^2b$
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$\text{Na}_6\text{Pt}_8\text{Ge}_8$ [1]; $\text{Ca}_6\text{Ni}_8\text{Ga}_8$ [2]

Structural features: Pt_4Ge_4 tetrahedron stars (a Pt_4 inner tetrahedron surrounded by a Ge_4 outer tetrahedron) are interconnected via additional Ge-Pt bonds to form a 3D-framework. See Fig. II.6.

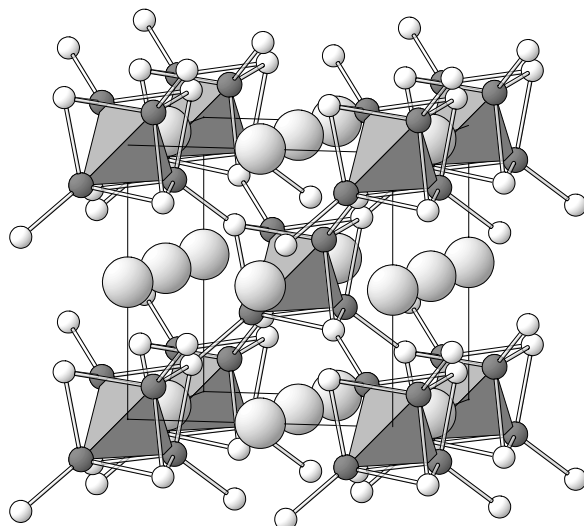


Fig. II.6. **$\text{Na}_6\text{Pt}_8\text{Ge}_8$**

Arrangement of $\text{Pt}_4\text{Ge}_4\text{Ge}_4$ extended tetrahedron stars (Pt atoms dark, Ge atoms light) and Na atoms (large).

Thronberens W., Schuster H.U. (1979) [1]

$\text{Ge}_4\text{Na}_3\text{Pt}_4$

$a = 0.7614 \text{ nm}$, $V = 0.4414 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pt1	8c	.3m	0.1366	0.1366	0.1366		tetrahedron Ge_4
Ge2	8c	.3m	0.3136	0.3136	0.3136		tetrahedron Pt_4
Na3	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		20-vertex polyhedron $\text{Ge}_8\text{Pt}_8\text{Na}_4$

Experimental: single crystal, diffractometer, X-rays, $R = 0.045$

References: [1] Thronberens W., Schuster H.U. (1979), Z. Naturforsch. B 34, 781-783. [2] Kim S.G., Gryn Y.N., Gladyshevskii E.I. (1983), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1983(8), 13-15.

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cI24

Ta_2O	<i>cI24</i>	(217) $I-43m - c^2ba$
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Ta_2O [1]

Structural features: Ta forms a W-type (b.c.c.) framework; O in linear coordination.

Steeb S., Renner J. (1965) [1]

OTa₂

$a = 0.668 \text{ nm}$, $V = 0.2981 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	8c	.3m	0.125	0.125	0.125		colinear Ta ₂
Ta2	8c	.3m	0.25	0.25	0.25		single atom O
Ta3	6b	-42.m	0	1/2	1/2		tetrahedron O ₄
Ta4	2a	-43m	0	0	0		tetrahedron O ₄

Experimental: thin film, electron diffraction, T = 653 K

Remarks: We deduced the space group from the coordinates of all atoms in the unit cell. Short interatomic distances: d(Ta-O) = 0.145 nm. An orthorhombic cell reported in [2] and a tetragonal cell reported in [3] are stated to be wrong.

References: [1] Steeb S., Renner J. (1965), J. Less-Common Met. 9, 181-189. [2] Wasilewski R.J. (1953), J. Am. Chem. Soc. 75, 1001-1002. [3] Norman N. (1962), J. Less-Common Met. 4, 52-61.

217
cI40

K[IO ₃]	cI40	(217) <i>I</i> -43m – gcba
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KIO₃ [1], perovskite family

Structural features: IO₆ octahedra share vertices to form a 3D-framework; K in cuboctahedral voids. Distortions towards single :IO₃ ψ-tetrahedra.

Ozerov R.P. et al. (1962) [1]

KO₃

$a = 0.8938 \text{ nm}$, $V = 0.7140 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	..m	0.25	0.25	0.0		non-colinear I ₂
I2	8c	.3m	0.24	0.24	0.24		octahedron O ₆
K3	6b	-42.m	0	1/2	1/2		cuboctahedron O ₁₂
K4	2a	-43m	0	0	0		cuboctahedron O ₁₂

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

Experimental: single crystal, diffractometer, neutrons

Remarks: Average structure. Space groups (199) *I*2₁3, (204) *Im*-3, (211) *I*432, and (229) *Im*-3m were tested and rejected, however, space group (197) *I*23 could not be excluded. We assigned an arbitrary value to the displacement of the iodine atoms along <111> since the correct space group for an undistorted structure would be (221) *Pm*-3m with 1/8 cell volume. The authors state that also the O atoms are displaced from the ideal positions, and that the real structure is rhombohedral, $a = 0.8938 \text{ nm}$, $\alpha = 89.50^\circ$, space group (160) *R*3m.

References: [1] Ozerov R.P., Rannev N.V., Pakhomov V.I., Rez I.S., Zhdanov G.S. (1962), Sov. Phys. Crystallogr. (Engl. Transl.) 7, 499-501.

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cI40

Li ₃ AsSe ₄ [NH ₃] ₁₂	cI40	(217) <i>I</i> -43m – gcba
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[Li(NH₃)₄]₃AsSe₄ [1]

Structural features: Single AsSe₄ tetrahedra and Li(NH₃)₄ tetrahedral units in a AuSb₃-type arrangement.

Korber N., Grothe M. (2001) [1]

AsH₃₆Li₃N₁₂Se₄

$a = 1.05038 \text{ nm}$, $V = 1.1589 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24g	..m	0.3872	0.3872	0.1191		single atom Li
Se2	8c	.3m	0.12788	0.12788	0.12788		single atom As
Li3	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron N ₄
As4	2a	-43m	0	0	0		tetrahedron Se ₄
H5	48h	1	0.113	0.322	0.391		
H6	24g	..m	0.401	0.401	0.181		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.013$, $T = 123 \text{ K}$

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

References: [1] Korber N., Grothe M. (2001), Z. Kristallogr., New Cryst. Struct. 216, 177-178.

217
cI44

U ₂ F ₉	cI44	(217) <i>I</i> -43m – gec
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U₂F₉ [2]

Structural features: UF₆F₃ tricapped trigonal prisms share atoms to form a 3D-framework.

Howard C.J. et al. (1982) [1]

F₉U₂

$a = 0.84716 \text{ nm}$, $V = 0.6080 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	24g	..m	0.2078	0.2078	0.4425		single atom U
F2	12e	2.mm	0.2262	0	0		non-colinear U ₂
U3	8c	.3m	0.1884	0.1884	0.1884		tricapped trigonal prism F ₉

Experimental: powder, diffractometer, neutrons, $R_B = 0.030$

Remarks: We took the space group and Wyckoff positions from [2].

References: [1] Howard C.J., Taylor J.C., Waugh A.B. (1982), J. Solid State Chem. 45, 396-398. [2] Zachariasen W.H. (1948), Acta Crystallogr. 1, 265-268.

217
cI46

Pd ₁₆ S ₇	cI46	(217) <i>I</i> -43m – gc ² b
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Pd₃₂S₁₄ [1]

Structural features: SPd₆ trigonal prisms and flattened SPd₄ tetrahedra share atoms to form a 3D-framework. Alternatively: S-Pd-S linear units share atoms to form a 3D-framework; additional Pd in trigonal voids (displaced out of the plane).

Romming C., Rost E. (1976) [1]

Pd_{16}S_7

$a = 0.8954 \text{ nm}$, $V = 0.7179 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pd1	24g	..m	0.16979	0.16979	0.41829		7-vertex polyhedron S_2Pd_5
Pd2	8c	.3m	0.11624	0.11624	0.11624		tricapped trigonal prism S_3Pd_6
S3	8c	.3m	0.34392	0.34392	0.34392		trigonal prism Pd_6
S4	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Pd_4

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

Remarks: Identical to the phase called Pd_{22}S in [3]. It is not clear if the atom coordinates reported in [2] were determined on the binary or a ternary phase ($\text{Cu}_3\text{Pd}_{13}\text{S}_7$).

References: [1] Romming C., Rost E. (1976), Acta Chem. Scand. A 30, 425-428. [2] Matkovic P., El Boragy M., Schubert K. (1976), J. Less-Common Met. 50, 165-176. [3] Gronvold F., Rost E. (1956), Acta Chem. Scand. 10, 1620-1634.

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cI46

$(\text{Cu}_{0.75}\text{Pd}_{0.25})_4\text{Pd}_{12}\text{S}_7$	cI46	(217) $I-43m - gc^2b$
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$\text{Pd}_{13}\text{Cu}_3\text{S}_7$ [1]

Structural features: $\text{S}(\text{Pd}_3(\text{Cu},\text{Pd})_3)$ trigonal prisms and flattened SPd_4 tetrahedra share atoms to form a 3D-framework. Alternatively: S-Pd-S linear units share atoms to form a 3D-framework; (Cu,Pd) in trigonal voids (displaced out of the plane). Ordering variant of Pd_{16}S_7 .

Matkovic P. et al. (1976) [1]

$\text{Cu}_3\text{Pd}_{13}\text{S}_7$

$a = 0.8874 \text{ nm}$, $V = 0.6988 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Pd1	24g	..m	0.1696	0.1696	0.4149		non-colinear S_2
M2	8c	.3m	0.1168	0.1168	0.1168		tricapped trigonal prism $\text{S}_3\text{Pd}_3\text{Cu}_3$
S3	8c	.3m	0.3476	0.3476	0.3476		trigonal prism Pd_3Cu_3
S4	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Pd_4

$\text{M2} = 0.75\text{Cu} + 0.25\text{Pd}$

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

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

References: [1] Matkovic P., El Boragy M., Schubert K. (1976), J. Less-Common Met. 50, 165-176.

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cI46

$(\text{Cs}_{0.7}\text{Ti}_{0.3})\text{Hg}_{5.5}\text{As}_4\text{S}_{12}$	cI46	(217) $I-43m - gdca$
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$(\text{Hg},\text{Cu},\text{Zn},\text{Fe},\text{Ti},\square)_6(\text{Cs},\text{Ti},\square)(\text{As},\text{Sb})_4\text{S}_{12}$ [2], galkhaite

Structural features: Single $(\text{As},\text{Sb})\text{S}_3$ ψ -tetrahedra.

Chen T.T., Szymanski J.T. (1981) [1]

$\text{As}_{3.93}\text{Cs}_{0.59}\text{Cu}_{0.86}\text{Fe}_{0.06}\text{Hg}_{4.24}\text{S}_{12}\text{Sb}_{0.07}\text{Ti}_{0.28}\text{Zn}_{0.52}$

$a = 1.0365 \text{ nm}$, $V = 1.1135 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	..m	0.11174	0.11174	0.33751		non-coplanar triangle AsHg ₂
M2	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	0.955	tetrahedron S ₄
M3	8c	.3m	0.25475	0.25475	0.25475		non-coplanar triangle S ₃
M4	2a	-43m	0	0	0	0.815	pseudo Frank-Kasper S ₁₂ As ₈

M2 = 0.74Hg + 0.15Cu + 0.09Zn + 0.01Fe + 0.01Tl; M3 = 0.983As + 0.017Sb; M4 = 0.73Cs + 0.27Tl

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

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

Remarks: Natural specimen from the Getchel mine, Humboldt County, Nevada. Composition (Hg_{4.42}Cu_{0.88}Zn_{0.48})Tl_{0.21}Cs_{0.67}(As_{3.55}Sb_{0.04})S₁₂ from electron microprobe analysis. Supersedes a structure proposal for so-called HgAsS₂ where the atoms in Wyckoff position 2a are statistically replaced by As₄ tetrahedra [3]. In [4] the occupations of the sites in Wyckoff positions 2a and 8c are interchanged with respect to the original report [3].

References: [1] Chen T.T., Szymanski J.T. (1981), Can. Mineral. 19, 571-581. [2] Divjakovic V., Nowacki W. (1975), Z. Kristallogr. 142, 262-270. [3] Kaplunnik L.N., Pobedinskaya E.A., Belov N.V. (1975), Dokl. Akad. Nauk SSSR 225, 561-563. [4] (1977), Structure Reports 41A, 21.

217
cI46

Zn₄B₆O₁₃

cI46

(217) I-43m – gdca

Zn₄B₆O₁₃ [2]; Ca₄Al₆O₁₃ [4], zeolite SOD

Structural features: BO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by OZn₄ tetrahedra. See Fig. II.7.

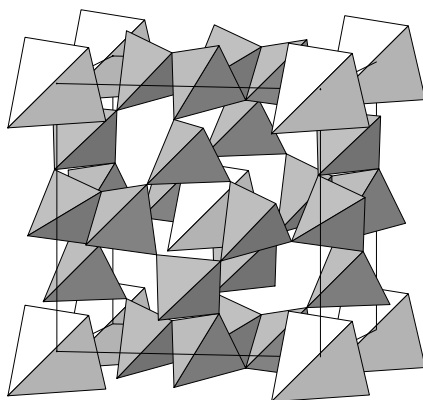


Fig. II.7. **Zn₄B₆O₁₃**

Arrangement of BO₄ (dark) and OZn₄ (light) tetrahedra.

Smith Verdier P., Garcia Blanco S. (1980) [1]

B₆O₁₃Zn₄

a = 0.74659 nm, *V* = 0.4161 nm³, *Z* = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	..m	0.1398	0.1398	0.41469		non-colinear B ₂
B2	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
Zn3	8c	.3m	0.15328	0.15328	0.15328		tetrahedron O ₄
O4	2a	-43m	0	0	0		tetrahedron Zn ₄

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

Remarks: Preliminary data in [3].

References: [1] Smith Verdier P., Garcia Blanco S. (1980), Z. Kristallogr. 151, 175-177. [2] Smith P., Garcia Blanco S., Rivoir L. (1964), Z. Kristallogr. 119, 375-383. [3] Smith P., Garcia Blanco S., Rivoir L. (1961), Z. Kristallogr. 115, 460-463. [4] Ponomarev V.I., Kheiker D.M., Belov N.V. (1971), Sov. Phys. Crystallogr. (Engl. Transl.) 15, 799-801.

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cI46

Na ₁₀ CaSn ₁₂	cI46	(217) <i>I</i> -43m – gdca
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Na₁₀CaSn₁₂ [1]

Structural features: CaSn₁₂ truncated tetrahedra are separated by Na atoms forming sodalite-type cages (14-face truncated octahedra).

Bobev S., Sevov S.C. (2001) [1]

CaNa₁₀Sn₁₂

$a = 1.11847$ nm, $V = 1.3992$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	24g	..m	0.09068	0.09068	0.278		tricapped trigonal prism Sn ₃ Na ₅ Ca
Na2	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron Sn ₄
Na3	8c	.3m	0.3061	0.3061	0.3061		16-vertex polyhedron Sn ₉ CaNa ₆
Ca4	2a	-43m	0	0	0		16-vertex Frank-Kasper Sn ₁₂ Na ₄

Experimental: single crystal, diffractometer, X-rays, R = 0.013, T = 294 K

References: [1] Bobev S., Sevov S.C. (2001), Inorg. Chem. 40, 5361-5364.

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cI46

Na ₄ (Al _{0.5} Si _{0.5}) ₆ IO ₁₂	cI46	(217) <i>I</i> -43m – gdca
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Ca₈Al₁₂O₂₄I₂ [1], zeolite SOD-I; Ca₈Al₁₂O₂₄(SO₄)₂ (see remark), ye'elemite, zeolite SOD-SO₄; Cd₄P₆N₁₂S [4]

Structural features: (Al,Si)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by I; Na near the centers of 6-rings.

Beagley B. et al. (1982) [1]

Al₃INa₄O₁₂Si₃

$a = 0.9008$ nm, $V = 0.7309$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	..m	0.1428	0.1428	0.4508		non-colinear Al ₂
M2	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
Na3	8c	.3m	0.198	0.198	0.198		non-coplanar triangle O ₃
I4	2a	-43m	0	0	0		tetrahedron Na ₄

M2 = 0.5Al + 0.5Si

Experimental: powder, film, X-rays

Remarks: Space group (218) *P*-43n was tested and rejected. The description of Ca₈Al₁₂O₂₄(SO₄)₂ (O of the sulfate not located) in space group (197) *I*23 in [2] does not take into consideration all symmetry elements of the proposed structure; the correct space group was used in [3].

References: [1] Beagley B., Henderson C.M.B., Taylor D. (1982), Mineral. Mag. 46, 459-464. [2] Kondo R. (1965), Yogyo Kyokaishi 73, 1-8. [3] Brenchley M.E., Weller M.T. (1992), J. Mater. Chem. 2, 1003-1005. [4] Ronis J., Krasnikov V., Bundars B., Vitola A., Millers T. (1988), Latv. PSR Zinat. Akad. Vestis, Kim. Ser. 1988, 643-646.

217
cI50

NaTh ₂ F ₉			cI50			(217) <i>I</i> -43 <i>m</i> – gecb	
NaTh₂F₉ [2]							
Structural features: ThF ₆ F ₃ tricapped trigonal prisms share atoms to form a 3D-framework; Na in octahedral voids.							
Zachariasen W.H. (1949) [1]							
F ₉ NaTh ₂							
<i>a</i> = 0.8723 nm, <i>V</i> = 0.6637 nm ³ , <i>Z</i> = 4							
site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	24 <i>g</i>	.. <i>m</i>	0.19	0.19	0.465		coplanar triangle NaTh ₂
F2	12 <i>e</i>	2.. <i>mm</i>	0.235	0	0		coplanar triangle NaTh ₂
Th3	8 <i>c</i>	.. <i>3m</i>	0.187	0.187	0.187		tricapped trigonal prism F ₉
Na4	6 <i>b</i>	-42.. <i>m</i>	0	¹ / ₂	¹ / ₂	0.667	octahedron F ₆

Experimental: powder, film, X-rays

Remarks: F positions from crystal-chemical considerations.

References: [1] Zachariasen W.H. (1949), Acta Crystallogr. 2, 390-393. [2] Zachariasen W.H. (1948), Acta Crystallogr. 1, 265-268.

217
cI52

Ca ₄ (Al _{0.67} Si _{0.33}) ₆ O ₁₂ [OH] ₄			cI52			(217) <i>I</i> -43 <i>m</i> – gdc ²	
Ca₈Al₈Si₄O₂₄(OH)₈ [2], bicchulite, zeolite SOD-OH							
Structural features: (Al,Si)O ₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); Ca and OH opposite 6-rings.							
Dann S.E. et al. (1996) [1]							
Al ₄ Ca ₄ H ₄ O ₁₆ Si ₂							
<i>a</i> = 0.88317 nm, <i>V</i> = 0.6889 nm ³ , <i>Z</i> = 2							
site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	.. <i>m</i>	0.35925	0.35925	0.07713		non-colinear Al ₂
M2	12 <i>d</i>	-4.. <i></i>	¹ / ₄	¹ / ₂	0		tetrahedron O ₄
O3	8 <i>c</i>	.. <i>3m</i>	0.11736	0.11736	0.11736		non-coplanar triangle Ca ₃
Ca4	8 <i>c</i>	.. <i>3m</i>	0.35627	0.35627	0.35627		octahedron O ₆
H5	24 <i>g</i>	.. <i>m</i>	0.1885	0.1885	0.1509	0.333	

M2 = 0.667Al + 0.333Si

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

Experimental: powder, diffractometer, neutrons, R_p = 0.027

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The data from [2] are also reported in [3].

References: [1] Dann S.E., Mead P.J., Weller M.T. (1996), Inorg. Chem. 35, 1427-1428. [2] Sahl K., Chatterjee N.D. (1977), Naturwissenschaften 64, 94. [3] Sahl K., Chatterjee N.D. (1977), Z. Kristallogr. 146, 35-41.

217
cI52

Cu_5Zn_8	<i>cI52</i>	(217) <i>I-43m</i> – <i>gec</i> ²
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Cu_5Zn_8 [2], γ -brass, Strukturbericht notation D8₂; Cu_5Cd_8 [1]

Structural features: 26-atom γ brass-type nested polyhedra units (a Zn_4 inner tetrahedron surrounded by a Cu_4 outer tetrahedron, a Cu_6 octahedron and a Zn_{12} cuboctahedron) in a W-type (b.c.c.) arrangement. See Fig. II.8.

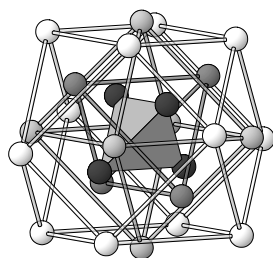


Fig. II.8. **Cu_5Zn_8**

26-atom (γ brass-type) nested polyhedra unit: Zn_4 inner tetrahedron + Cu_4 outer tetrahedron + Cu_6 octahedron + Zn_{12} cuboctahedron.

Brandon J.K. et al. (1974) [1]

Cu_5Zn_8

$a = 0.8878 \text{ nm}$, $V = 0.6998 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	24g	$\dots m$	0.3128	0.3128	0.0366		pentacapped trigonal prism Cu_6Zn_5
Cu2	12e	$2.mmm$	0.3558	0	0		pseudo Frank-Kasper $\text{Zn}_{10}\text{Cu}_3$
Zn3	8c	$.3m$	0.1089	0.1089	0.1089		icosahedron Cu_6Zn_6
Cu4	8c	$.3m$	0.328	0.328	0.328		pseudo Frank-Kasper $\text{Zn}_{10}\text{Cu}_3$

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

References: [1] Brandon J.K., Brizard R.Y., Chieh P.C., McMillan R.K., Pearson W.B. (1974), Acta Crystallogr. B 30, 1412-1417. [2] (1931), Strukturberichte 1, 497.

217
cI52

$\text{Zn}_9(\text{Zn}_{0.5}\text{Fe}_{0.5})_2\text{Fe}_2$	<i>cI52</i>	(217) <i>I-43m</i> – <i>gec</i> ²
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$\text{Fe}_3\text{Zn}_{10}$ [2], γ -brass, Strukturbericht notation D8₁

Structural features: 26-atom γ brass-type nested polyhedra units (a $(\text{Fe},\text{Zn})_4$ inner tetrahedron surrounded by a Fe_4 outer tetrahedron, a Zn_6 octahedron and a Zn_{12} cuboctahedron) in a W-type (b.c.c.) arrangement. Ordering variant of Cu_5Zn_8 of ideal composition $\text{A}_9\text{A}'_2\text{A}''_2$.

Brandon J.K. et al. (1974) [1]

$\text{Fe}_3\text{Zn}_{10}$

$a = 0.9018 \text{ nm}$, $V = 0.7334 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zn1	24g	..m	0.3045	0.3045	0.0491		15-vertex Frank-Kasper Fe ₃ Zn ₁₂
Zn2	12e	2.mm	0.3538	0	0		pseudo Frank-Kasper Fe ₄ Zn ₉
M3	8c	.3m	0.1028	0.1028	0.1028		icosahedron Fe ₆ Zn ₆
Fe4	8c	.3m	0.3327	0.3327	0.3327		icosahedron Fe ₃ Zn ₉

M3 = 0.5Fe + 0.5Zn

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

Remarks: Additional reflections indicate a possible superstructure with 64-fold cell volume (a = 3.6 nm).

References: [1] Brandon J.K., Brizard R.Y., Chieh P.C., McMillan R.K., Pearson W.B. (1974), Acta Crystallogr. B 30, 1412-1417. [2] (1931), Strukturberichte 1, 499.

217
cI54

Ba ₄ (Ga _{0.36} Sn _{0.64}) ₂₂ Sn	cI54	(217) I-43m – gdc ² a
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Ba₈Ga₁₆Sn₃₀ [1], clathrate I

Structural features: Ga and Sn form a tetrahedral 3D-framework; Ba in 20-vertex polyhedra.

Eisenmann B. et al. (1986) [1]

Ba₄Ga_{8.70}Sn_{14.30}

a = 1.15945 nm, V = 1.5587 nm³, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24g	..m	0.0841	0.0841	0.3509		tetrahedron GaSn ₃
M2	12d	-4..	1/4	1/2	0		tetrahedron Sn ₄
M3	8c	.3m	0.1344	0.1344	0.1344		tetrahedron Sn ₄
Ba4	8c	.3m	0.3154	0.3154	0.3154		pseudo Frank-Kasper Ga ₄ Sn ₁₆
Sn5	2a	-43m	0	0	0		tetrahedron Ga ₄

M1 = 0.67Sn + 0.33Ga; M2 = 0.65Sn + 0.35Ga; M3 = 0.66Ga + 0.34Sn

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

Experimental: single crystal, diffractometer, X-rays, R = 0.073

References: [1] Eisenmann B., Schäfer H., Zagler R. (1986), J. Less-Common Met. 118, 43-55.

217
cI54

HgAsS ₂	cI54	(217) I-43m – gdc ² a
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HgAsS₂ [1], galkhaite

Structural features: Ignoring partly occupied sites, HgS₄ tetrahedra and :AsS₃ ψ-tetrahedra share vertices to form a 3D-framework. Disordered arrangement of additional As atoms and As₄ tetrahedra.

Kaplunnik L.N. et al. (1975) [1]

AsHgS₂

a = 1.0422 nm, V = 1.1320 nm³, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	..m	0.1127	0.1127	0.3382		tetrahedron As ₂ Hg ₂
Hg2	12d	-4..	1/4	1/2	0		tetrahedron S ₄
As3	8c	.3m	0.07	0.07	0.07	0.333	

As4	8c	.3m	0.2564	0.2564	0.2564	non-coplanar triangle S ₃
As5	2a	-43m	0	0	0	0.667

Experimental: single crystal, diffractometer, X-rays, R = 0.098

Remarks: Natural specimen from Galkhai, Yakutiya. Composition (Hg_{0.74}Cu_{0.17}Zn_{0.14}Tl_{0.01})₂(As_{0.98}Sb_{0.02})S_{2.01} from chemical analysis. Short interatomic distances for partly occupied site(s). The structure was redetermined in [2] (no As₄ tetrahedra found).

References: [1] Kaplunnik L.N., Pobedinskaya E.A., Belov N.V. (1975), Dokl. Akad. Nauk SSSR 225, 561-563. [2] Chen T.T., Szymanski J.T. (1981), Can. Mineral. 19, 571-581.

217
cI56

Na ₃ SbO ₃	cI56	(217) <i>I</i> -43m – g ² c
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Na₃SbO₃ [1]

Structural features: Single :SbO₃ ψ-tetrahedra. Derivative of NaCl with ¹/₄ of the anion sites vacant, [Na₃Sb][O₃□].

Stöver H.D., Hoppe R. (1980) [1]

Na₃O₃Sb

a = 0.9564 nm, *V* = 0.8748 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24g	..m	0.1346	0.1346	0.3431		single atom Sb
Na2	24g	..m	0.3767	0.3767	0.1035		square pyramid O ₅
Sb3	8c	.3m	0.1458	0.1458	0.1458		non-coplanar triangle O ₃

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

Remarks: In the abstracts of [1] the space group is misprinted as *F*-43m instead of *I*-43m (given on page 140).

References: [1] Stöver H.D., Hoppe R. (1980), Z. Anorg. Allg. Chem. 468, 137-147.

217
cI56

(Na _{0.875} [H ₂ O] _{0.125}) ₄ (Al _{0.48} Si _{0.52}) ₆ S _{2.25} O ₁₂	cI56	(217) <i>I</i> -43m – gedc
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Na_{7.5}Al₆Si₆O₂₄S_{4.5} [1], lazurite-1C, zeolite SOD-S

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by S₂ dumbbells (orientational disorder); (Na,H₂O) above the centers of 6-rings.

Tarling S.E. et al. (1988) [1]

Al_{2.85}DNa_{3.50}O_{12.50}S_{2.25}Si_{3.15}

a = 0.90338 nm, *V* = 0.7372 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24g	..m	0.35	0.35	0.018		non-colinear Si ₂
S2	12e	2.mm	0.079	0	0	0.375	
M3	12d	-4..	¹ / ₄	¹ / ₂	0		tetrahedron O ₄
M4	8c	.3m	0.182	0.182	0.182		

M3 = 0.525Si + 0.475Al; M4 = 0.875Na + 0.125OD₂

Experimental: powder, diffractometer, neutrons, $wR_p = 0.147$, $T = 4$ K

Remarks: Si/Al ratio 1.11 from chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. An ordered model in space group (218) $P-43n$ was tested and rejected.

References: [1] Tarling S.E., Barnes P., Klinowski J. (1988), Acta Crystallogr. B 44, 128-135.

217
cI56

Cu_3SbS_3	<i>cI56</i>	(217) <i>I-43m</i> – gedc
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Cu_3SbS_3 [2], tetrahedrite

Structural features: Single SbS_3 ψ -tetrahedra in an α Po-type (primitive cubic) arrangement.

Avilov A.S. et al. (1971) [1]

$\text{Cu}_3\text{S}_3\text{Sb}$

$a = 1.024$ nm, $V = 1.0737$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	$\dots m$	0.117	0.117	0.36		tetrahedron Cu_3Sb
Cu2	12e	$2.mm$	0.22	0	0		non-collinear S_2
Cu3	12d	$-4..$	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S_4
Sb4	8c	$.3m$	0.27	0.27	0.27		non-coplanar triangle S_3

Experimental: thin film, electron diffraction, $R = 0.205$

Remarks: No electron density was detected in Wyckoff position $2a$. According to most authors this position is occupied by additional S in tetrahedrite. The data from [2] are also reported in [3].

References: [1] Avilov A.S., Imamov R.M., Muradyan L.A. (1971), Sov. Phys. Crystallogr. (Engl. Transl.) 15, 616-619. [2] Machatschki F. (1928), Nor. Geol. Tidsskr. 10, 23-32. [3] Machatschki F. (1928), Z. Kristallogr. 68, 204-222.

217
cI56

$\text{Ag}_3\text{Ge}_5\text{P}_6$	<i>cI56</i>	(217) <i>I-43m</i> – gedc
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$\text{Ag}_6\text{Ge}_{10}\text{P}_{12}$ [1]

Structural features: GeP_3 ψ -tetrahedra and GeP_4 tetrahedra share atoms to form a 3D-framework; empty Ag_6 octahedra in large voids.

Von Schnering H.G., Häusler K.G. (1976) [1]

$\text{Ag}_3\text{Ge}_5\text{P}_6$

$a = 1.0322$ nm, $V = 1.0997$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	24g	$\dots m$	0.12832	0.12832	0.3605		tetrahedron Ge_3Ag
Ag2	12e	$2.mm$	0.1954	0	0		square antiprism $\text{P}_2\text{Ag}_4\text{Ge}_2$
Ge3	12d	$-4..$	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron P_4
Ge4	8c	$.3m$	0.2885	0.2885	0.2885		non-coplanar triangle P_3

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

References: [1] Von Schnering H.G., Häusler K.G. (1976), Rev. Chim. Miner. 13, 71-81.

Mn	<i>cI58</i>	(217) <i>I-43m</i> – g^2ca
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Mn α [2], Strukturbericht notation A12; P white rt [3]

Structural features: 29-atom α Mn-type nested polyhedra units (a central atom surrounded by a Mn_4 tetrahedron, a Mn_{12} truncated tetrahedron and a Mn_{12} cuboctahedron) in a W-type (b.c.c.) arrangement. See Fig. II.9.

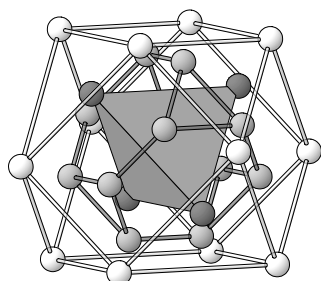


Fig. II.9. **Mn α**

29-atom (α Mn-type) nested polyhedra unit: Mn central atom + Mn_4 tetrahedron + Mn_{12} truncated tetrahedron + Mn_{12} cuboctahedron.

Oberteuffer J.A., Ibers J.A. (1970) [1]

Mn

$a = 0.8911$ nm, $V = 0.7076$ nm³, $Z = 58$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	24g	$\bar{3}m$	0.08958	0.08958	0.28194		icosahedron Mn_{12}
Mn2	24g	$\bar{3}m$	0.35706	0.35706	0.03457		pseudo Frank-Kasper Mn_{13}
Mn3	8c	$\bar{3}m$	0.31787	0.31787	0.31787		16-vertex Frank-Kasper Mn_{16}
Mn4	2a	$\bar{4}3m$	0	0	0		16-vertex Frank-Kasper Mn_{16}

Experimental: single crystal, diffractometer, X-rays, $R = 0.084$

Remarks: Phase stable at $T < 947$ K. The atom coordinates correspond to the centers of P_4 tetrahedra for white phosphorus ([3], [4]), rotational disorder is observed at room temperature. In [6] the z -coordinate of former P(IV) is misprinted as 0.04 instead of 0.28 (see [5]).

References: [1] Oberteuffer J.A., Ibers J.A. (1970), Acta Crystallogr. B 26, 1499-1504. [2] (1937), Strukturberichte 2, 2. [3] Sugawara T., Sakamoto T., Kanda E. (1949), Sci. Rep. Res. Inst. Tokyo Univ., Ser. A 1, 29-32. [4] Sugawara T., Sakamoto T., Kanda E. (1949), Sci. Rep. Res. Inst. Tokyo Univ., Ser. A 1, 153-155. [5] Donohue P.C. (1974), The Structure of the Elements, Wiley-Interscience Publ., 1974, p. 297-299. [6] (1954), Structure Reports 13, 165.

$Mg_{17}Al_{12}$	<i>cI58</i>	(217) <i>I-43m</i> – g^2ca
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$Mg_{17}Al_{12}$ [2]

Structural features: 29-atom α Mn-type nested polyhedra units (a central Mg atom surrounded by a Mg_4 tetrahedron, an Al_{12} truncated tetrahedron and a Mg_{12} cuboctahedron) in a W-type (b.c.c.) arrangement. Ordering variant of α -Mn.

Schobinger Papamantellos P., Fischer P. (1970) [1]

$Al_{12}Mg_{17}$

$a = 1.05438$ nm, $V = 1.1722$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	24g	..m	0.0954	0.0954	0.2725		icosahedron Al ₃ Mg ₉
Mg2	24g	..m	0.3582	0.3582	0.0393		pseudo Frank-Kasper Al ₅ Mg ₈
Mg3	8c	.3m	0.324	0.324	0.324		16-vertex Frank-Kasper Mg ₇ Al ₉
Mg4	2a	-43m	0	0	0		16-vertex Frank-Kasper Al ₁₂ Mg ₄

Experimental: powder, diffractometer, neutrons, $wR_p = 0.063$

Remarks: Identical to the phase called (MgAl) γ , for which the homogeneity range 48.0-51.3 at.% Mg was, however, reported in [3]. Too short interatomic distances exist both in the ordered and the disordered structures proposed for Mg₁₇Al₁₂ in (229) $Im-3m$ in [4] (the Wyckoff positions refer to space group (204) $Im-3$, however, the authors state that the structure can be described in (229) $Im-3m$).

References: [1] Schobinger Papamantellos P., Fischer P. (1970), Naturwissenschaften 57, 128-129. [2] Laves L., Löhberg K., Rahlfs P. (1934), Nachr. Ges. Wiss. Goettingen, Math.-Phys. Kl., Fachgruppe 1 1, 67-71. [3] Schürmann E., Geissler I.K. (1980), Giessereiforschung 32, 167-170. [4] Takeoshi K. (1971), Jpn. J. Appl. Phys. 10, 1311-1328.

217
cI58

Ti ₅ Re ₂₄	cI58	(217) $I-43m - g^2ca$
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Ti₅Re₂₄ [1]

Structural features: 29-atom α Mn-type nested polyhedra units (a central Ti atom surrounded by a Ti₄ tetrahedron, a Re₁₂ truncated tetrahedron and a Re₁₂ cuboctahedron) in a W-type (b.c.c.) arrangement. Ordering variant of α -Mn.

Trzebiatowski W., Niemiec J. (1955) [1]

Re₂₄Ti₅

$a = 0.9609$ nm, $V = 0.8872$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Re1	24g	..m	0.089	0.089	0.278		icosahedron Re ₈ Ti ₄
Re2	24g	..m	0.356	0.356	0.042		pseudo Frank-Kasper Re ₁₁ Ti ₂
Ti3	8c	.3m	0.317	0.317	0.317		16-vertex Frank-Kasper Re ₁₅ Ti
Ti4	2a	-43m	0	0	0		16-vertex Frank-Kasper Re ₁₂ Ti ₄

Experimental: powder, Debye-Scherrer film, X-rays

References: [1] Trzebiatowski W., Niemiec J. (1955), Roczn. Chem. 29, 277-283.

217
cI58

La ₆ Ni ₆ P ₁₇	cI58	(217) $I-43m - gedca$
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La₆Ni₆P₁₇ [1]; Ce₆Ni₆P₁₇ [1]

Structural features: :PP₃ ψ -tetrahedra are interconnected via Ni atoms to form a 3D-framework; additional P in La₆ octahedra. See Fig. II.10.

Braun D.J., Jeitschko W. (1978) [1]

La₆Ni₆P₁₇

$a = 1.0168$ nm, $V = 1.0513$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
P1	24g	..m	0.20148	0.20148	0.43226		non-coplanar triangle Ni ₂ P
La2	12e	2.mm	0.28997	0	0		13-vertex polyhedron P ₉ Ni ₄
Ni3	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron P ₄
P4	8c	.3m	0.21483	0.21483	0.21483		non-coplanar triangle P ₃
P5	2a	-43m	0	0	0		octahedron La ₆

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

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

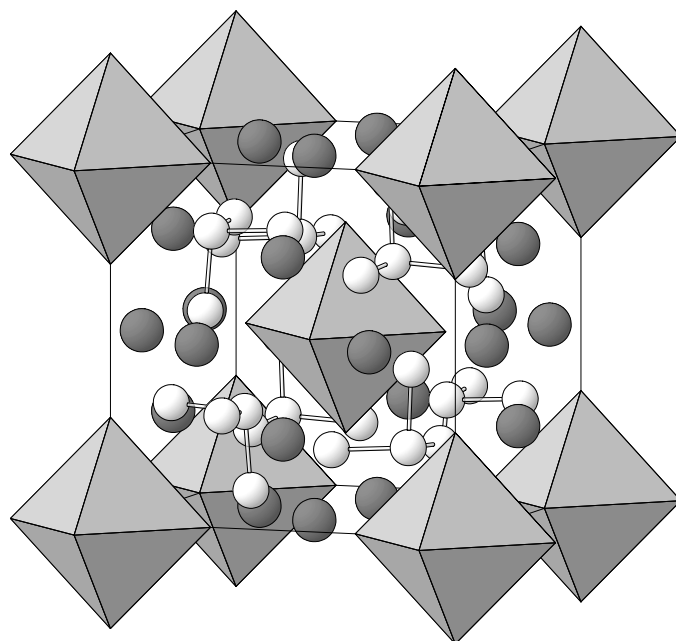


Fig. II.10. **La₆Ni₆P₁₇**

Arrangement of PLa₆ octahedra, :PP₃ ψ -tetrahedra (P atoms light) and Ni atoms (dark).

References: [1] Braun D.J., Jeitschko W. (1978), Acta Crystallogr. B 34, 2069-2074.

217
c158

Cu ₁₀ Te ₄ S ₁₃	c158	(217) I-43m – gedca
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Cu_{12-x}Te₄S₁₃ [1], goldfieldite; "Cu₁₂Sb₄S₁₃" (see remark)

Structural features: Four single :TeS₃ ψ -tetrahedra for one single S in a Cu₆ octahedron.

Kalbskopf R. (1974) [1]

Cu_{10.02}S₁₃Te₄

$a = 1.0263$ nm, $V = 1.0810$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	..m	0.107	0.107	0.353		tetrahedron Cu ₃ Te
Cu2	12e	2.mm	0.207	0	0	0.67	coplanar triangle S ₃
Cu3	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S ₄
Te4	8c	.3m	0.259	0.259	0.259		non-coplanar triangle S ₃
S5	2a	-43m	0	0	0		octahedron Cu ₆

Experimental: powder, diffractometer, X-rays, $R_B = 0.035$

Remarks: In the English summary of [1] the S site at the origin is omitted in the structural formula.

References: [1] Kalbskopf R. (1974), TMPM, Tschermaks Mineral. Petrogr. Mitt. 21, 1-10.

217
cI58

$\text{Cu}_6(\text{Cu}_{0.083}\text{Fe}_{0.917})_6\text{As}_4\text{S}_{13}$	<i>cI58</i>	(217) <i>I-43m</i> – gedca
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$\text{Cu}_6(\text{Cu}_{0.48}\text{Fe}_{5.52})\text{As}_4\text{S}_{13}$ [2], tennantite; $\text{Cu}_{10}\text{Zn}_2\text{Sb}_4\text{S}_{13}$ [2], tetrahedrite

Structural features: Four AsS_3 ψ -tetrahedra for one single S in a $(\text{Fe,Cu})_6$ octahedron. Ordering variant of $\text{Cu}_{10}\text{Te}_4\text{S}_{13}$.

Ochando L.E. et al. (1998) [1]

$\text{As}_4\text{Cu}_{6.48}\text{Fe}_{5.52}\text{S}_{13}$

$a = 1.02157 \text{ nm}$, $V = 1.0661 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	$\bar{3}m$	0.1108	0.1108	0.358		tetrahedron FeCu_2As
M2	12e	$2.mm$	0.2161	0	0		coplanar triangle S_3
Cu3	12d	$\bar{4}..$	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S_4
As4	8c	$\bar{3}m$	0.2596	0.2596	0.2596		non-coplanar triangle S_3
S5	2a	$\bar{4}3m$	0	0	0		octahedron Fe_6

$\text{M2} = 0.92\text{Fe} + 0.08\text{Cu}$

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

Remarks: Natural specimen from Villahermosa del Rio, Castellon, Spain. Composition $\text{Cu}_{10.62}\text{Fe}_{1.26}\text{As}_4\text{S}_{12.75}$ from electron microprobe analysis. The existence of stoichiometric tennantite $\text{Cu}_{12}\text{As}_4\text{S}_{13}$ and tetrahedrite $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ [3] is questioned in [5] (decomposition into a Cu-rich and a Cu-poor phase), however, refinements of $\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$ at different temperatures are reported in [4].

References: [1] Ochando L.E., Casanova J.M., Esteve V.J., Reventos M.M., Amigo J.M. (1998), An. Quim. Int. Ed. 94, 359-362. [2] Pauling L., Neumann E.W. (1934), Z. Kristallogr. 88, 54-62. [3] Wuensch B.J. (1964), Z. Kristallogr. 119, 437-453. [4] Pfitzner A., Evain M., Petricek V. (1997), Acta Crystallogr. B 53, 337-345. [5] Makovicky E., Skinner B.J. (1979), Can. Mineral. 17, 619-634.

217
cI62

$\text{Ca}_4\text{Al}_6[\text{SO}_4]\text{O}_{12}$	<i>cI62</i>	(217) <i>I-43m</i> – gdc^3a
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$\text{Ca}_8\text{Al}_{12}\text{O}_{24}(\text{SO}_4)_2$ [1], ye'elemite, zeolite SOD- SO_4

Structural features: AlO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO_4 tetrahedra; Ca at and near the centers of 6-rings (split site).

Saalfeld H., Depmeier W. (1972) [1]

$\text{Al}_6\text{Ca}_4\text{O}_{16}\text{S}$

$a = 0.92 \text{ nm}$, $V = 0.7787 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	$\bar{3}m$	0.337	0.337	0.056		non-collinear Al_2
Al2	12d	$\bar{4}..$	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4
O3	8c	$\bar{3}m$	0.079	0.079	0.079		single atom S
Ca4	8c	$\bar{3}m$	0.259	0.259	0.259	0.5	

Ca5	8c	.3m	0.33	0.33	0.33	0.5	
S6	2a	-43m	0	0	0		tetrahedron O ₄

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

Experimental: powder, X-rays, $R = 0.162$

Remarks: Average structure; additional reflections could be indexed in a cell with 8-fold volume, probable space group (214) $I4_132$. Short interatomic distances for partly occupied site(s). In table 2 of [1] the number of atoms per unit cell of former Ca(I) and Ca(II) is misprinted as 8 instead of 4 (agreement with the nominal composition).

References: [1] Saalfeld H., Depmeier W. (1972), Krist. Tech. 7, 229-233.

217
cI64

Li ₃ NbO ₄	cI64	(217) $I-43m - g^2c^2$
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Li₃NbO₄ [2]

Structural features: Close-packed O layers in c stacking, Li and Nb occupy all octahedral voids. LiO₆ and NbO₆ octahedra share edges to form a 3D-framework. Substitution derivative of NaCl of ideal composition A₃A'B₄.

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

Li₃NbO₄

$a = 0.8412$ nm, $V = 0.5952$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Li1	24g	..m	0.1218	0.1218	0.3954		octahedron O ₆
O2	24g	..m	0.3753	0.3753	0.1399		octahedron NbLi ₅
O3	8c	.3m	0.109	0.109	0.109		non-coplanar triangle Nb ₃
Nb4	8c	.3m	0.35972	0.35972	0.35972		octahedron O ₆

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

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

References: [1] Ukei K., Suzuki H., Shishido T., Fukuda T. (1994), Acta Crystallogr. C 50, 655-656. [2] Blasse G. (1963), Z. Anorg. Allg. Chem. 326, 44-46.

217
cI64

K ₃ TeS ₃ [SH]	cI64	(217) $I-43m - gedcba$
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K₃(SH)TeS₃ [1]

Structural features: Close-packed (S,SH) layers in c stacking; K and Te in octahedral voids (Te strongly displaced from the octahedron center). One :TeS₃ ψ-tetrahedron for one SH unit.

Dittmar G., Schäfer H. (1978) [1]

HK₃S₄Te

$a = 1.27$ nm, $V = 2.0484$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	..m	0.25	0.25	0.0463		single atom Te
K2	12e	2.mm	0.2503	0	0		octahedron (SH) ₂ S ₄
K3	12d	-4..	¹ / ₄	¹ / ₂	0		octahedron (SH) ₂ S ₄
Te4	8c	.3m	0.2287	0.2287	0.2287		non-coplanar triangle S ₃

(SH)5	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	octahedron K ₆
(SH)6	2a	-43m	0	0	0	octahedron K ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.073

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

References: [1] Dittmar G., Schäfer H. (1978), Z. Anorg. Allg. Chem. 439, 212-218.

217
cI70

Sr ₄ Al ₆ [CrO ₄] ₁₂	cI70	(217) <i>I</i> -43m – g ² dca
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Sr₈Al₁₂O₂₄(CrO₄)₂ ht [1], zeolite SOD-CrO₄

Structural features: AlO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by CrO₄ tetrahedra (orientational disorder); Sr at the centers of 6-rings.

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

Al₆CrO₁₆Sr₄

$a = 0.9427$ nm, $V = 0.8378$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	..m	0.125	0.125	0.036	0.333	
O2	24g	..m	0.1595	0.1595	0.4982		non-colinear Al ₂
Al3	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
Sr4	8c	.3m	0.2476	0.2476	0.2476		
Cr5	2a	-43m	0	0	0		

Experimental: single crystal, diffractometer, X-rays, R = 0.045, T = 330 K

Remarks: Phase stable at T > ~293 K. Short interatomic distances for partly occupied site(s). Space group (229) *Im*-3m could not be rejected.

References: [1] Depmeier W., Schmid H., Setter N., Werk M.L. (1987), Acta Crystallogr. C 43, 2251-2255.

217
cI72

Cu ₉ Fe ₈ S ₁₆	cI72	(217) <i>I</i> -43m – gedc ² ba
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Cu₁₈Fe₁₆S₃₂ [1], talnakhite

Structural features: Close-packed S layers in c stacking; Fe and Cu in tetrahedral voids (partial order).

Hall S.R., Gabe E.J. (1972) [1]

Cu_{10.06}Fe_{7.06}S₁₆

$a = 1.0593$ nm, $V = 1.1887$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24g	..m	0.3737	0.3737	0.1209		trigonal bipyramid Cu ₅
M2	12e	2.mmm	0.2571	0	0		tetrahedron S ₄
M3	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S ₄
S4	8c	.3m	0.1245	0.1245	0.1245		trigonal bipyramid FeCu ₄
Cu5	8c	.3m	0.2528	0.2528	0.2528		tetrahedron S ₄

M6	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.04	fourcapped trigonal prism S_4Cu_6
Fe7	2a	-43m	0	0	0		fourcapped trigonal prism S_4Cu_6

M2 = 0.5Cu + 0.5Fe; M3 = 0.5Cu + 0.5Fe; M6 = 0.5Cu + 0.5Fe

Experimental: single crystal, diffractometer, X-rays, R = 0.045

Remarks: Natural specimen from the Noril'sk or Talnakh deposit, western Siberia. Composition $Cu_{17.9}Fe_{15.9}Ni_{0.4}S_{31.8}$ from electron microprobe analysis. An additional partly occupied site in Wyckoff position 24g was reported for synthetic $FeCuS_2$ β in [2] (idealized coordinates).

References: [1] Hall S.R., Gabe E.J. (1972), Am. Mineral. 57, 368-380. [2] Hiller J.E., Probsthain K. (1956), Z. Kristallogr. 108, 108-129.

217
c/80

$Yb_3Sb_5O_{12}$	c/80	(217) $I-43m - g^2edc$
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$Yb_3Sb_5O_{12}$ [2]

Structural features: $:SbO_3$ ψ -tetrahedra and $:SbO_4$ square ψ -pyramids share atoms to form a 3D-framework; Yb in cubic voids. See Fig. II.11.

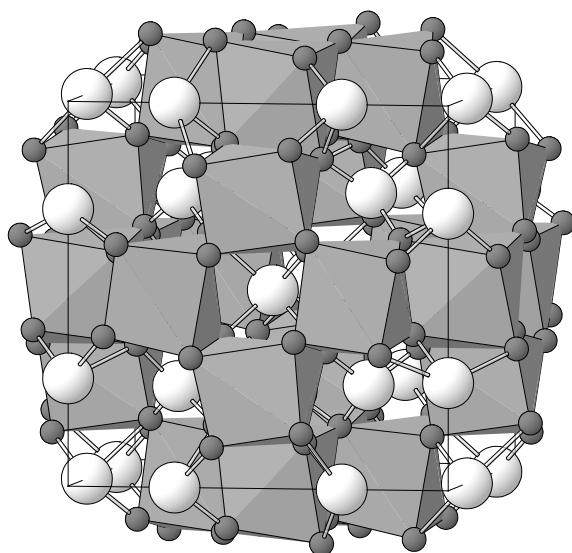


Fig. II.11. $Yb_3Sb_5O_{12}$

Arrangement of YbO_8 cubes, $:SbO_3$ ψ -tetrahedra and $:SbO_4$ square ψ -pyramids (Sb atoms large, O atoms small).

Cascales C. et al. (1989) [1]

$O_{12}Sb_5Yb_3$

$a = 1.06767$ nm, $V = 1.2171$ nm³, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24g	..m	0.112	0.112	0.397		non-coplanar triangle $SbYb_2$
O2	24g	..m	0.347	0.347	0.14		single atom Sb
Sb3	12e	2.mm	0.28	0	0		non-coplanar square O_4
Yb4	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		square prism (cube) O_8
Sb5	8c	.3m	0.254	0.254	0.254		non-coplanar triangle O_3

Experimental: powder, X-rays, $R_B = 0.036$

References: [1] Cascales C., Marcano C.M., Rasines I., Fernandez F., Saez Puche R. (1989), J. Less-Common Met. 149, 63-66. [2] Rannev N.V. (1984), Sov. Phys. Crystallogr. (Engl. Transl.) 29, 467-468.

217
cI82

$\text{Cu}_{14}\text{Sb}_4\text{S}_{13}$	<i>cI82</i>	(217) <i>I-43m</i> – g^2edca
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$\text{Cu}_{13.8}\text{Sb}_4\text{S}_{13}$ [1], tetrahedrite

Structural features: Four single SbS_3 ψ -tetrahedra for one single S in a Cu_6 octahedron.

Makovicky E., Skinner B.J. (1979) [1]

$\text{Cu}_{11.22}\text{S}_{13}\text{Sb}_4$

$a = 1.0448 \text{ nm}$, $V = 1.1405 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	24 <i>g</i>	<i>..m</i>	0.1137	0.1137	0.3613		7-vertex polyhedron Cu_6Sb
Cu2	24 <i>g</i>	<i>..m</i>	0.29	0.29	0.03	0.1	octahedron $\text{S}_3\text{Cu}_2\text{Sb}$
Cu3	12 <i>e</i>	2 <i>mm</i>	0.2157	0	0		coplanar triangle S_3
Cu4	12 <i>d</i>	-4 $..$	$\frac{1}{4}$	$\frac{1}{2}$	0	0.67	8-vertex polyhedron Cu_4S_4
Sb5	8 <i>c</i>	.3 <i>m</i>	0.2663	0.2663	0.2663		9-vertex polyhedron S_3Cu_6
S6	2 <i>a</i>	-43 <i>m</i>	0	0	0		octahedron Cu_6

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

Remarks: Cu-rich sample. Part of Cu not located. Space group (197) *I23* was tested and rejected. Supersedes a similar structure proposal for Cu_3SbS_3 with Wyckoff position 2*a* vacant ([2], [3]). A report on tetrahedrite with Cu_3VS_4 -type structure [2] (Cu_3SbS_4 , original description in space group (219) *F-43c* with 8-fold cell volume) is also superseded (see [4]); so are also the structure proposals for unsubstituted tennantite ($\text{Cu}_{12}\text{As}_4\text{S}_{13}$) and tetrahedrite ($\text{Cu}_{12}\text{Sb}_4\text{S}_{13}$) with Wyckoff position 24*g* vacant.

References: [1] Makovicky E., Skinner B.J. (1979), Can. Mineral. 17, 619-634. [2] Machatschki F. (1928), Z. Kristallogr. 68, 204-222. [3] Avilov A.S., Imamov R.M., Muradyan L.A. (1971), Sov. Phys. Crystallogr. (Engl. Transl.) 15, 616-619. [4] (1931), Strukturberichte 1, 335.

217
cI82

$\text{Th}_{11}\text{Ru}_{12}\text{C}_{18}$	<i>cI82</i>	(217) <i>I-43m</i> – g^2edca
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$\text{Th}_{11}\text{Ru}_{12}\text{C}_{18}$ [2]; $\text{Sm}_{11}\text{Fe}_{12}\text{C}_{18}$ [4]

Structural features: One C_2 dumbbell (double bond) for four single C in Th_4Ru_2 octahedra. See Fig. II.12.

Wachtmann K.H. et al. (1995) [1]

$\text{C}_{18}\text{Ru}_{12}\text{Th}_{11}$

$a = 1.0754 \text{ nm}$, $V = 1.2437 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ru1	24 <i>g</i>	<i>..m</i>	0.0845	0.0845	0.2799		non-coplanar triangle C_3
C2	24 <i>g</i>	<i>..m</i>	0.265	0.265	0.048		non-colinear Ru_2
C3	12 <i>e</i>	2 <i>mm</i>	0.43	0	0		coplanar triangle CRu_2
Th4	12 <i>d</i>	-4 $..$	$\frac{1}{4}$	$\frac{1}{2}$	0		8-vertex polyhedron C_8
Th5	8 <i>c</i>	.3 <i>m</i>	0.2968	0.2968	0.2968		octahedron C_6
Th6	2 <i>a</i>	-43 <i>m</i>	0	0	0		16-vertex Frank-Kasper $\text{Ru}_{12}\text{Th}_4$

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

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

Remarks: Identical to the phase called $\text{Th}_3\text{Ru}_4\text{C}_5$ in [3].

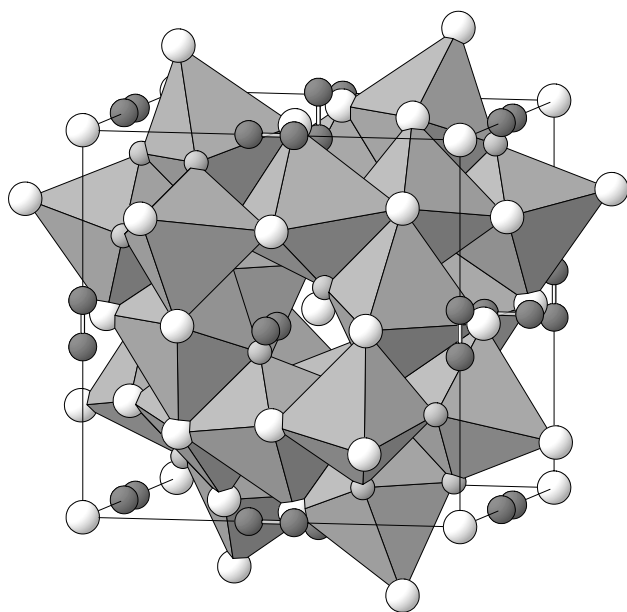


Fig. II.12. $\text{Th}_{11}\text{Ru}_{12}\text{C}_{18}$

Arrangement of $\text{C}(\text{Th}_4\text{Ru}_2)$ octahedra (Th atoms large, Ru atoms small), C_2 dumbbells (C atoms dark) and additional Th atoms.

References: [1] Wachtmann K.H., Moss M.A., Hoffmann R.D., Jeitschko W. (1995), J. Alloys Compd. 219, 279-284. [2] Aksel'rud L.G., Bodak O.I., Marusin E.P., Aslan A.M. (1990), Sov. Phys. Crystallogr. (Engl. Transl.) 35, 282-284. [3] Holleck H. (1977), J. Nucl. Mater. 66, 273-282. [4] Putyatyn A.A., Nesterenko S.N. (1992), Sov. Phys. Crystallogr. (Engl. Transl.) 37, 111-112.

217
c/82

$\text{Dy}_{10}(\text{Dy}_{0.14}\text{Mn}_{0.86})\text{Mn}_{12}\text{C}_{18}$

c/82

(217) $I-43m - g^2edca$

$\text{Dy}_{10.14}\text{Mn}_{12.86}\text{C}_{18}$ [1]

Structural features: One C_2 dumbbell (double bond) for four single C in Dy_4Mn_2 octahedra. Ordering variant of $\text{Th}_{11}\text{Ru}_{12}\text{C}_{18}$.

Kahnert G.E., Jeitschko W. (1993) [1]

$\text{C}_{18}\text{Dy}_{10.14}\text{Mn}_{12.86}$

$a = 1.0138 \text{ nm}$, $V = 1.0420 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Mn1	24g	$..m$	0.07802	0.07802	0.25964		4-vertex polyhedron C_3Mn
C2	24g	$..m$	0.2598	0.2598	0.0378		non-collinear Mn_2
C3	12e	$2.mm$	0.4322	0	0		single atom C
Dy4	12d	$-4..$	$\frac{1}{4}$	$\frac{1}{2}$	0		8-vertex polyhedron C_8
Dy5	8c	$.3m$	0.29436	0.29436	0.29436		octahedron C_6
M6	2a	$-43m$	0	0	0		12-vertex polyhedron Mn_{12}

$\text{M6} = 0.858\text{Mn} + 0.142\text{Dy}$

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

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

References: [1] Kahnert G.E., Jeitschko W. (1993), J. Alloys Compd. 196, 199-205.

217
cI84

$\text{Sr}_4\text{Al}_6[\text{TeO}_3]\text{O}_{12}$	<i>cI84</i>	(217) <i>I-43m</i> – g^2dc^3
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Sr₄Al₆O₂₄(TeO₃)₂ [1], zeolite SOD-TeO₃Structural features: AlO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); :TeO₃ ψ-tetrahedra near cage centers (orientational disorder), Sr at and above the centers of 6-rings (split site).

Dann S.E., Weller M.T. (1996) [1]

Al₆O₁₅Sr₄Te $a = 0.94206 \text{ nm}$, $V = 0.8361 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	.. <i>m</i>	0.1228	0.1228	0.0302	0.25	non-collinear Al ₂ tetrahedron O ₄
O2	24 <i>g</i>	.. <i>m</i>	0.15795	0.15795	0.4924		
Al3	12 <i>d</i>	-4.. <i>i</i>	$\frac{1}{4}$	$\frac{1}{2}$	0		
Te4	8 <i>c</i>	.3 <i>m</i>	0.0599	0.0599	0.0599	0.25	
Sr5	8 <i>c</i>	.3 <i>m</i>	0.2426	0.2426	0.2426	0.504	
Sr6	8 <i>c</i>	.3 <i>m</i>	0.2973	0.2973	0.2973	0.496	

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.028$

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

References: [1] Dann S.E., Weller M.T. (1996), J. Mater. Chem. 6, 1717-1721.

217
cI88

Na_6PbO_4	<i>cI88</i>	(217) <i>I-43m</i> – g^3cba
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Na₆PbO₄ [1]Structural features: Approximately close-packed O layers in c stacking; Na and Pb in tetrahedral voids. Pb₄O₁₃ units consisting of four PbO₄ tetrahedra sharing a central vertex; additional O in Na₈ square antiprisms.

Panek P., Hoppe R. (1973) [1]

Na₆O₄Pb $a = 1.101 \text{ nm}$, $V = 1.3346 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Na1	24 <i>g</i>	.. <i>m</i>	0.134	0.134	0.409		tetrahedron O ₄
O2	24 <i>g</i>	.. <i>m</i>	0.256	0.256	0.039		7-vertex polyhedron Na ₆ Pb
Na3	24 <i>g</i>	.. <i>m</i>	0.393	0.393	0.17		tetrahedron O ₄
Pb4	8 <i>c</i>	.3 <i>m</i>	0.1252	0.1252	0.1252		tetrahedron O ₄
O5	6 <i>b</i>	-42.. <i>m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		square antiprism Na ₈
O6	2 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron Pb ₄

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.082$

References: [1] Panek P., Hoppe R. (1973), Z. Anorg. Allg. Chem. 400, 229-241.

217
cI88

$\text{Na}_{23}\text{In}_5\text{O}_{15}$	<i>cI88</i>	(217) <i>I-43m</i> – g^3cba
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Na₂₃In₅O₁₅ [2]

Structural features: In₅O₁₂ units (an [InIn₄]⁷⁺ tetrahedron surrounded by an O₁₂ cuboctahedron) and ONa₈ square antiprisms. Ordering variant of Na₆PbO₄ with part of O replaced by In.

Deiseroth H.J. et al. (1998) [1]

In₅Na_{21.49}O₁₅

$a = 1.1075$ nm, $V = 1.3584$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Na1	24g	..m	0.1328	0.1328	0.417	0.925	tetrahedron O ₄
O2	24g	..m	0.2601	0.2601	0.051		7-vertex polyhedron InNa ₆
Na3	24g	..m	0.3921	0.3921	0.1768	0.866	tetrahedron O ₄
In4	8c	.3m	0.14351	0.14351	0.14351		non-coplanar triangle O ₃
O5	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$		square antiprism Na ₈
In6	2a	-43m	0	0	0		tetrahedron In ₄

Experimental: single crystal, diffractometer, X-rays, $R = 0.024$, $T = 293$ K

Remarks: Refinement of the site occupancies showed no significant deviation from unity, except for the Na sites. The compound was reported as Na₂₄In₅O₁₅ in [2]. The structural studies in [1], scanning electron microscopy and extended Huckel calculations give, however, strong evidence for the presence of an [InIn₄]⁷⁺ polycation and the corresponding chemical formula Na₂₃In₅O₁₅.

References: [1] Deiseroth H.J., Kerber H., Hoppe R. (1998), Z. Anorg. Allg. Chem. 624, 541-549. [2] Wagner G., Hoppe R. (1986), J. Less-Common Met. 116, 129-136.

217
cI96

(Cu _{0.5} Fe _{0.5}) _{1.1} S	cI96	(217) $I-43m - g^2edc^2ba$
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Cu_{17.6}Fe_{17.6}S₃₂ [1]

Structural features: Close-packed S layers in c stacking; (Cu,Fe) in tetrahedral voids (partial disorder).

Hiller J.E., Probsthain K. (1956) [1]

Cu_{0.55}Fe_{0.55}S

$a = 1.0605$ nm, $V = 1.1927$ nm³, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24g	..m	0.25	0.25	0.0	0.12	fourcapped trigonal prism S ₄ Cu ₆
S2	24g	..m	0.375	0.375	0.125		square prism (cube) Cu ₈
M3	12e	2.mm	0.25	0	0	0.893	fourcapped trigonal prism S ₄ Cu ₆
M4	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	0.893	fourcapped trigonal prism S ₄ Cu ₆
S5	8c	.3m	0.125	0.125	0.125		square prism (cube) Cu ₈
M6	8c	.3m	0.25	0.25	0.25		fourcapped trigonal prism S ₄ Cu ₆
M7	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.15	fourcapped trigonal prism S ₄ Cu ₆
M8	2a	-43m	0	0	0		fourcapped trigonal prism S ₄ Cu ₆

M1 = 0.5Cu + 0.5Fe; M3 = 0.5Cu + 0.5Fe; M4 = 0.5Cu + 0.5Fe; M6 = 0.5Cu + 0.5Fe; M7 = 0.5Cu + 0.5Fe; M8 = 0.5Cu + 0.5Fe

Experimental: powder, Debye-Scherrer film, X-rays

Remarks: Correct symmetry is space group (225) $Fm-3m$ with $\frac{1}{8}$ cell volume if all cation sites have the same occupancy.

References: [1] Hiller J.E., Probsthain K. (1956), Z. Kristallogr. 108, 108-129.

217
cI96

$\text{Tl}(\text{O}_{0.5}\text{F}_{0.5})_2$	<i>cI96</i>	(217) <i>I-43m</i> – $\text{g}^3\text{c}^2\text{ba}$
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TlOF [1]

Structural features: Close-packed Tl layers, (F,O) occupies all tetrahedral voids. Distorted $\text{Tl}(\text{F},\text{O})_8$ cubes share edges to form a 3D-framework. Derivative of CaF_2 (fluorite).

Vlasse M. et al. (1972) [1]

FOTl

 $a = 1.078 \text{ nm}$, $V = 1.2527 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	24g	<i>..m</i>	0.1	0.1	0.345		6-vertex polyhedron Tl_3F_3
Tl2	24g	<i>..m</i>	0.2633	0.2633	0.037		square prism (cube) F_8
M3	24g	<i>..m</i>	0.391	0.391	0.145		7-vertex polyhedron F_3Tl_4
M4	8c	<i>.3m</i>	0.145	0.145	0.145		6-vertex polyhedron Tl_3F_3
M5	8c	<i>.3m</i>	0.363	0.363	0.363		7-vertex polyhedron F_3Tl_4
Tl6	6b	<i>-42.m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		square prism (cube) F_8
Tl7	2a	<i>-43m</i>	0	0	0		square prism (cube) F_8

 $\text{M1} = 0.5\text{F} + 0.5\text{O}$; $\text{M3} = 0.5\text{F} + 0.5\text{O}$; $\text{M4} = 0.5\text{F} + 0.5\text{O}$; $\text{M5} = 0.5\text{F} + 0.5\text{O}$ Experimental: single crystal, Weissenberg and precession photographs, X-rays, $R = 0.048$

Remarks: In table 1 of [1] the *x*-coordinate of former Tl(2) is misprinted as $\frac{1}{2}$ instead of 0 (given in the text, agreement with Wyckoff position 6b).

References: [1] Vlasse M., Grannec J., Portier J. (1972), Acta Crystallogr. B 28, 3426-3428.

217
cI120

$\text{SbP}[\text{SCN}]_3\text{Cl}_3\text{O}$	<i>cI120</i>	(217) <i>I-43m</i> – g^4c^3
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[SbCl₃·OP(NCS)₃]₄ [1]

Structural features: $[\text{SbCl}_3 \cdot \text{OP}(\text{NCS})_3]_4$ molecules where four SbCl_3 ψ -tetrahedra and four $\text{P}[\text{O}(\text{NCS})_3]$ tetrahedral units (isothiocyanate linear units) are loosely interconnected so that a central Sb_4O_4 cube is formed.

Sienkiewicz A.V., Kapshuk A.A. (1994) [1]

 $\text{C}_3\text{Cl}_3\text{N}_3\text{OPS}_3\text{Sb}$ $a = 1.3927 \text{ nm}$, $V = 2.7013 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	24g	<i>..m</i>	0.1307	0.1307	0.4704		single atom C
C2	24g	<i>..m</i>	0.1472	0.1472	0.366		non-colinear NS
N3	24g	<i>..m</i>	0.1608	0.1608	0.2829		non-colinear CP
Cl4	24g	<i>..m</i>	0.4008	0.4008	0.226		single atom Sb
O5	8c	<i>.3m</i>	0.1133	0.1133	0.1133		single atom P
P6	8c	<i>.3m</i>	0.1733	0.1733	0.1733		tetrahedron ON_3
Sb7	8c	<i>.3m</i>	0.39381	0.39381	0.39381		octahedron Cl_3O_3

Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.033$, $T = 293 \text{ K}$

References: [1] Sienkiewicz A.V., Kapshuk A.A. (1994), Z. Naturforsch. B 49, 441-444.

217
cI128

ZrFe ₁₂ Si ₂ B	cI128	(217) <i>I</i> -43 <i>m</i> – g ³ edc ³ ba
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ZrFe₁₂Si₂B [1]

Structural features: Distorted substitution derivative of W (prototype for a b.c.c. atom arrangement).

Khan Y. (1992) [1]

BFe₁₂Si₂Zr $a = 1.216 \text{ nm}$, $V = 1.7980 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	24 <i>g</i>	.. <i>m</i>	0.155	0.155	0.345		4-vertex polyhedron Fe ₃ Si
Fe2	24 <i>g</i>	.. <i>m</i>	0.326	0.326	0.0		tricapped trigonal prism Fe ₈ Zr
Fe3	24 <i>g</i>	.. <i>m</i>	0.35	0.35	0.2		single atom B
Fe4	12 <i>e</i>	2.. <i>mm</i>	0.25	0	0		tetrahedron Si ₂ Fe ₂
Fe5	12 <i>d</i>	-4..	¹ / ₄	¹ / ₂	0		tetrahedron Fe ₄
Si6	8 <i>c</i>	.. <i>3m</i>	0.087	0.087	0.087		colinear SiZr
Si7	8 <i>c</i>	.. <i>3m</i>	0.17	0.17	0.17		tetrahedron SiFe ₃
B8	8 <i>c</i>	.. <i>3m</i>	0.337	0.337	0.337		non-coplanar triangle Fe ₃
Zr9	6 <i>b</i>	-42.. <i>m</i>	0	¹ / ₂	¹ / ₂		18-vertex polyhedron Fe ₁₈
Zr10	2 <i>a</i>	-43 <i>m</i>	0	0	0		tetrahedron Si ₄

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

Experimental: powder, film, X-rays

Remarks: Phase observed in melt-spun ribbons. Short interatomic distances: d(Si6-Zr10) = 0.183 nm.

References: [1] Khan Y. (1992), Phys. Status Solidi A 130, K7-K12.

217
cI144

H ₆ (Al _{0.25} Si _{0.75}) ₂₄ O ₄₈	cI144	(217) <i>I</i> -43 <i>m</i> – h ² g ²
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H₁₂Al₁₂Si₃₆O₉₆ [1], zeolite RHO-HStructural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings.

Robson H.E. et al. (1973) [1]

Al₆O₄₈Si₁₈ $a = 1.5 \text{ nm}$, $V = 3.3750 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>h</i>	1	0.0013	0.2215	0.383		non-colinear Si ₂
M2	48 <i>h</i>	1	0.1076	0.2581	0.4039		tetrahedron O ₄
O3	24 <i>g</i>	.. <i>m</i>	0.1825	0.1825	0.366		non-colinear Si ₂
O4	24 <i>g</i>	.. <i>m</i>	0.3451	0.3451	0.1307		non-colinear Si ₂

M2 = 0.75Si + 0.25Al

Experimental: powder, Debye-Scherrer film, X-rays, R = 0.077

Remarks: H not located. Unreasonable interatomic distances: d(M2-O) = 0.150-0.172 nm. The authors suggest that a better model may be obtained in space group (228) *Fd*-3*c* with 8-fold cell volume. Space group (229) *Im*-3*m* could not be rejected for the average structure (R = 0.109, but better interatomic

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

References: [1] Robson H.E., Shoemaker D.P., Ogilvie R.A., Manor P.C. (1973), Adv. Chem. Ser. 121, 106-115.

217
cI150

$\text{H}_{4.6}\text{Cs}_{0.6}(\text{Al}_{0.22}\text{Si}_{0.78})_{24}\text{O}_{48}$	<i>cI150</i>	(217) <i>I-43m</i> – h^2g^2b
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Cs_{1.2}H_{9.2}Al_{10.4}Si_{37.6}O₉₆ [2], zeolite RHO-H,Cs

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings.

Parise J.B. et al. (1984) [1]

$\text{Al}_{5.16}\text{Cs}_{1.90}\text{O}_{48}\text{Si}_{18.84}$

$a = 1.47237 \text{ nm}$, $V = 3.1919 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	48 <i>h</i>	1	0.0817	0.2274	0.3829		tetrahedron O ₄
O2	48 <i>h</i>	1	0.1125	0.2868	0.4746		non-colinear Si ₂
O3	24 <i>g</i>	.. <i>m</i>	0.1356	0.1356	0.3778		non-colinear Si ₂
O4	24 <i>g</i>	.. <i>m</i>	0.2915	0.2915	0.107		non-colinear Si ₂
Cs5	6 <i>b</i>	-42.. <i>m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$	0.633	tetrahedron O ₄

$\text{M1} = 0.785\text{Si} + 0.215\text{Al}$

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

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.049$, $T = 295 \text{ K}$

Remarks: The authors explain the large occupation factor refined for the Cs site by a partial substitution by D or D₂O. Additional peaks in difference Fourier maps could not be assigned with certainty. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Parise J.B., Abrams L., Gier T.E., Corbin D.R., Jorgensen J.D., Prince E. (1984), J. Phys. Chem. 88, 2303-2307. [2] Parise J.B., Prince E. (1983), Mater. Res. Bull. 18, 841-852.

217
cI162

$[\text{NH}_4]_6(\text{Al}_{0.25}\text{Si}_{0.75})_{24}\text{O}_{48}[\text{H}_2\text{O}]_{1.2}$	<i>cI162</i>	(217) <i>I-43m</i> – h^2g^2eb
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(NH₄)₁₂Al₁₂Si₃₆O₉₆·xH₂O [1], zeolite RHO-NH₄ residual water; Cs_{0.22}Cd_{4.8}Al₁₁Si₃₇O₉₆ rt [2], zeolite RHO-Cd,Cs

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; H₂O between 8-rings, NH₄ near the centers of 8-rings.

McCusker L.B. (1984) [1]

$\text{Al}_6\text{H}_{26.40}\text{N}_6\text{O}_{49.20}\text{Si}_{18}$

$a = 1.4821 \text{ nm}$, $V = 3.2556 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	48 <i>h</i>	1	0.0897	0.2352	0.3865		tetrahedron O ₄
O2	48 <i>h</i>	1	0.1132	0.2891	0.48		non-colinear Si ₂
O3	24 <i>g</i>	.. <i>m</i>	0.1377	0.1377	0.3809		non-colinear Si ₂
O4	24 <i>g</i>	.. <i>m</i>	0.3064	0.3064	0.1068		non-colinear Si ₂

(NH ₄) ₅	12e	2.mm	0.3842	0	0		single atom (OH ₂)
(OH ₂) ₆	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.4	colinear (NH ₄) ₂

M1 = 0.75Si + 0.25Al

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

Experimental: powder, diffractometer, X-rays, R_B = 0.078, T = 373 K

Remarks: We assume that the not identified non-framework species in Wyckoff position 6b are water molecules, f(O) was used in the refinement. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 1 of [1] the space group is misprinted as *I*-4*m* instead of *I*-43*m* (given elsewhere).

References: [1] McCusker L.B. (1984), Zeolites 4, 51-56. [2] Parise J.B., Liu X., Corbin D.R., Jones G.A. (1991), Mater. Res. Soc. Symp. Proc. 233, 267-272.

217
cI164

Rb ₅ (Al _{0.21} Si _{0.79}) ₂₄ O ₄₈	cI164	(217) <i>I</i> -43 <i>m</i> – h ² g ² ec
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Rb₁₀Al₁₀Si₃₈O₉₆ [1], zeolite RHO-Rb

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Rb between 8-rings (split site) and near the centers of 6-rings.

Parise J.B. et al. (1992) [1]

Al_{4.99}O₄₈Rb₅Si_{19.01}

a = 1.4374 nm, *V* = 2.9698 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>h</i>	1	0.0393	0.2095	0.3863		non-colinear Si ₂
M2	48 <i>h</i>	1	0.1261	0.2758	0.4272		tetrahedron O ₄
O3	24 <i>g</i>	. <i>m</i>	0.2235	0.2235	0.3984		non-colinear Si ₂
O4	24 <i>g</i>	. <i>m</i>	0.3783	0.3783	0.1214		non-colinear Si ₂
Rb5	12 <i>e</i>	2. <i>mm</i>	0.4805	0	0	0.167	
Rb6	8 <i>c</i>	.3 <i>m</i>	0.1903	0.1903	0.1903		non-coplanar triangle O ₃

M2 = 0.792Si + 0.208Al

Experimental: powder, diffractometer, neutrons, time-of-flight, R_B = 0.034, T = 297 K

Remarks: Short interatomic distances for partly occupied site(s). In table 3 of [1] the Wyckoff position of former Rb(1) is misprinted as 6*b* instead of 12*e* (splitting ignored); we assume that the occupancy of the same site is misprinted as 1.0 instead of 0.333 for 6*b* or 0.167 for 12*e* (fixed in agreement with the nominal composition).

References: [1] Parise J.B., Corbin D.R., Gier T.E., Harlow R.L., Abrams L., Dreele R.B.V. (1992), Zeolites 12, 360-368.

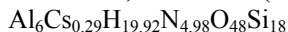
217
cI168

Cs _{0.5} [NH ₄] _{5.5} (Al _{0.25} Si _{0.75}) ₂₄ O ₄₈	cI168	(217) <i>I</i> -43 <i>m</i> – h ² g ² e ²
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Cs(NH₄)₁₁Al₁₂Si₃₆O₉₆ rt [1], zeolite RHO-NH₄,Cs rt

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings (split site), NH₄ near the centers of 8-rings.

Bieniok A., Baur W.H. (1993) [1]



$$a = 1.48168 \text{ nm}, V = 3.2528 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	1	0.0866	0.2368	0.3864		tetrahedron O ₄
O2	48h	1	0.11	0.292	0.4778		non-colinear Si ₂
O3	24g	..m	0.1392	0.1392	0.3838		non-colinear Si ₂
O4	24g	..m	0.298	0.298	0.1173		non-colinear Si ₂
(NH ₄) ₅	12e	2.mm	0.399	0	0	0.83	
Cs6	12e	2.mm	0.48	0	0	0.048	

$$\text{M1} = 0.75\text{Si} + 0.25\text{Al}$$

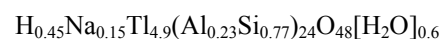
Transformation from published data: -x,-y,-z

Experimental: powder, diffractometer, X-rays, R_B = 0.037, T = 295 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bieniok A., Baur W.H. (1993), Acta Crystallogr. B 49, 817-822.

217
c/180



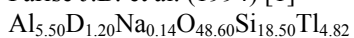
c/180

(217) $I-43m - h^2g^2ec^3$

(Cs_{0.11}Na_{0.30}Tl_{9.8}H_{0.79})Al₁₁Si₃₇O₉₆·xH₂O [1], zeolite RHO-Tl,Na residual water

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Tl between 8-rings (split site), (Tl,Na) and H₂O opposite 6-rings (disorder).

Parise J.B. et al. (1994) [1]



$$a = 1.44636 \text{ nm}, V = 3.0257 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	1	0.0752	0.226	0.3772		tetrahedron O ₄
O2	48h	1	0.1129	0.2916	0.464		non-colinear Si ₂
O3	24g	..m	0.1246	0.1246	0.3771		non-colinear Si ₂
O4	24g	..m	0.2793	0.2793	0.0997		non-colinear Si ₂
Tl5	12e	2.mm	0.478	0	0	0.5	
M6	8c	.3m	0.151	0.151	0.151	0.43	non-coplanar triangle O ₃
M7	8c	.3m	0.3	0.3	0.3	0.06	
(OD ₂) ₈	8c	.3m	0.35	0.35	0.35	0.15	

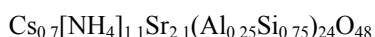
$$\text{M1} = 0.771\text{Si} + 0.229\text{Al}; \text{M6} = 0.929\text{Tl} + 0.071\text{Na}; \text{M7} = 0.929\text{Tl} + 0.071\text{Na}$$

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

Experimental: powder, diffractometer, neutrons, R_B = 0.045, T = 300 K

Remarks: Composition (Tl_{9.8}Na_{0.30}Cs_{0.11}H_{0.79})Al₁₁Si₃₇O₉₆ from chemical analysis, protons were added to achieve charge balance. Small amounts of Cs (not located) are ignored in the chemical formula given above. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

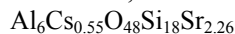
References: [1] Parise J.B., Corbin D.R., Abrams L., Northrup P., Rakovan J., Nenoff T.M., Stucky G.D. (1994), Zeolites 14, 25-34.

217
cI186

cI186

(217) *I*-43 m – h²g³eb**Cs_{1.4}(NH₄)_{2.2}Sr_{4.2}Al₁₂Si₃₆O₉₆ rt [2]**, zeolite RHO-Sr rtStructural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings, Sr near the centers of 8-rings (split site).

Bieniok A., Baur W.H. (1991) [1]

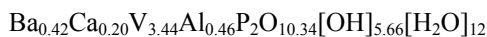
 $a = 1.45882$ nm, $V = 3.1046$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.0304	0.2108	0.3896		non-colinear Si ₂
M2	48h	1	0.1195	0.2676	0.4203		tetrahedron O ₄
Sr3	24g	..m	0.021	0.021	0.3825	0.142	
O4	24g	..m	0.2135	0.2135	0.3906		non-colinear Si ₂
O5	24g	..m	0.3659	0.3659	0.1129		non-colinear Si ₂
Sr6	12e	2.mm	0.446	0	0	0.092	
Cs7	6b	-42.m	0	1/2	1/2	0.183	

M2 = 0.75Si + 0.25Al

Experimental: powder, diffractometer, X-rays, $R_B = 0.073$, $T = 293$ KRemarks: Phase stable at $T < 373$ K. NH₄ not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

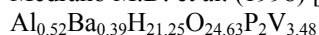
References: [1] Bieniok A., Baur W.H. (1991), Mater. Sci. Forum 79/81, 721-726. [2] Bieniok A., Baur W.H. (1991), J. Solid State Chem. 90, 173-177.

217
cI188

cI188

(217) *I*-43 m – hg⁵dc**(Ba_{0.38}Ca_{0.20}K_{0.06}Na_{0.02})[P₂(V_{3.44}Al_{0.46})O_{10.34}(OH)_{5.66}·12H₂O [1]**, phosphovanadyliteStructural features: (V,Al)₄(O,OH)₁₆ units consisting of four edge-sharing (V,Al)(O₃[OH]₃) octahedra (a (V,Al)₄(OH)₄ cube with three additional O bonded to each (V,Al)) share atoms with PO₄ tetrahedra to form a 3D-framework; Ba and H₂O in voids (partial disorder).

Medrano M.D. et al. (1998) [1]

 $a = 1.547$ nm, $V = 3.7023$ nm³, $Z = 6$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.065	0.193	0.45		non-colinear PV
(OH)2	24g	..m	0.058	0.058	0.566		non-colinear V ₂
M3	24g	..m	0.0706	0.0706	0.4172		octahedron O ₃ (OH) ₃
O4	24g	..m	0.08	0.08	0.316		single atom V
M5	24g	..m	0.257	0.257	0.028	0.92	10-vertex polyhedron (OH ₂) ₄ O ₆
(OH ₂)6	24g	..m	0.352	0.352	0.186		single atom (OH)
P7	12d	-4..	1/4	1/2	0		tetrahedron O ₄

M8 8c .3m 0.16 0.16 0.16 octahedron (OH₂)₃O₃

M3 = 0.87V + 0.13Al; M5 = 0.924OH₂ + 0.076Ba; M8 = 0.92OH₂ + 0.08Ba

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

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

Remarks: Natural specimen from the Monsanto's Enoch Valley mine, Soda Springs, Idaho. Composition Ba_{1.52}Ca_{0.82}Cd_{0.02}Zn_{0.13}Na_{0.16}K_{0.47}P_{8.04}V_{13.82}Al_{1.83}O_{73.14}F_{0.04} from electron microprobe analysis. Small amounts of K, Na, Zn, Cd and F are ignored in the chemical formula given above. Part of OH not identified. Space group (211) *I*432 was tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Medrano M.D., Evans J.H.T., Wenk H.R., Piper D.Z. (1998), Am. Mineral. 83, 889-895.

217
c/I190

Cs_{4.5}Na₆(Ga_{0.45}Si_{0.55})₂₄O₄₈

c/I190

(217) *I*-43m – h²g³c²b

Cs_{9.5}Na_{11.9}Ga_{21.4}Si_{26.6}O₉₆ [1], zeolite RHO(Ga)-Cs,Na

Structural features: (Si,Ga)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings and opposite 6-rings, Na opposite 6- and 8-rings (split site).

Newsam J.M. et al. (1995) [1]

Cs_{4.41}Ga_{10.70}Na_{4.92}O₄₈Si_{13.30}

a = 1.4545 nm, *V* = 3.0771 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
M1	48 <i>h</i>	1	0.0686	0.2228	0.371		tetrahedron O ₄
O2	48 <i>h</i>	1	0.1174	0.2897	0.4537		non-collinear Si ₂
Na3	24 <i>g</i>	..m	0.044	0.044	0.611	0.14	
O4	24 <i>g</i>	..m	0.1133	0.1133	0.3711		non-collinear Si ₂
O5	24 <i>g</i>	..m	0.2657	0.2657	0.0934		non-collinear Si ₂
Na6	8 <i>c</i>	.3m	0.1713	0.1713	0.1713	0.81	non-coplanar triangle O ₃
Cs7	8 <i>c</i>	.3m	0.3139	0.3139	0.3139	0.6	non-coplanar triangle O ₃
Cs8	6 <i>b</i>	-42..m	0	1/2	1/2	0.67	tetrahedron Na ₄

M1 = 0.554Si + 0.446Ga

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

Experimental: powder, diffractometer, neutrons, R_B = 0.016, T = 298 K

Remarks: Chemical formula given as Na_{2.7}Cs_{2.1}Si_{6.9}Ga_{4.8}O₂₄ (Si/Ga = 1.4) in the abstract; composition Cs_{9.5}Na_{11.6}Ga_{21.4}Si_{26.4}Al_{0.2}O₉₆ from chemical analysis. Short interatomic distances for partly occupied site(s). In table 6 of [1] the *y*-coordinate of former O3 is misprinted as 0.1289 instead of identical to *x* (checked on interatomic distances).

References: [1] Newsam J.M., Vaughan D.E.W., Strohmaier K.G. (1995), J. Phys. Chem. 99, 9924-9932.

217
c/I192

H_{2.65}Cs_{0.35}(Al_{0.125}Si_{0.875})₂₄O₄₈

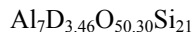
c/I192

(217) *I*-43m – h²g⁴

Cs_{0.7}H_{5.3}Al₆Si₄₂O₉₆ [1], zeolite RHO-H,Cs

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; AlO_x near the centers of 6-rings, H part of bridging OH units.

Fischer R.X. et al. (1988) [1]



$a = 1.48803 \text{ nm}$, $V = 3.2948 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48h	1	0.0883	0.236	0.383		tetrahedron O ₄
O2	48h	1	0.1127	0.2861	0.4799		non-colinear Si ₂
O3	24g	..m	0.1416	0.1416	0.3743		non-colinear Si ₂
O4	24g	..m	0.172	0.172	0.112	0.192	
Al5	24g	..m	0.233	0.233	0.187	0.333	
O6	24g	..m	0.3029	0.3029	0.1144		non-coplanar triangle Si ₂ Al
D7	48h	1	0.107	0.353	0.471	0.144	

$\text{M1} = 0.875\text{Si} + 0.125\text{Al}$

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

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_p = 0.031$

Remarks: Cs not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Fischer R.X., Baur W.H., Shannon R.D., Staley R.H., Abrams L., Vega A.J., Jorgensen J.D. (1988), Acta Crystallogr. B 44, 321-334.

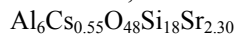
217
cI198

$\text{H}_{1.1}\text{Cs}_{0.7}\text{Sr}_{2.1}(\text{Al}_{0.25}\text{Si}_{0.75})_{24}\text{O}_{48}$	$cI198$	$(217) I-43m - h^3g^2b$
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Cs_{1.4}H_{2.2}Sr_{4.2}Al₁₂Si₃₆O₉₆ [2], zeolite RHO-Sr,Cs

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs and Sr between 8-rings (Sr displaced from the center, split site).

Bieniok A., Baur W.H. (1991) [1]



$a = 1.41729 \text{ nm}$, $V = 2.8469 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sr1	48h	1	0.012	0.027	0.531	0.096	
M2	48h	1	0.0698	0.2241	0.3752		tetrahedron O ₄
O3	48h	1	0.1075	0.2979	0.4592		non-colinear Si ₂
O4	24g	..m	0.1216	0.1216	0.3868		non-colinear Si ₂
O5	24g	..m	0.271	0.271	0.0935		non-colinear Si ₂
Cs6	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.183	

$\text{M2} = 0.75\text{Si} + 0.25\text{Al}$

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.052$, $T = 573 \text{ K}$

Remarks: Composition Cs_{1.4}(NH₄)_{2.2}Sr_{4.2}Al₁₂Si₃₆O₉₆ from chemical analysis performed before heating to 473 K in vacuum. 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] Bieniok A., Baur W.H. (1991), Mater. Sci. Forum 79/82, 721-726. [2] Bieniok A., Baur W.H. (1991), J. Solid State Chem. 90, 173-177.

217
cI204

$\text{H}_{1.4}\text{Cs}_{0.35}[\text{NH}_4]_{3.7}(\text{Al}_{0.23}\text{Si}_{0.77})_{24}\text{O}_{48}$	<i>cI204</i>	(217) <i>I-43m</i> – $\text{h}^3\text{g}^2\text{e}$
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Cs_{0.7}(NH₄)_{7.4}H_{2.8}Al_{10.9}Si_{37.1}O₉₆ [1], zeolite RHO-NH₄

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; NH₄ between 8-rings and opposite 8-rings in α cages.

Fischer R.X. et al. (1989) [1]

 $\text{Al}_{5.50}\text{D}_{25.25}\text{N}_{6.31}\text{O}_{48}\text{Si}_{18.50}$ $a = 1.45265 \text{ nm}$, $V = 3.0654 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(ND ₄)1	48 <i>h</i>	1	0.033	0.077	0.214	0.138	
O2	48 <i>h</i>	1	0.0342	0.214	0.3853		non-collinear Si ₂
M3	48 <i>h</i>	1	0.1242	0.2712	0.4256		tetrahedron O ₄
O4	24 <i>g</i>	.. <i>m</i>	0.2197	0.2197	0.3999		non-collinear Si ₂
O5	24 <i>g</i>	.. <i>m</i>	0.3691	0.3691	0.1227		non-collinear Si ₂
(ND ₄)6	12 <i>e</i>	2. <i>mm</i>	0.47	0	0	0.5	

M3 = 0.771Si + 0.229Al

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.039$

Remarks: H and Cs not located. We changed the amount of H in the chemical formula from 2.5 to 2.8 (also given as *x* in the paper) to achieve charge balance. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Fischer R.X., Baur W.H., Shannon R.D., Parise J.B., Faber J., Prince E. (1989), Acta Crystallogr. C 45, 983-989.

217
cI208

$[\text{NH}_4]_8\text{V}_{18}[\text{SO}_4]_{42}[\text{H}_2\text{O}]_{25}$	<i>cI208</i>	(217) <i>I-43m</i> – $\text{g}^7\text{e}^2\text{cba}$
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(NH₄)₈[V₁₈O₄₂(SO₄)]·25H₂O [1]

Structural features: SV₁₈O₄₆ extended Keggin units consisting of eighteen VO₅ square pyramids sharing edges and vertices (O₂₄ polyhedron with V atoms above square faces, one additional O bonded to each V) around a central SO₄ tetrahedron (orientational disorder); NH₄ and H₂O between the units.

Müller A., Döring J. (1991) [1]

 $\text{H}_{82.01}\text{N}_8\text{O}_{71}\text{SV}_{18}$ $a = 1.56 \text{ nm}$, $V = 3.7964 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>g</i>	.. <i>m</i>	0.0819	0.0819	0.2019		non-coplanar triangle V ₃
(NH ₄)2	24 <i>g</i>	.. <i>m</i>	0.094	0.094	0.5	0.667	single atom (OH ₂)
(OH ₂)3	24 <i>g</i>	.. <i>m</i>	0.1627	0.1627	0.354		non-coplanar triangle (NH ₄)(OH ₂) ₂
V4	24 <i>g</i>	.. <i>m</i>	0.165	0.165	0.0		square pyramid O ₅
O5	24 <i>g</i>	.. <i>m</i>	0.2365	0.2365	0.0		single atom V
(OH ₂)6	24 <i>g</i>	.. <i>m</i>	0.339	0.339	0.1471		tetrahedron (NH ₄)O(OH ₂) ₂
O7	24 <i>g</i>	.. <i>m</i>	0.4178	0.4178	0.2843		non-coplanar triangle V ₃
V8	12 <i>e</i>	2. <i>mm</i>	0.2515	0	0		square pyramid O ₅
O9	12 <i>e</i>	2. <i>mm</i>	0.3545	0	0		single atom V
O10	8 <i>c</i>	.. <i>3m</i>	0.0552	0.0552	0.0552		single atom S

(OH ₂) ₁₁	6b	-42.m	0	$\frac{1}{2}$	$\frac{1}{2}$	0.333	octahedron (NH ₄) ₄ O ₂
S12	2a	-43m	0	0	0		tetrahedron O ₄

Experimental: single crystal, diffractometer, X-rays, wR = 0.040, T = 294 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 6 of [1] the occupancies of former N(1) and O(8) are misprinted as implicit 1 instead of $\frac{2}{3}$ and $\frac{1}{3}$, respectively (from the chemical formula).

References: [1] Müller A., Döring J. (1991), Z. Anorg. Allg. Chem. 595, 251-274.

217
cI218

Sr ₃ Ce ₁₀ Al ₁₂ Si ₁₈ N ₃₆ O ₁₈	cI218	(217) <i>I</i> -43m – g ⁸ eda
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Sr₃Ce₁₀Al₁₂Si₁₈O₁₈N₃₆ [1]

Structural features: SiN₄, Si(ON₃) and Al(ON₃) tetrahedra share vertices to form a 3D-framework with double 3-rings of Si(ON₃) and Al(ON₃) tetrahedra; additional O in (Ce,Sr)₄ tetrahedra (distinct positions for Ce and Sr, split site).

Lauterbach R. et al. (2000) [1]

Al₁₂Ce_{9.96}N₃₆O₁₈Si₁₈Sr_{3.04}

a = 1.3382 nm, *V* = 2.3964 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24g	..m	0.0772	0.0772	0.2287		non-coplanar triangle SiAl ₂
Sr2	24g	..m	0.1294	0.1294	0.441	0.17	
Ce3	24g	..m	0.1294	0.1294	0.4504	0.83	
Al4	24g	..m	0.2054	0.2054	0.0454		tetrahedron ON ₃
N5	24g	..m	0.2676	0.2676	0.4177		non-coplanar triangle Si ₂ Al
O6	24g	..m	0.2862	0.2862	0.1022		non-collinear SiAl
Si7	24g	..m	0.3498	0.3498	0.19		tetrahedron ON ₃
N8	24g	..m	0.428	0.428	0.1238		non-collinear Si ₂
Si9	12e	2.mm	0.3	0	0		tetrahedron N ₄
O10	12d	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		
Sr11	2a	-43m	0	0	0		12-vertex polyhedron N ₁₂

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

Experimental: single crystal, diffractometer, X-rays, R = 0.033, T = 296 K

Remarks: Short interatomic distances for partly occupied site(s). Ordering of O and N was confirmed by neutron diffraction on isotypic Sr₃Pr₁₀Al₁₂Si₁₈N₃₆O₁₈ [1].

References: [1] Lauterbach R., Irran E., Henry P.F., Weller M.T., Schnick W. (2000), J. Mater. Chem. 10, 1357-1364.

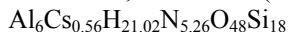
217
cI228

Cs _{0.5} [NH ₄] _{5.5} (Al _{0.25} Si _{0.75}) ₂₄ O ₄₈	cI228	(217) <i>I</i> -43m – h ³ g ³ e
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Cs(NH₄)₁₁Al₁₂Si₃₆O₉₆ ht [1], zeolite RHO-NH₄,Cs ht

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs between 8-rings, NH₄ near the centers of 6-rings and above 8-rings in α cages (disorder).

Bieniok A., Baur W.H. (1993) [1]



$a = 1.44803 \text{ nm}$, $V = 3.0362 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(NH ₄)1	48h	1	0.022	0.08	0.176	0.09	single atom (NH ₄)
M2	48h	1	0.077	0.2282	0.378		tetrahedron O ₄
O3	48h	1	0.1116	0.2896	0.4636		non-colinear Si ₂
O4	24g	..m	0.1292	0.1292	0.3845		non-colinear Si ₂
O5	24g	..m	0.2825	0.2825	0.1017		non-colinear Si ₂
(NH ₄)6	24g	..m	0.288	0.288	0.339	0.258	
Cs7	12e	2.mm	0.466	0	0	0.094	

$\text{M2} = 0.75\text{Si} + 0.25\text{Al}$

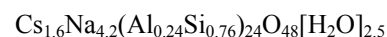
Transformation from published data: $-x, -y, -z$

Experimental: powder, diffractometer, X-rays, $R_B = 0.027$, $T = 573 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bieniok A., Baur W.H. (1993), Acta Crystallogr. B 49, 817-822.

217
cI254



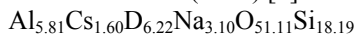
cI254

(217) $I-43m - h^2g^6cb$

Cs_{3.2}Na_{8.4}Al_{11.6}Si_{36.4}O₉₆·5H₂O [1], zeolite RHO-Na,Cs hydrated

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via double 8-rings; Cs and Na between 8-rings (Na displaced from the center, split site), additional Na near the centers of 6-rings, disordered arrangement of H₂O in the cages.

Baur W.H. et al. (1989) [1]



$a = 1.46566 \text{ nm}$, $V = 3.1485 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.0294	0.2099	0.3864		non-colinear Si ₂
M2	48h	1	0.1207	0.2692	0.42		tetrahedron O ₄
(OD ₂)3	24g	..m	0.04	0.04	0.169	0.092	non-coplanar triangle (OD ₂) ₃
Na4	24g	..m	0.04	0.04	0.504	0.175	
O5	24g	..m	0.2092	0.2092	0.3949		non-colinear Si ₂
(OD ₂)6	24g	..m	0.218	0.218	0.12	0.088	non-colinear (OD ₂) ₂
O7	24g	..m	0.3667	0.3667	0.1232		non-colinear Si ₂
(OD ₂)8	24g	..m	0.432	0.432	0.282	0.079	non-colinear (OD ₂) ₂
Na9	8c	.3m	0.305	0.305	0.305	0.25	octahedron O ₃ (OD ₂) ₃
Cs10	6b	-42.m	0	1/2	1/2	0.533	

$\text{M2} = 0.758\text{Si} + 0.242\text{Al}$

Experimental: powder, diffractometer, neutrons, $R_p = 0.071$, $T = 373 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Baur W.H., Bieniok A., Shannon R.D., Prince E. (1989), Z. Kristallogr. 187, 253-266.

217
cI282

$V_{10}As_2O_{26}[H_2O]_9$	<i>cI282</i>	(217) <i>I</i> -43 <i>m</i> – $h^2g^6e^2db$
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[As₂V₁₀O₂₆(H₂O)]·8H₂O [2]

Structural features: (H₂O)V₁₀O₂₆ units (a central H₂O molecule surrounded by ten edge-linked VO₅ square pyramids) share vertices with AsO₄ tetrahedra to form a 3D-framework; additional H₂O in channels along $\langle 111 \rangle$.

Zhao Y. et al. (2001) [1]

As₂H₁₈O₃₅V₁₀

$a = 1.6708$ nm, $V = 4.6642$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	48 <i>h</i>	1	0.0043	0.30636	0.4171		non-coplanar triangle AsV ₂
O2	48 <i>h</i>	1	0.0097	0.1077	0.3903		non-colinear V ₂
V3	24 <i>g</i>	.. <i>m</i>	0.1125	0.1125	0.4285		square pyramid O ₅
O4	24 <i>g</i>	.. <i>m</i>	0.1705	0.1705	0.3678		single atom V
(OH ₂)5	24 <i>g</i>	.. <i>m</i>	0.2343	0.2343	0.0243		single atom (OH ₂)
(OH ₂)6	24 <i>g</i>	.. <i>m</i>	0.2583	0.2583	0.155		pentagonal pyramid O ₃ (OH ₂) ₃
O7	24 <i>g</i>	.. <i>m</i>	0.3444	0.3444	0.1522		non-colinear V(OH ₂)
V8	24 <i>g</i>	.. <i>m</i>	0.3875	0.3875	0.0768		square pyramid O ₅
O9	12 <i>e</i>	2. <i>mm</i>	0.2557	0	0		single atom V
V10	12 <i>e</i>	2. <i>mm</i>	0.3527	0	0		square pyramid O ₅
As11	12 <i>d</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
(OH ₂)12	6 <i>b</i>	-42. <i>m</i>	0	$\frac{1}{2}$	$\frac{1}{2}$		10-vertex polyhedron V ₂ O ₈

Experimental: single crystal, diffractometer, X-rays, $R = 0.110$, $T = 293$ K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The same data are reported in [2] and [3]. In [1] the number of formula units per unit cell Z is misprinted as 4 instead of 6. In [2] the chemical formula is misprinted as [AsV₁₀O₂₆(μ-H₂O)]·8H₂O instead of [As₂V₁₀O₂₆(μ-H₂O)]·8H₂O and the number of formula units per cell Z as 4 instead of 6. In the title of [3] the chemical formula is misprinted As₂V⁴⁺V⁵⁺O₂₆(OH)]·8H₂O instead of [As₂V⁴⁺₈V⁵⁺₂O₂₆(H₂O)]·8H₂O (given on page 164) and the number of formula units per cell Z as 4 instead of 6.

References: [1] Zhao Y., Liu Q., Li Y., Chen X., Mai Z. (2001), J. Mater. Chem. 11, 1553-1554. [2] Bu W.M., Ye L., Yang G.Y., Shao M.C., Fan Y.G., Xu J.Q. (2000), Chem. Commun. 2000, 1279-1280. [3] Zhao Y., Li Y., Liu Q., Chen X., Wang Y., Li X., Li M., Mai Z. (2002), J. Solid State Chem. 169, 160-167.

217
cI392

$Cd_{40}Pt_8$	<i>cI392</i>	(217) <i>I</i> -43 <i>m</i> – $h^2g^9fe^2c^4$
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Pt₈Cd₄₀ [1]

Structural features: 26-atom γ brass- (an inner tetrahedron surrounded by an outer tetrahedron, an octahedron and a cuboctahedron) and 22-atom Ti₂Ni-type (an octahedron surrounded by a tetrahedron and a cuboctahedron) nested polyhedra units in the ratio 10:6.

Arnberg L. (1980) [1]

Cd_{40.40}Pt₈

$a = 1.98042$ nm, $V = 7.7673$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cd1	48h	1	0.097	0.229	0.414		16-vertex Frank-Kasper Pt ₂ Cd ₁₄
Cd2	48h	1	0.142	0.36	0.468		icosahedron Pt ₂ Cd ₁₀
Cd3	24g	..m	0.096	0.096	0.27		15-vertex Frank-Kasper Pt ₂ Cd ₁₃
Pt4	24g	..m	0.0985	0.0985	0.4112		bicapped square prism Cd ₁₀
Cd5	24g	..m	0.151	0.151	0.023		pseudo Frank-Kasper Pt ₂ Cd ₁₁
Cd6	24g	..m	0.194	0.194	0.314		pseudo Frank-Kasper Cd ₉ Pt ₄
Cd7	24g	..m	0.247	0.247	0.428		pseudo Frank-Kasper Cd ₁₁ Pt ₂
Cd8	24g	..m	0.255	0.255	0.069		pseudo Frank-Kasper Cd ₁₁ Pt ₂
Pt9	24g	..m	0.3343	0.3343	0.164		icosahedron Cd ₁₂
Cd10	24g	..m	0.351	0.351	0.021		icosahedron Pt ₂ Cd ₁₀
Cd11	24g	..m	0.411	0.411	0.266		15-vertex Frank-Kasper Cd ₁₃ Pt ₂
Cd12	24f	2..	0.158	1/2	0		pseudo Frank-Kasper Pt ₂ Cd ₁₁
Cd13	12e	2.mm	0.178	0	0		pseudo Frank-Kasper Cd ₁₁ Pt ₂
Cd14	12e	2.mm	0.373	0	0		15-vertex Frank-Kasper Cd ₁₃ Pt ₂
Cd15	8c	.3m	0.043	0.043	0.043	0.4	icosahedron Cd ₉ Pt ₃
Pt16	8c	.3m	0.1699	0.1699	0.1699		icosahedron Cd ₁₂
Cd17	8c	.3m	0.299	0.299	0.299		icosahedron Pt ₃ Cd ₉
Pt18	8c	.3m	0.416	0.416	0.416		icosahedron Cd ₁₂

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

Remarks: Phase referred to as γ -(CdPt); the homogeneity range, Cd_{100-x}Pt_x, 14.5 < x < 17.5, includes also a structure with a smaller, primitive cubic cell. Short interatomic distances for partly occupied site(s). Similar models with the atoms differently distributed around the origin were tested and rejected. In table 6 of [1] the Wyckoff position corresponding to 0 0 z is misprinted as 12d instead of 12e; the occupation of former A:IT is misprinted as 0.8 instead of 0.4 (2.9 ± 0.8 Cd atoms/site given in the text).

References: [1] Arnberg L. (1980), Acta Crystallogr. B 36, 527-532.

217
cI528

YFe ₂ H _{1.75}	cI528	(217) <i>I</i> -43m – h ⁶ g ⁹ c ² ba
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YFe₂H_{1.75} [1]

Structural features: Filled-up derivative of MgCu₂ with H in tetrahedral (mainly Y₂Fe₂) voids.

Paul Boncour V. et al. (1999) [1]

D_{2.01}Fe₂Y

a = 1.5336 nm, V = 3.6069 nm³, Z = 64

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	48h	1	0.002	0.111	0.259	0.765	
D2	48h	1	0.008	0.141	0.354	0.358	non-collinear DFe
D3	48h	1	0.029	0.133	0.239	0.327	
Fe4	48h	1	0.06	0.19	0.444		non-coplanar triangle D ₃
D5	48h	1	0.092	0.158	0.272	0.167	single atom D
D6	48h	1	0.129	0.242	0.378	0.308	non-collinear Fe ₂
D7	24g	..m	0.012	0.012	0.633	0.454	
D8	24g	..m	0.018	0.018	0.142	0.683	
Fe9	24g	..m	0.07	0.07	0.319		
D10	24g	..m	0.107	0.107	0.496	0.217	tetrahedron Fe ₂ Y ₂
Fe11	24g	..m	0.198	0.198	0.316		non-collinear D ₂
D12	24g	..m	0.241	0.241	0.119	0.167	non-collinear D ₂

Y13	24g	$\bar{1}m$	0.26	0.26	0.006	single atom D
Y14	24g	$\bar{1}m$	0.365	0.365	0.116	square pyramid D ₅
Fe15	24g	$\bar{1}m$	0.426	0.426	0.318	non-coplanar square D ₄
Y16	8c	$\bar{3}m$	0.127	0.127	0.127	18-vertex polyhedron D ₁₈
Fe17	8c	$\bar{3}m$	0.315	0.315	0.315	octahedron Fe ₆
Y18	6b	$\bar{4}2m$	0	$\frac{1}{2}$	$\frac{1}{2}$	
Y19	2a	$\bar{4}3m$	0	0	0	

Experimental: powder, diffractometer, neutrons, $R_p = 0.054$, $T = 300$ K

Remarks: Short interatomic distances for partly occupied site(s). We assume that in table 4 of [1] the z -coordinate of former Y5 is misprinted as 0.384 instead of -0.384 (interatomic distances closer to expected ones). The metal atom substructure was refined in [2].

References: [1] Paul Boncour V., Guénée L., Latroche M., Percheron Guégan A., Ouladdiaf B., Bourée Vigneron F. (1999), J. Solid State Chem. 142, 120-129. [2] Paul Boncour V., Latroche M., Guénée L., Percheron Guégan A. (1997), J. Alloys Compd. 255, 195-202.