$[H_3O]_5Zr_6BCl_{18}[H_2O]_{19}$	$cI98$	(229) $Im\text{-}3m$ – khe^{2}a

(H$_3$O)$_5$[(Zr$_6$BCl$_{12}$)Cl$_6$]·19H$_2$O [1]

Structural features: BZr$_6$Cl$_{18}$ clusters (a central B atom surrounded by a Zr$_6$ octahedron, a Cl$_{12}$ cuboctahedron and a Cl$_6$ octahedron) are loosely interconnected via water molecules.

Xie X., Hughbanks T. (1999) [1]

BCl$_{18}$H$_{53.04}$O$_{24}$Zr$_6$
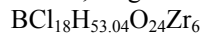
$a = 1.38749$ nm, $V = 2.6711$ nm^3, $Z = 2$

| site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	48k	..m	0.1605	0.1605	0.3987		non-coplanar triangle (OH$_2$)$_3$
Cl2	24h	$m.m2$	0	0.1831	0.1831		non-colinear Zr$_2$
Zr3	12e	4$m.m$	0.1657	0	0		octahedron BCl$_5$
Cl4	12e	4$m.m$	0.3575	0	0		single atom Zr
B5	2a	$m\text{-}3m$	0	0	0		octahedron Zr$_6$

M1 = 0.79OH$_2$ + 0.21OH$_3$

Experimental: single crystal, diffractometer, X-rays, R = 0.022, T = 213 K

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

References: [1] Xie X., Hughbanks T. (1999), Angew. Chem. Int. Ed. 38, 1777-1779.
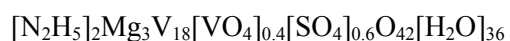
[N$_2$H$_5$]$_2$Mg$_3$V$_{18}$[VO$_4$]$_{0.4}$[SO$_4$]$_{0.6}$O$_{42}$[H$_2$O]$_{36}$	*cI*288	(229) *Im-3m* – k^{2}j^{2}h^{2}fe^{2}ba
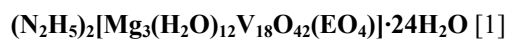
(N$_2$H$_5$)$_2$[Mg$_3$(H$_2$O)$_{12}$V$_{18}$O$_{42}$(EO$_4$)]·24H$_2$O [1]

Structural features: (V,S)V$_{18}$O$_{46}$ units consisting of eighteen VO$_5$ square pyramids sharing edges and vertices around a (V,S)O$_4$ tetrahedron (orientational disorder) are loosely interconnected via Mg(H$_2$O)$_4$ units to form two interpenetrating 3D-frameworks.
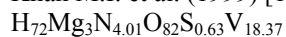
Khan M.I. et al. (1999) [1]
H$_{72}$Mg$_3$N$_{4.01}$O$_{82}$S$_{0.63}$V$_{18.37}$
a = 1.54913 nm, V = 3.7176 nm^3, Z = 2

site	Wyck.sym.		x	y	z	occ.	atomic environment
O1	48k	..m	0.08248	0.08248	0.21259		non-coplanar triangle V$_3$
O2	48k	..m	0.16132	0.16132	0.35578		
N3	48j	m..	0	0.253	0.4497	0.167	
O4	48j	m..	0	0.3883	0.4311	0.5	
V5	24h	$m.m$2	0	0.16685	0.16685		square pyramid O$_5$
O6	24h	$m.m$2	0	0.23947	0.23947		single atom V
O7	16f	.3m	0.058	0.058	0.058	0.5	4-vertex polyhedron SO$_3$
V8	12e	4$m.m$	0.25971	0	0		square pyramid O$_5$
O9	12e	4$m.m$	0.3659	0	0		colinear VMg
Mg10	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		
M11	2a	m-3m	0	0	0		square prism (cube) O$_8$
H12	96l	1	0.1552	0.2163	0.3448	0.5	
H13	48k	..m	0.1081	0.1081	0.4565		
H14	48k	..m	0.1449	0.1449	0.3182		

M11 = 0.63S + 0.37V

Experimental: single crystal, diffractometer, X-rays, R = 0.028, T = 133 K

Remarks: H of N$_2$H$_5$ 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] Khan M.I., Yohannes E., Doedens R.J., Tabussum S., Cevik S., Manno L., Powell D. (1999), Cryst. Eng. 2, 171-179.
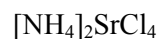
[NH₄]₂SrCl₄	cI16	(229) $Im\text{-}3m$ – cba

(NH₄)₂SrCl₄ [1]

Structural features: Substitution derivative of CsCl of ideal composition [A₃B][Cl₄], with part of the A positions vacant (disorder).

Stehlik B., Weidenthaler P. (1958) [1]

$Cl_4H_8N_2Sr$

$a = 0.715$ nm, $V = 0.3655$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	8c	.-3m	¼	¼	¼		rhombic dodecahedron Sr₂(NH₄)₆Cl₆
(NH₄)2	6b	4/mm.m	0	½	½	0.667	rhombic dodecahedron Cl₈Sr₂(NH₄)₄
Sr3	2a	m-3m	0	0	0		rhombic dodecahedron Cl₈(NH₄)₆

Experimental: powder, X-rays

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The description by the authors in space group (211) I432 does not take into consideration all symmetry elements of the proposed structure.
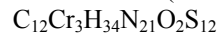
References: [1] Stehlik B., Weidenthaler P. (1958), Chem. Zvesti 12, 197-200.

[NH$_4$]$_3$Cr$_3$[SCN]$_{12}$[NH$_3$]$_6$[H$_2$O]$_2$	*cI*100	(229) *Im*-3*m* – h^{3}ecba

NH$_4$[Cr(SCN)$_4$(NH$_3$)$_2$]·H$_2$O [1], Reinecke's salt, reineckate NH$_4$
Structural features: Single Cr[(NCS)$_4$(NH$_3$)$_2$] octahedral complexes with N=C=S linear units parallel to <110> and NH$_3$ in axial positions.

Saito Y. et al. (1955) [1]
C$_{12}$Cr$_3$H$_{34}$N$_{21}$O$_2$S$_{12}$
a = 1.325 nm, V = 2.3262 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24*h*	*m.m*2	0	0.238	0.238		single atom C
C2	24*h*	*m.m*2	0	0.334	0.334		single atom N
N3	24*h*	*m.m*2	0	0.395	0.395		single atom C
(NH$_3$)4	12*e*	4*m.m*	0.338	0	0		single atom Cr
M5	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		octahedron S$_6$
Cr6	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		octahedron N$_4$(NH$_3$)$_2$
M7	2*a*	*m*-3*m*	0	0	0		18-vertex polyhedron S$_{12}$(NH$_3$)$_6$

M5 = 0.6NH$_4$ + 0.4OH$_2$; M7 = 0.6NH$_4$ + 0.4OH$_2$
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.116

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

References: [1] Saito Y., Takeuchi Y., Pepinsky R. (1955), Z. Kristallogr. 106, 476-477.

Ag$_{1.5}$(S$_{0.5}$I$_{0.5}$)		cI34	(229) Im-3m – gca

Ag$_3$SI α [1]
Structural features: (S,I) forms a W-type (b.c.c.) framework; Ag in tetrahedral and linear voids (partial disorder).

Didisheim J.J. et al. (1986) [1]
Ag$_{1.55}$I$_{0.50}$S$_{0.50}$
$a = 0.4934$ nm, $V = 0.1201$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24g	mm2..	0.156	0	$^1/_2$	0.104	
Ag2	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$	0.075	
M3	2a	m-3m	0	0	0		square prism (cube) Ag$_8$

M3 = 0.5I + 0.5S
Experimental: single crystal, diffractometer, neutrons, R = 0.029, T = 596 K

Remarks: Phase stable at T > 509 K. Short interatomic distances for partly occupied site(s).

References: [1] Didisheim J.J., McMullan R.K., Wuensch B.J. (1986), Solid State Ionics 18/19, 1150-1162.

Ag$_{1.8}$Au$_{0.2}$S				cI52			(229) Im-3m – hdcba

Ag$_{1.8}$Au$_{0.2}$S [1]

Structural features: S forms a W-type (b.c.c.) framework; Au in linear coordination; Ag distributed over 42 positions per unit cell.

Folmer J.C.W. et al. (1976) [1]
Ag$_{1.80}$Au$_{0.22}$S
a = 0.4905 nm, V = 0.1180 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24h	m.m2	0	0.375	0.375	0.075	
Ag2	12d	-4m.2	$^1/_4$	0	$^1/_2$	0.12	
Au3	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$	0.054	
Ag4	6b	4/mm.m	0	$^1/_2$	$^1/_2$	0.061	
S5	2a	m-3m	0	0	0		square prism (cube) Au$_8$

Experimental: powder, diffractometer, X-rays, T = 563 K

Remarks: Phase stable at T > 386 K, homogeneity range Ag$_{2-x}$Au$_x$S, x = 0-0.28 at 473 K. Idealized coordinates. Short interatomic distances for partly occupied site(s).

References: [1] Folmer J.C.W., Hofman P., Wiegers G.A. (1976), J. Less-Common Met. 48, 251-268.

Ag$_2$S		cI20	(229) Im-3m – dba

Ag$_2$S β [1], argentite; K$_{0.33}$Pb$_{0.67}$F$_{1.67}$ [4]
Structural features: S forms a W-type (b.c.c.) framework; Ag in tetrahedral and octahedral voids (disorder).

Cava R.J. et al. (1980) [1]
Ag$_2$S
a = 0.486 nm, V = 0.1148 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	12d	-4m.2	$^1/_4$	0	$^1/_2$	0.266	
Ag2	6b	4/mm.m	0	$^1/_2$	$^1/_2$	0.135	
S3	2a	m-3m	0	0	0		octahedron Ag$_6$

Experimental: single crystal, diffractometer, neutrons, R = 0.026, T = 459 K
Remarks: Phase stable at 450 < T < 866 K. Above 473 K the octahedral site is vacant. Short interatomic distances for partly occupied site(s). Supersedes a structure proposal reported in [2]. Ag$_2$S α (acanthite) is referred to as Ag$_2$S β in [3].

References: [1] Cava R.J., Reidinger F., Wuensch B.J. (1980), J. Solid State Chem. 31, 69-80. [2] Rahlfs P. (1936), Z. Phys. Chem., Abt. B 31, 157-194. [3] Frueh A.J. Jr. (1958), Z. Kristallogr. 110, 136-144. [4] Hull S., Berastegui P., Eriksson S.G., Gardner N.J.G. (1998), J. Phys.: Condens. Matter 10, 8429-8446.

AgI α [2]

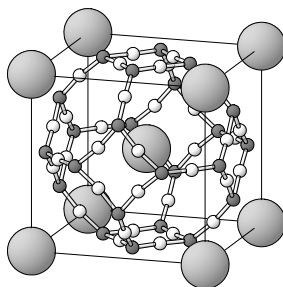Structural features: I forms a W-type (b.c.c.) framework; Ag in tetrahedral and trigonal voids. See Fig. I.9.

Fig. I.9. **AgI α**

Arrangement of Ag (partly occupied sites: tetrahedral coordination dark, trigonal coordination light) and I (large) atoms.

Cooper M.J., Sakata M. (1979) [1]
AgI
$a = 0.5062$ nm, $V = 0.1297$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ag1	24*h*	*m.m*2	0	0.385	0.385	0.07	
Ag2	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$	0.027	
I3	2*a*	*m*-3*m*	0	0	0		

Experimental: powder, diffractometer, neutrons, R = 0.031, T = 453 K

Remarks: Phase stable at high temperature. Diffraction data from [2]; we took the cell parameter from the same reference. Short interatomic distances for partly occupied site(s). The present model is considered to be a good approximation, however, the authors state that the best agreement was obtained for a model with Ag only in Wyckoff position 12*d* (V$_2$H α type), but including higher-order harmonics in the representation of thermal motion. Strukturbericht notation B23 was defined on a structure proposal where Ag partly occupies also Wyckoff position 6*b*.

References: [1] Cooper M.J., Sakata M. (1979), Acta Crystallogr. A 35, 989-991. [2] Wright A.F., Fender B.E.F. (1977), J. Phys. C: Solid State Phys. 10, 2261-2267.

AuSb₃		*cI*8	(229) *Im-3m* – ba

AuSb₃ [1]

Structural features: Infinite 3D-framework of fused (Au₂Sb₆) cubes. Substitution derivative of α-Po and NaCl.

Palatnik L.S. et al. (1961) [1]

AuSb₃

$a = 0.608$ nm, $V = 0.2248$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sb1	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		octahedron Au₂Sb₄
Au2	2*a*	*m*-3*m*	0	0	0		octahedron Sb₆

Experimental: thin film, electron diffraction

Remarks: Metastable phase.

References: [1] Palatnik L.S., Kosevich V.M., Tyrina L.V. (1961), Phys. Met. Metallogr. 11(2), 75-80 (Fiz. Met. Metalloved. 11, 229-235).

Ba$_{0.25}$Bi$_{0.75}$O$_{1.375}$		*cI*8	(229) *Im-3m* – ba

BaBi$_3$O$_{5.5}$ ht [2]

Structural features: Superposition of two ReO$_3$-type structures (frameworks of vertex-sharing (Bi,Ba)O$_6$ octahedra) with 64% vacancies on the O sites.

Esmaeilzadeh S. et al. (2000) [1]
Ba$_{0.25}$Bi$_{0.75}$O$_{1.08}$
a = 0.43798 nm, V = 0.0840 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$	0.36	octahedron Bi$_2$O$_4$
M2	2*a*	*m*-3*m*	0	0	0		octahedron O$_6$

M2 = 0.75Bi + 0.25Ba
Experimental: single crystal, diffractometer, neutrons, wR = 0.053

Remarks: Incommensurate structure, q$_1$ = 0.3835a*, q$_2$ = 0.3835b*, q$_3$ = 0.3835c*.

References: [1] Esmaeilzadeh S., Berastegui P., Grins J., Rundlöf H. (2000), J. Solid State Chem. 152, 435-440.
[2] Abbattista F., Hervieu M., Vallino M., Michel C., Raveau B. (1993), J. Solid State Chem. 104, 338-344.

| C | | | | cI16 | | | | (229) *Im*-3*m* – f |

C₈ [1]

Structural features: Distorted tetrahedral 3D-framework. C_8 cubes centered at 0 0 0 and $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ are interconnected via short C-C bonds to form a 3D-framework.

Matyushenko N.N. et al. (1981) [1]
C
$a = 0.4279$ nm, $V = 0.0784$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	16*f*	.3*m*	0.1667	0.1667	0.1667		tetrahedron C_4

Experimental: thin film, electron diffraction

Remarks: Idealized coordinates. The description by the authors in space group (204) *Im*-3 does not take into consideration all symmetry elements of the proposed structure.

References: [1] Matyushenko N.N., Strel'nitskii V.E., Gusev V.A. (1981), Sov. Phys. Crystallogr. (Engl. Transl.) 26, 274-276.

C_2Cl_6			$cI28$		(229) $Im\text{-}3m$ – fe

C_2Cl_6 form III [1], hexachloroethane

Structural features: $Cl_3C\text{-}CCl_3$ molecules in staggered conformation (Cl_6 octahedron) parallel to <111> (4-fold orientational disorder).

Gerlach P. et al. (1981) [1]
C_2Cl_6
$a = 0.755$ nm, $V = 0.4304$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
C1	16f	.3m	0.0579	0.0579	0.0579	0.25	
Cl2	12e	4m.m	0.2681	0	0		

Experimental: single crystal, diffractometer, neutrons, R = 0.110, T = 423 K

Remarks: Phase stable at T > 344 K. Cell parameter taken from figure. Short interatomic distances for partly occupied site(s). Wyckoff position 12e was used as approximation for a theoretical position 48k with $^1/_4$ occupancy.

References: [1] Gerlach P., Hohlwein D., Prandl W., Schulz F.W. (1981), Acta Crystallogr. A 37, 904-908.

| Ca₄Rh₃H₁₂ | | | *cI*38 | | | (229) *Im-3m* – edcb |

Ca₄Rh₃H₁₂ [1]

Structural features: RhH_6 octahedra share vertices to form a 3D-framework.

Bronger W., Breil L. (1998) [1]

$Ca_4D_{12}Rh_3$

$a = 0.7283$ nm, $V = 0.3863$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12*e*	4*m*.m	0.2622	0	0		single atom Rh
D2	12*d*	-4*m*.2	¹/₄	0	¹/₂		colinear Rh_2
Ca3	8*c*	.-3*m*	¹/₄	¹/₄	¹/₄		cuboctahedron D_{12}
Rh4	6*b*	4/*mm*.m	0	¹/₂	¹/₂		octahedron D_6

Experimental: powder, diffractometer, neutrons, R = 0.021

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

References: [1] Bronger W., Breil L. (1998), Z. Anorg. Allg. Chem. 624, 1819-1822.

$Cs_{0.1}Na_{0.6}Cd_{2.4}(Al_{0.23}Si_{0.77})_{24}O_{48}$	$cI166$	(229) $Im\text{-}3m$ – kjifb

$Cs_{0.2}Na_{1.2}Cd_{4.8}Al_{11}Si_{37}O_{96}$ ht [1], zeolite RHO-Cd,Cs ht
Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; Cs at the centers of octagonal prisms, Cd near the centers of 6-rings.

Parise J.B. et al. (1991) [1]
$Al_{5.52}Cd_{2.40}Cs_{0.11}O_{48}Si_{18.48}$
$a = 1.502$ nm, $V = 3.3885$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.168	0.168	0.374		non-colinear Si$_2$
O2	48j	m..	0	0.219	0.38		non-colinear Si$_2$
M3	48i	..2	$^1/_4$	0.1023	0.3977		tetrahedron O$_4$
Cd4	16f	.3m	0.237	0.237	0.237	0.3	
Cs5	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$	0.037	square prism (cube) O$_8$

M3 = 0.77Si + 0.23Al
Experimental: powder, diffractometer, X-rays, wR_p = 0.230, T = 783 K

Remarks: Phase stable at T > 573 K. Composition $Cs_{0.22}Na_{0.06}Cd_{4.8}Al_{11}Si_{37}O_{96}$ from chemical analysis, fixed for the refinement. We adjusted the charge balance in the chemical formula given above by adding more Na (not located). Short interatomic distances for partly occupied site(s).

References: [1] Parise J.B., Liu X., Corbin D.R., Jones G.A. (1991), Mater. Res. Soc. Symp. Proc. 233, 267-272.
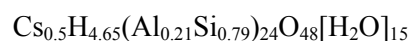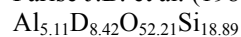
$Cs_{0.5}H_{4.65}(Al_{0.21}Si_{0.79})_{24}O_{48}[H_2O]_{15}$	$cI282$	(229) $Im\text{-}3m$ – lkjiheb

$Cs_{0.95}H_{9.35}Al_{10.3}Si_{37.7}O_{96}\cdot30H_2O$ [1], zeolite RHO-H hydrated
Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; water molecules clustered close to the framework (disorder).

Parise J.B. et al. (1984) [1]
$Al_{5.11}D_{8.42}O_{52.21}Si_{18.89}$
$a = 1.5027$ nm, $V = 3.3933$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OD_2)1	96l	1	0.05	0.095	0.335	0.014	
O2	48k	..m	0.1645	0.1645	0.3762		non-colinear Si$_2$
O3	48j	m..	0	0.2072	0.3834		non-colinear Si$_2$
M4	48i	..2	$^1/_4$	0.1055	0.3945		tetrahedron O$_4$
(OD_2)5	24h	$m.m$2	0	0.25	0.25	0.125	non-colinear O$_2$
(OD_2)6	12e	4$m.m$	0.393	0	0	0.24	
(OD_2)7	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$	0.2	colinear $(OD_2)_2$

M4 = 0.787Si + 0.213Al
Experimental: powder, diffractometer, neutrons, $R_B = 0.075$, T = 423 K

Remarks: Composition $D_{9.15}Cs_{0.95}Al_{10.3}Si_{37.7}O_{96}$ from chemical analysis. We adjusted the charge balance in the formula given above by adding H. The authors state that Cs probably substitutes for H_2O in Wyckoff position 6b; major part of H_2O 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. Contrary to dehydrated zeolite RHO, hydrated zeolite RHO remains centrosymmetric at room temperature (see [2]; 30 H_2O per unit cell not located).

References: [1] Parise J.B., Gier T.E., Corbin D.R., Cox D.E. (1984), J. Phys. Chem. 88, 1635-1640. [2] 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.

| Eu[NH$_3$]$_6$ | | | | | *cI*14 | | | (229) *Im-3m* – ea | |

Eu·6NH$_3$ [2]; Ca·6NH$_3$ [1]

Structural features: Single Eu(NH$_3$)$_6$ octahedral units in a W-type (b.c.c.) arrangement; :NH$_3$ ψ-tetrahedra in 4-fold orientational disorder (data for isotypic Ca(NH$_3$)$_6$).

Von Dreele R.B. et al. (1975) [1]
CaD$_{18}$N$_6$
$a = 0.90137$ nm, $V = 0.7323$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12*e*	4*m.m*	0.298	0	0		single atom Ca
Ca2	2*a*	*m-3m*	0	0	0		octahedron N$_6$
D3	96*l*	1	0.082	0.13	0.286	0.25	
D4	48*j*	*m*..	0	0.1	0.328	0.25	

Experimental: powder, diffractometer, neutrons, wR$_p$ = 0.098, T = 75 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In [1] the occupancy of former D2 is misprinted as 50% instead of 25% (agreement with the nominal composition).

References: [1] Von Dreele R.B., Glaunsinger W.S., Bowman A.L., Yarnell J.L. (1975), J. Phys. Chem. 79, 2992-2995. [2] Oesterreicher H., Mammano N., Sienko M.J. (1969), J. Solid State Chem. 1, 10-18.
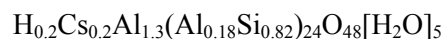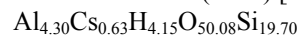
| $H_{0.2}Cs_{0.2}Al_{1.3}(Al_{0.18}Si_{0.82})_{24}O_{48}[H_2O]_5$ | *cI*186 | (229) *Im-3m* – kjiheb |

$Cs_{0.4}H_{0.4}Al_{2.6}[Al_{8.6}Si_{39.4}O_{96}]\cdot xH_2O$ [1], zeolite RHO-Cs,H (Al_2O_3) residual water
Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; Cs at the centers of octagonal prisms, H_2O at the centers of 8-rings.
Gameson I. et al. (1988) [1]
$Al_{4.30}Cs_{0.63}H_{4.15}O_{50.08}Si_{19.70}$
$a = 1.5012$ nm, $V = 3.3831$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48*k*	..*m*	0.1721	0.1721	0.3702		non-colinear Si$_2$
O2	48*j*	*m*..	0	0.2014	0.406		non-colinear Si$_2$
M3	48*i*	..2	$^1/_4$	0.0987	0.4013		tetrahedron O$_4$
(OH$_2$)4	24*h*	*m.m*2	0	0.25	0.25	0.008	non-colinear O$_2$
(OH$_2$)5	12*e*	4*m.m*	0.4	0	0	0.33	
Cs6	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$	0.21	

M3 = 0.821Si + 0.179Al
Experimental: powder, diffractometer, X-rays, wR$_p$ = 0.171, T = 25 K

Remarks: Approximate composition, ~2.6 additional Al per unit cell 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. Ambiguous data: part of the water molecules are stated to be at the centers of 6-rings ($^1/_4$ $^1/_4$ $^1/_4$), however, the atom coordinates of this site are given as $^1/_4$ $^1/_4$ $^1/_2$ (twice).

References: [1] Gameson I., Rayment T., Thomas J.M., Wright P.A. (1988), J. Phys. Chem. 92, 988-991.

$H_{1.05}Cs_{0.55}(Al_{0.07}Si_{0.93})_{24}O_{48}$	$cI162$	(229) Im-$3m$ – kjieb

$Cs_{1.1}H_{2.1}Al_{3.2}Si_{44.8}O_{96}$ [1], zeolite RHO-Cs calcined
Structural features: (Si,Al)O_4 tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; Cs at the centers of octagonal prisms, additional Al near the centers of 8-rings.

Fischer R.X. et al. (1986) [1]
$Al_{2.39}Cs_{0.54}O_{48}Si_{22.39}$
$a = 1.485$ nm, $V = 3.2748$ nm^3, $Z = 2$

site	Wyck.sym.		x	y	z	occ.	atomic environment
O1	48k	..m	0.1654	0.1654	0.3728		non-colinear Si$_2$
O2	48j	m..	0	0.2175	0.383		non-colinear Si$_2$
M3	48i	..2	$^1/_4$	0.1035	0.3965		tetrahedron O$_4$
Al4	12e	4m.m	0.35	0	0	0.13	
Cs5	6b	4/mm.m	0	$^1/_2$	$^1/_2$	0.18	

M3 = 0.933Si + 0.067Al
Experimental: powder, diffractometer, neutrons, $wR_p = 0.087$, T = 13 K

Remarks: Deep-bed calcined sample. $D_{2.1-x}H_xCs_{1.1}Al_{3.2}Si_{44.8}O_{96}$, $0 < x < 0.2$. 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., Vega A.J., Abrams L., Prince E. (1986), J. Phys. Chem. 90, 4414-4423.

$H_{2.65}Cs_{0.35}Al_{2.5}(Al_{0.125}Si_{0.875})_{24}O_{51.75}$	$cI252$	(229) Im-$3m$ – k^{3}jie

$Cs_{0.7}H_{5.3}Al_6Si_{42}O_{96} \cdot 2.5Al_2O_3$ [1], zeolite RHO-Cs,H (Al$_2$O$_3$)

Structural features: (Si,Al)O$_4$ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; Cs near the centers of octagonal prisms, additional AlO$_x$ near 6-rings, H is assumed to form bridging OH groups.

Fischer R.X. et al. (1987) [1]
$Al_{5.76}Cs_{0.84}D_{4.20}O_{50.45}Si_{21}$
$a = 1.5062$ nm, $V = 3.4170$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.1667	0.1667	0.376		non-colinear Si$_2$
O2	48k	..m	0.197	0.197	0.125	0.102	
Al3	48k	..m	0.208	0.208	0.263	0.115	
O4	48j	m..	0	0.2173	0.3841		non-colinear Si$_2$
M5	48i	..2	$^1/_4$	0.1029	0.3971		tetrahedron O$_4$
Cs6	12e	4m.m	0.452	0	0	0.14	
D7	48j	m..	0	0.154	0.381	0.175	

M5 = 0.875Si + 0.125Al

Experimental: powder, diffractometer, neutrons, time-of-flight, wR$_p$ = 0.037, T = 623 K

Remarks: Shallow-bed calcined sample. Approximate composition. The H content was calculated from the charge balance of the framework, additional Al is assumed to be compensated for by additional O. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The same data are also reported in [2].

References: [1] Fischer R.X., Baur W.H., Shannon R.D., Staley R.H. (1987), J. Phys. Chem. 91, 2227-2230. [2] 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.

$H_2PF_7[H_2O]_5$		*cI*62	(229) *Im*-3*m* – kda

HPF$_6$·5H$_2$O·HF [1]

Structural features: (H$_2$O,F) forms a clathrate-type framework with PF$_6$ octahedra in truncated octahedral voids (orientational disorder).

Wiebcke M., Mootz D. (1986) [1]
F$_7$H$_{12}$O$_5$P
$a = 0.7544$ nm, $V = 0.4293$ nm^3, $Z = 2$

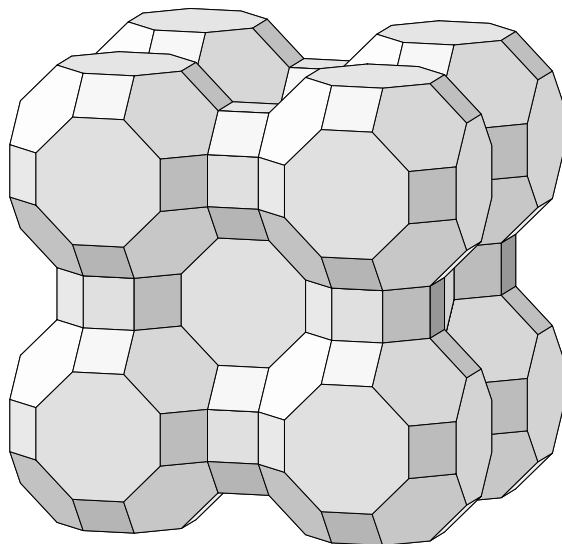| site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	48*k*	..*m*	0.1363	0.1363	0.0751	0.25	
M2	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$		tetrahedron O$_4$
P3	2*a*	*m*-3*m*	0	0	0		
H4	48*j*	*m*..	0	0.291	0.428	0.5	

M2 = 0.833O + 0.167F
Experimental: single crystal, diffractometer, X-rays, R = 0.030, T = 107 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. Supersedes a structure proposal for so-called HPF$_6$·6H$_2$O [2].

References: [1] Wiebcke M., Mootz D. (1986), Z. Kristallogr. 177, 291-299. [2] Bode H., Teufer G. (1955), Acta Crystallogr. 8, 611-614.

$H_6(Al_{0.25}Si_{0.75})_{24}O_{48}$	$cI144$	(229) $Im\text{-}3m$ – kji

$H_{12}Al_{12}Si_{36}O_{96}$ ht [2], zeolite RHO-H ht

Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form a RHO-type zeolite framework with α cages (26-face truncated cuboctahedra) interconnected via octagonal prisms; H is bonded to the O site in Wyckoff position 48j. See Fig. I.13.

Fig. I.13. **$H_{12}Al_{12}Si_{36}O_{96}$**

RHO-type (Si,Al) framework.

Baur W.H. et al. (1987) [1]

$Al_{4.51}D_{1.90}O_{48}Si_{19.49}$
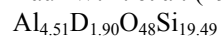
$a = 1.50696$ nm, $V = 3.4222$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.167	0.167	0.374		non-colinear Si$_2$
O2	48j	m..	0	0.2195	0.382		non-colinear Si$_2$
M3	48i	..2	$^1/_4$	0.1025	0.3975		tetrahedron O$_4$
D4	48j	m..	0	0.164	0.415	0.079	

M3 = 0.812Si + 0.188Al

Experimental: powder, diffractometer, neutrons, time-of-flight, R$_p$ = 0.021, T = 623 K

Remarks: Phase stable at high temperature. Hydrated zeolite RHO remains centrosymmetric at room temperature (see [3]; 30 H$_2$O per unit cell not located). No non-framework Al was detected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Baur W.H., Fischer R.X., Shannon R.D., Staley R.H., Vega A.J., Abrams L., Corbin D.R., Jorgensen J.D. (1987), Z. Kristallogr. 179, 281-304. [2] Robson H.E., Shoemaker D.P., Ogilvie R.A., Manor P.C. (1973), Adv. Chem. Ser. 121, 106-115. [3] 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.

HPF$_6$[H$_2$O]$_6$		*cI*110	(229) *Im*-3*m* – lda

HPF$_6$·6H$_2$O [1]

Structural features: Single PF$_6$ octahedra (orientational disorder) in (H$_2$O)$_{24}$ truncated octahedra that share faces to form a 3D-framework.

Bode H., Teufer G. (1955) [1]
F$_6$H$_{12}$O$_6$P
a = 0.7678 nm, V = 0.4526 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	96*l*	1	0.072	0.124	0.174	0.125	
O2	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$		
P3	2*a*	*m*-3*m*	0	0	0		
H4	48*j*	*m*..	0	0.345	0.403	0.5	

Experimental: powder, Debye-Scherrer, X-rays, R = 0.104

Remarks: H not belonging to H$_2$O was 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. On page 613 of [1] the Wyckoff position of the F site is misprinted as 96*e* instead of 96*l*. The structure was redetermined on single crystal data in [2].

References: [1] Bode H., Teufer G. (1955), Acta Crystallogr. 8, 611-614. [2] Wiebcke M., Mootz D. (1986), Z. Kristallogr. 177, 291-299.

| Hg$_4$Pt | | | | | | | *cI*10 | | (229) *Im*-3*m* – ca |

PtHg$_4$ [1]; NiHg$_4$ [2]
Structural features: PtHg$_8$ cubes share vertices to form a 3D-framework.

Bauer E. et al. (1953) [1]
Hg$_4$Pt
a = 0.61865 nm, V = 0.2368 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		8-vertex polyhedron Pt$_2$Hg$_6$
Pt2	2a	m-3m	0	0	0		square prism (cube) Hg$_8$

Experimental: powder, film, X-rays

Remarks: The description by the authors in space group (211) *I*432 does not take into consideration all symmetry elements of the proposed structure (see [3]).

References: [1] Bauer E., Nowotny H., Stempfl A. (1953), Monatsh. Chem. 84, 692-700. [2] Lihl F., Nowotny H. (1953), Z. Metallkd. 44, 359. [3] Fischer W., Koch E. (1983), Acta Crystallogr. A 39, 907-915.

K$_{4.5}$U$_3$O$_{11.25}$		*cI*40	(229) *Im*-3*m* – edcba

K$_9$U$_6$O$_{22.5}$ [1], perovskite A$_4$AB$_3$O$_{12}$

Structural features: UO$_6$ octahedra share vertices to form a 3D-framework; K in remaining octahedral and cuboctahedral voids. Distorted perovskite of ideal composition A$_4$[AB$_3$]O$_{12}$.

Saine M.C. et al. (1987) [1]
K$_{4.50}$O$_{11.28}$U$_3$
a = 0.8722 nm, V = 0.6635 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*e*	4*m.m*	0.3064	0	0		single atom U
O2	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$	0.88	colinear U$_2$
K3	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron O$_{12}$
U4	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		octahedron O$_6$
K5	2*a*	*m*-3*m*	0	0	0	0.5	octahedron O$_6$

Experimental: single crystal, diffractometer, X-rays, R = 0.092

References: [1] Saine M.C., Gasperin M., Jove J., Cousson A. (1987), J. Less-Common Met. 132, 141-148.

$Li_2Zr_6MnCl_{15}$	$cI56$	(229) Im-$3m$ – hedba

$Li_2Zr_6MnCl_{15}$ [1]; $Na_xTh_6FeBr_{15}$ [2]

Structural features: $MnZr_6Cl_{18}$ clusters (a central Mn atom surrounded by a Zr_6 octahedron, a Cl_{12} cuboctahedron and a Cl_6 octahedron) share vertices of the Cl_6 octahedron to form a 3D-framework.

Zhang J., Corbett J.D. (1991) [1]
$Cl_{15}Li_2MnZr_6$
$a = 1.03459$ nm, $V = 1.1074$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24h	$m.m2$	0	0.248	0.248		coplanar square Zr_2Li_2
Zr2	12e	$4m.m$	0.2331	0	0		octahedron $MnCl_5$
Li3	12d	$-4m.2$	$^1/_4$	0	$^1/_2$	0.333	octahedron Cl_6
Cl4	6b	$4/mm.m$	0	$^1/_2$	$^1/_2$		octahedron Li_4Zr_2
Mn5	2a	m-$3m$	0	0	0		octahedron Zr_6

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

Remarks: The occupancy of the Li site was fixed in agreement with the nominal composition.

References: [1] Zhang J., Corbett J.D. (1991), Inorg. Chem. 30, 431-435. [2] Böttcher F., Simon A., Kremer R.K., Buchkremer Hermanns H., Cockcroft J.K. (1991), Z. Anorg. Allg. Chem. 598/599, 25-44.

Li$_6$V$_{18}$Mn$_3$[VO$_4$]$_{0.5}$[SO$_4$]$_{0.5}$O$_{42}$[H$_2$O]$_{36}$	*cI*312	(229) *Im-3m* – k^{2}j^{2}h^{3}fe^{2}ba

Li$_6$[Mn$_3$(H$_2$O)$_{12}$V$_{18}$O$_{42}$(V,SO$_4$)]·24H$_2$O [1]
Structural features: (V,S)V$_{18}$O$_{46}$ units consisting of eighteen VO$_5$ square pyramids sharing edges and vertices around a (V,S)O$_4$ tetrahedron (orientational disorder) are loosely interconnected via Mn(H$_2$O)$_4$ units to form two interpenetrating 3D-frameworks.

Khan M.I. et al. (1999) [1]
H$_{72}$Li$_6$Mn$_3$O$_{82}$S$_{0.50}$V$_{18.50}$
$a = 1.55378$ nm, $V = 3.7512$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48*k*	..*m*	0.08211	0.08211	0.2098		non-coplanar triangle V$_3$
O2	48*k*	..*m*	0.16143	0.16143	0.3544		single atom (OH$_2$)
Li3	48*j*	*m*..	0	0.251	0.444	0.25	
(OH$_2$)4	48*j*	*m*..	0	0.3737	0.4398	0.305	
V5	24*h*	*m.m*2	0	0.16563	0.16563		square pyramid O$_5$
O6	24*h*	*m.m*2	0	0.2379	0.2379		single atom V
(OH$_2$)7	24*h*	*m.m*2	0	0.4023	0.4023	0.39	
O8	16*f*	.3*m*	0.0568	0.0568	0.0568	0.5	4-vertex polyhedron SO$_3$
V9	12*e*	4*m.m*	0.25621	0	0		square pyramid O$_5$
O10	12*e*	4*m.m*	0.3612	0	0		colinear VMn
Mn11	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		
M12	2*a*	*m-3m*	0	0	0		square prism (cube) O$_8$
H13	96*l*	1	0.14	0.209	0.355	0.5	
H14	48*k*	..*m*	0.137	0.137	0.311		

M12 = 0.50S + 0.50V
Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 183 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] Khan M.I., Yohannes E., Doedens R.J., Tabussum S., Cevik S., Manno L., Powell D. (1999), Cryst. Eng. 2, 171-179.

$Li_8La_{16}Fe_{3.2}O_{33.44}$	$cI158$	(229) $Im\text{-}3m$ – khgfe^{2}dca

$Li_{0.5}LaFe_{0.2}O_{2.09}$ [1]
Structural features: FeO_6 octahedra, high degree of disorder.

Mazza D. et al. (1985) [1]
$Fe_{3.21}La_{15.96}Li_8O_{33.72}$
$a = 1.2231$ nm, $V = 1.8297$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.1386	0.1386	0.3046	0.89	non-colinear FeLi
La2	24h	$m.m$2	0	0.30568	0.30568	0.88	10-vertex polyhedron O_{10}
O3	24g	mm2..	0.134	0	$^1/_2$	0.4	single atom O
Li4	16f	.3m	0.133	0.133	0.133		8-vertex polyhedron O_6Fe_2
O5	12e	4$m.m$	0.143	0	0	0.88	single atom Fe
La6	12e	4$m.m$	0.34724	0	0	0.9	tricapped trigonal prism O_9
O7	12d	-4m.2	$^1/_4$	0	$^1/_2$	0.38	colinear O_2
Fe8	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$	0.6	8-vertex polyhedron O_6Li_2
Fe9	2a	m-3m	0	0	0	0.81	octahedron O_6

Experimental: single crystal, diffractometer, X-rays, wR = 0.033

Remarks: Partial substitution of Li for Fe could not be excluded. Space group (204) Im-3 was tested and rejected.

References: [1] Mazza D., Abbattista F., Vallino M., Ivaldi G. (1985), J. Less-Common Met. 106, 277-285.

LiBa$_4$Sb$_3$O$_{12}$		*cI*40	(229) *Im*-3*m* – edcba

LiBa$_4$Sb$_3$O$_{12}$ [2], perovskite A$_4$BB'$_3$O$_{12}$; K$_6$Ba$_2$CaU$_6$O$_{24}$ [3]
Structural features: LiO$_6$ and SbO$_6$ octahedra share vertices to form a 3D-framework; Ba in cuboctahedral voids.
See Fig. I.10.

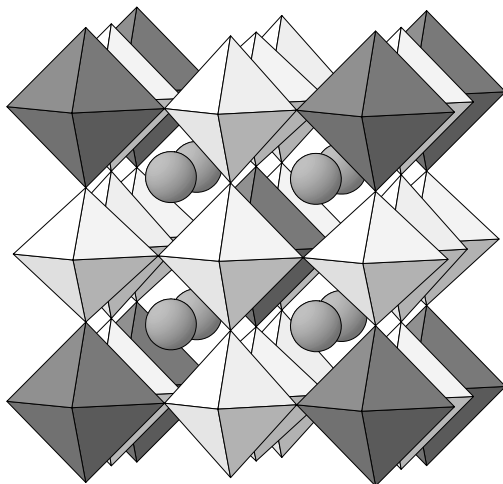Fig. I.10. **LiBa$_4$Sb$_3$O$_{12}$**

Arrangement of LiO$_6$ octahedra (dark),
SbO$_6$ octahedra (light) and Ba atoms.

Alonso J.A. et al. (1987) [1]
Ba$_4$LiO$_{12}$Sb$_3$
$a = 0.8224$ nm, $V = 0.5562$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*e*	4*m.m*	0.272	0	0		colinear SbLi
O2	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$		colinear Sb$_2$
Ba3	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron O$_{12}$
Sb4	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		octahedron O$_6$
Li5	2*a*	*m*-3*m*	0	0	0		octahedron O$_6$

Experimental: powder, X-rays, R = 0.025

Remarks: Perovskite of ideal composition A$_4$BB'$_3$O$_{12}$. Site occupation (K$_{0.75}$Ba$_{0.25}$)$_8$(Ca$_{0.5}$ $_{0.5}$)$_2$U$_6$O$_{24}$ was reported for K$_6$Ba$_2$CaU$_6$O$_{24}$.

References: [1] Alonso J.A., Mzayek E., Rasines I. (1987), Mater. Res. Bull. 22, 69-74. [2] Jacobson A.J., Collins B.M., Fender B.E.F. (1974), Acta Crystallogr. B 30, 1705-1711. [3] Saine M.C. (1987), J. Less-Common Met. 134, 245-248.

LiCa$_4$(BN$_2$)$_3$ [1]; NaSr$_4$(BN$_2$)$_3$ [2]
Structural features: N-B-N linear units parallel to <100>. Ordering variant of Sr$_{4.5}$B$_3$N$_6$. See Fig. I.7.
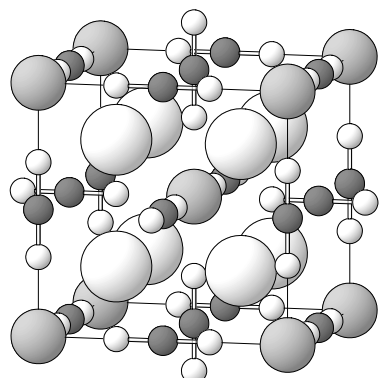

Fig. I.7. **LiCa$_4$(BN$_2$)$_3$**

Arrangement of N-B-N units (N atoms light, B atoms dark), Li (medium) and Ca (large) atoms.

Somer M. et al. (1994) [1]
B$_3$Ca$_4$LiN$_6$
a = 0.7115 nm, *V* = 0.3602 nm^3, *Z* = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
N1	12*e*	4*m.m*	0.313	0	0		single atom B
Ca2	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		octahedron N$_6$
B3	6*b*	4/*mm.m*	0	$^1/_2$	$^1/_2$		colinear N$_2$
Li4	2*a*	*m*-3*m*	0	0	0		octahedron N$_6$

Experimental: single crystal, diffractometer, X-rays, R = 0.032, T = 293 K

Remarks: The atom coordinates of NaSr$_4$B$_3$N$_6$ have not been published.

References: [1] Somer M., Herterich U., Curda J., Peters K., Von Schnering H.G. (1994), Z. Kristallogr. 209, 182-182. [2] Womelsdorf H., Meyer H.J. (1994), Z. Anorg. Allg. Chem. 620, 262-265.
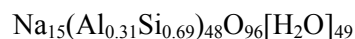
$Na_{15}(Al_{0.31}Si_{0.69})_{48}O_{96}[H_2O]_{49}$	$cI304$	(229) Im-$3m$ – lk^{2}jif

$Na_{15}Al_{15}Si_{33}O_{96} \cdot 98H_2O$ [1], zeolite KFI-Na

Structural features: (Si,Al)O_4 tetrahedra share vertices to form a KFI-type zeolite framework with α (26-face truncated cuboctahedra) and γ (18-face truncated octahedra) cages; Na near the centers of 6-rings.

Meier W.M., Kokotailo G.T. (1965) [1]
$Al_{14.88}Na_8O_{96}Si_{33.12}$
a = 1.875 nm, V = 6.5918 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	96l	1	0.084	0.2015	0.322		tetrahedron O_4
O2	48k	..m	0.1245	0.1245	0.321		non-colinear Si_2
O3	48k	..m	0.2475	0.2475	0.0955		non-colinear Si_2
O4	48j	m..	0	0.183	0.327		non-colinear Si_2
O5	48i	..2	$^1/_4$	0.1125	0.3875		non-colinear Si_2
Na6	16f	.3m	0.1315	0.1315	0.1315		non-coplanar triangle O_3

M1 = 0.69Si + 0.31Al
Experimental: powder, diffractometer, X-rays, R = 0.180

Remarks: ~14 Na and 98 H_2O per cell not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Meier W.M., Kokotailo G.T. (1965), Z. Kristallogr. 121, 211-219.
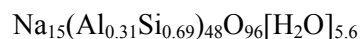
$Na_{15}(Al_{0.31}Si_{0.69})_{48}O_{96}[H_2O]_{5.6}$	*cI*288	(229) *Im*-3*m* – lk^{2}ji

$Na_{30}Al_{30}Si_{66}O_{192} \cdot xH_2O$ [1], zeolite KFI-Na hydrated
Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form a FKI-type zeolite framework with α (26-face truncated cuboctahedra) and γ (18-face truncated octahedra) cages.

Meier W.M., Kokotailo G.T. (1965) [1]
$Al_{14.88}O_{96}Si_{33.12}$
$a = 1.866$ nm, $V = 6.4973$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	96*l*	1	0.085	0.204	0.323		tetrahedron O_4
O2	48*k*	..*m*	0.1265	0.1265	0.325		non-colinear Si_2
O3	48*k*	..*m*	0.249	0.249	0.1015		non-colinear Si_2
O4	48*j*	*m*..	0	0.187	0.328		non-colinear Si_2
O5	48*i*	..2	$^1/_4$	0.1095	0.3905		non-colinear Si_2

M1 = 0.69Si + 0.31Al
Experimental: powder, diffractometer, X-rays, R = 0.110, T = 423 K

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

References: [1] Meier W.M., Kokotailo G.T. (1965), Z. Kristallogr. 121, 211-219.

$Na_3W_4O_{12}$	$cI110$	(229) $Im\text{-}3m$ – k^{2}cb

Na$_{0.75}$WO$_3$ [1], tungsten bronze cubic
Structural features: WO_6 octahedra share vertices to form a 3D-framework (distorted O sublattice).

Atoji M., Rundle R.E. (1960) [1]
$Na_3O_{12}W_4$
$a = 0.769$ nm, $V = 0.4548$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.235	0.235	0.011	0.25	
O2	48k	..m	0.267	0.267	0.011	0.25	
W3	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		
Na4	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		

Experimental: twinned crystal, neutrons, R = 0.170

Remarks: Cell parameter from [2]. Short interatomic distances for partly occupied site(s).

References: [1] Atoji M., Rundle R.E. (1960), J. Chem. Phys. 32, 627-628. [2] Brown B.W., Banks E. (1954), J. Am. Chem. Soc. 76, 963-966.

| $Na_4Ca_4Al_7F_{33}$ | | $cI136$ | (229) Im-$3m$ – k^{2}edcba |

$Na_4Ca_4Al_7F_{33}$ [1]
Structural features: CaF_6 and AlF_6 octahedra share all vertices to form a 3D-framework.

Hemon A., Courbion G. (1990) [1]
$Al_7Ca_4F_{33}Na_{4.03}$
$a = 1.0781$ nm, $V = 1.2531$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	48k	..m	0.0239	0.0239	0.1633	0.25	
F2	48k	..m	0.1159	0.1159	0.3363		single atom Al
Al3	12e	4m.m	0.3298	0	0		
Na4	12d	-4m.2	$^1/_4$	0	$^1/_2$	0.672	10-vertex polyhedron F_{10}
Ca5	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		octahedron F_6
F6	6b	4/mm.m	0	$^1/_2$	$^1/_2$		colinear Al_2
Al7	2a	m-3m	0	0	0		

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

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

References: [1] Hemon A., Courbion G. (1990), J. Solid State Chem. 84, 153-164.

Nb$_3$(Sb$_{0.5}$Te$_{0.5}$)$_4$Te$_3$	cI40	(229) Im-3m – fed

Nb$_3$Sb$_2$Te$_5$ [1]

Structural features: Nb(Sb,Te)$_8$ square antiprisms share atoms to form a 3D-framework. Partly ordered variant of Ru$_3$Sn$_7$.

Jensen P., Kjekshus A. (1967) [1]
Nb$_3$Sb$_2$Te$_5$

$a = 0.98155$ nm, $V = 0.9457$ nm^3, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	16f	.3m	0.165	0.165	0.165		pseudo Frank-Kasper Nb$_3$Sb$_4$Te$_6$
Nb2	12e	4m.m	0.3426	0	0		tricapped trigonal prism Sb$_4$Te$_4$Nb
Te3	12d	-4m.2	$^1/_4$	0	$^1/_2$		16-vertex Frank-Kasper Nb$_4$Te$_4$Sb$_8$

M1 = 0.5Sb + 0.5Te
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.089

References: [1] Jensen P., Kjekshus A. (1967), J. Less-Common Met. 13, 357-359.

| NdO$_{1.5}$ | | *cI*26 | (229) *Im-3m* – ga |

Nd$_2$O$_3$ form X [1]; La$_2$O$_3$ form X [1], sesquioxide X; AgI α [2]
Structural features: Nd forms a W-type (b.c.c.) framework; O in tetrahedral voids (disorder).

Aidebert P., Traverse J.P. (1979) [1]
NdO$_{1.50}$
$a = 0.441$ nm, $V = 0.0858$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24*g*	*mm*2..	0.18	0	$^1/_2$	0.125	
Nd2	2*a*	*m-3m*	0	0	0		24-vertex polyhedron O$_{24}$

Experimental: powder, diffractometer, neutrons, R$_B$ = 0.055, T = 2498 K

Remarks: Phase stable at T > 2423 K. The *x*-coordinate of the O site could not be determined with accuracy. Short interatomic distances for partly occupied site(s). Several models were tested (atom coordinates published). A similar model with x(O) = $^1/_2$ gave R = 0.041 but was rejected because of short interatomic distances. On page 318 of [1] the occupancy of the O site is misprinted as $^1/_4$ instead of $^1/_8$.

References: [1] Aidebert P., Traverse J.P. (1979), Mater. Res. Bull. 14, 303-323. [2] Wright A.F., Fender B.E.F. (1977), J. Phys. C: Solid State Phys. 10, 2261-2267.

NiCl$_2$[NCNH$_2$]$_4$	cI114	(229) Im-$3m$ – kh^{2}eb

Ni(NCNH$_2$)$_4$Cl$_2$ [1]

Structural features: Single Ni[(NCNH$_2$)$_4$Cl$_2$] octahedral complexes with NCNH$_2$ (cyanamide) units parallel to <110>.

Liu X. et al. (2001) [1]

C$_4$Cl$_2$H$_8$N$_8$Ni
a = 1.2593 nm, V = 1.9970 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	48k	..m	0.2497	0.2497	0.0252	0.5	
C2	24h	$m.m$2	0	0.32203	0.32203		
N3	24h	$m.m$2	0	0.38499	0.38499		
Cl4	12e	4$m.m$	0.30281	0	0		single atom Ni
Ni5	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		octahedron N$_4$Cl$_2$
H6	48j	m..	0	0.183	0.266		

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

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

References: [1] Liu X., Kroll P., Dronskowski R. (2001), Z. Anorg. Allg. Chem. 627, 1682-1686.

| Pt_3O_4 | | | | | | $cI14$ | | (229) $Im\text{-}3m$ – cb |

Pt_3O_4 [1]

Structural features: PtO_8 cubes share faces and edges to form a 3D-framework.

Galloni E.E., Roffo A.E. Jr. (1941) [1]
O_4Pt_3
$a = 0.6226$ nm, $V = 0.2413$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron Pt_6O_6
Pt2	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		cuboctahedron O_8Pt_4

Experimental: powder, film, X-rays

Remarks: This structure proposal is stated to be doubtful in [3]. Composition Pt_3O_8 ($Pt_3[O_2]_4$) was proposed in [2] (see discussion in [3]).

References: [1] Galloni E.E., Roffo A.E. Jr. (1941), J. Chem. Phys. 9, 875-877. [2] Shishakov N.A., Andreeva V.V., Andrushchenko N.M. (1959), Stroenie i Mekhanism Obrazovaniya Okisnykh Plenok na Metallakh, Akad. Nauk SSSR, Moscow. [3] Muller O., Roy R. (1968), J. Less-Common Met. 16, 129-146.

| Ru$_3$Sn$_7$ | | | | | | *cI*40 | (229) *Im*-3*m* – fed | |

Ru$_3$Sn$_7$ [1], Strukturbericht notation D8$_f$; Co$_3$Al$_3$Si$_4$ [3]; Ir$_3$Ge$_7$ [2]; Ir$_3$Sn$_7$ [1]
Structural features: RuSn$_8$ square antiprisms share atoms to form a 3D-framework.

Nial O. (1947) [1]
Ru$_3$Sn$_7$
$a = 0.9351$ nm, $V = 0.8177$ nm^3, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sn1	16*f*	.3*m*	0.156	0.156	0.156		7-vertex polyhedron Ru$_3$Sn$_4$
Ru2	12*e*	4*m.m*	0.342	0	0		tricapped trigonal prism Sn$_8$Ru
Sn3	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$		16-vertex Frank-Kasper Ru$_4$Sn$_{12}$

Experimental: powder, film, X-rays

Remarks: The Strukturbericht notation was defined on Ir$_3$Ge$_7$. The authors of [3] could not determine whether Al and Si are ordered or randomly distributed over Wyckoff positions 16*f* and 12*d*.
References: [1] Nial O. (1947), Sven. Kem. Tidskr. 59, 172-183. [2] Pfisterer H., Schubert K. (1950), Naturwissenschaften 37, 112-113. [3] Burger K.O., Wittmann A., Nowotny H. (1962), Monatsh. Chem. 93, 9-14.

SF$_6$							cI14	(229) Im-$3m$ – ea	

SF$_6$ rt [2]

Structural features: Single SF$_6$ octahedra in a W-type (b.c.c.) arrangement.

Cockcroft J.K., Fitch A.N. (1988) [1]

F$_6$S

a = 0.57951 nm, V = 0.1946 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	12e	4$m.m$	0.2685	0	0		single atom S
S2	2a	m-3m	0	0	0		octahedron F$_6$

Experimental: powder, diffractometer, neutrons, R$_B$ = 0.039, T = 115 K

Remarks: Phase stable at T > 96 K. Refinement with symmetry-adapted spherical-harmonic functions, F shell radius 0.1556(3) nm. An approximated model ignoring rotational disorder, used by the authors to calculate interatomic distances, is reported here. Rotational disorder is also studied in [3].

References: [1] Cockcroft J.K., Fitch A.N. (1988), Z. Kristallogr. 184, 123-145. [2] Taylor J.C., Waugh A.B. (1976), J. Solid State Chem. 18, 241-246. [3] Powell B.M., Dolling G. (1988), Can. J. Chem. 66, 897-903.

$Sr_{39}Co_{12}N_{31}$		*cI*200	(229) *Im*-3*m* – k²h³edba

$Sr_{39}Co_{12}N_{31}$ [1]
Structural features: Single N-Co-N linear units parallel to <110>, additional N in Sr_6 octahedra.

Kowach G.R. et al. (1998) [1]
$Co_{12}N_{31}Sr_{39}$
$a = 1.491$ nm, $V = 3.3146$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Sr1	48*k*	..*m*	0.0331	0.0331	0.1646	0.25	
Sr2	48*k*	..*m*	0.1228	0.1228	0.3143		7-vertex polyhedron N_4SrCo_2
N3	24*h*	*m.m*2	0	0.201	0.201		single atom Co
Co4	24*h*	*m.m*2	0	0.2879	0.2879		colinear N_2
N5	24*h*	*m.m*2	0	0.373	0.373		octahedron $CoSr_5$
N6	12*e*	4*m.m*	0.328	0	0		
Sr7	12*d*	-4*m*.2	¹/₄	0	¹/₂		tetrahedron N_4
Sr8	6*b*	4/*mm.m*	0	¹/₂	¹/₂		octahedron N_6
N9	2*a*	*m*-3*m*	0	0	0		

Experimental: single crystal, diffractometer, X-rays, wR = 0.063, T = 291 K

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

References: [1] Kowach G.R., Lin H.Y., DiSalvo F.J. (1998), J. Solid State Chem. 141, 1-9.

| $Sr_{4.5}B_3N_6$ | | $cI28$ | | (229) $Im\text{-}3m$ – ecba |

$Sr_3(BN_2)_2$ [1]; $Ca_3(BN_2)_2$ α [2]; $K_5H(CN_2)_3$ [3]
Structural features: N-B-N linear units parallel to <100>.

Womelsdorf H., Meyer H.J. (1994) [1]
$B_3N_6Sr_{4.49}$
$a = 0.76456$ nm, $V = 0.4469$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	12e	4$m.m$	0.3224	0	0		single atom B
Sr2	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		octahedron N$_6$
B3	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		colinear N$_2$
Sr4	2a	m-3m	0	0	0	0.49	octahedron N$_6$

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

References: [1] Womelsdorf H., Meyer H.J. (1994), Z. Anorg. Allg. Chem. 620, 262-265. [2] Wörle M., Meyer H., Nesper R. (1998), J. Alloys Compd. 264, 107-114. [3] Becker M., Jansen M., Lieb A., Milius W., Schnick W. (1998), Z. Anorg. Allg. Chem. 624, 113-118.

$Sr_4Al_6[CrO_4]O_{12}$		*cI*70	(229) *Im*-3*m* – h^{2}dca

$Sr_8Al_{12}O_{24}(CrO_4)_2$ ht [1], sodalite SACR ht, zeolite SOD-Sr (CrO_4) ht
Structural features: AlO_4 tetrahedra share vertices to form a SOD-type zeolite framework with β cages (14-face truncated octahedra) centered by CrO_4 tetrahedra (orientational disorder); Sr at the centers of 6-rings.

Depmeier W. et al. (1987) [1]
$Al_6CrO_{16}Sr_4$
a = 0.9427 nm, V = 0.8378 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24*h*	*m.m*2	0	0.125	0.125	0.333	5-vertex polyhedron O_4Cr
O2	24*h*	*m.m*2	0	0.3407	0.3407		non-colinear Al_2
Al3	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$		tetrahedron O_4
Sr4	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		icosahedron O_{12}
Cr5	2*a*	*m*-3*m*	0	0	0		cuboctahedron O_{12}

Experimental: single crystal, diffractometer, X-rays, R = 0.048, T = 330 K

Remarks: Phase stable at T > ~293 K. Space group (217) *I*-43*m* could not be rejected.

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

| $Tb_3Ni_6Al_2H_{0.5}$ | | | | | | *cI*94 | | (229) *Im*-3*m* – jheca |

$Tb_3Ni_6Al_2H_{0.5}$ [1]

Structural features: Filled-up derivative of $Ce_3Ni_6Si_2$ with H in tetrahedral ($TbNi_3$) and octahedral (Tb_6) voids.
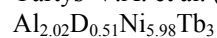
Yartys' V.A. et al. (1992) [1]
$Al_{2.02}D_{0.51}Ni_{5.98}Tb_3$
$a = 0.89413$ nm, $V = 0.7148$ nm^3, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	48*j*	*m*..	0	0.189	0.437	0.036	
M2	24*h*	*m*.*m*2	0	0.335	0.335		
Tb3	12*e*	4*m*.*m*	0.292	0	0		non-coplanar square D_4
M4	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		octahedron Ni_6
D5	2*a*	*m*-3*m*	0	0	0	0.147	octahedron Tb_6

M2 = 0.96Ni + 0.04Al; M4 = 0.89Al + 0.11Ni
Experimental: powder, diffractometer, neutrons, $R_B = 0.089$

Remarks: In table 2 of [1] the cell parameter is misprinted as 0.9841 nm instead of 0.8941 nm.

References: [1] Yartys' V.A., Pavlenko V.V., Khidirov I. (1992), Sov. J. Coord. Chem. 18, 371-377 (Koord. Khim. 18, 428-435).

$Tb_3Ni_6Al_2H_{6.5}$						$cI120$		(229) $Im\text{-}3m$ – jhfedc

$Tb_3Ni_6Al_2H_{6.5}$ [1]
Structural features: Filled-up derivative of $Ce_3Ni_6Si_2$ with H in tetrahedral ($TbNi_3$, Tb_3Al and Ni_4) voids.

Yartys' V.A. et al. (1992) [1]
$Al_{2.02}D_{6.48}Ni_{5.98}Tb_3$
$a = 0.9064$ nm, $V = 0.7447$ nm^3, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	48j	m..	0	0.175	0.458	0.183	
M2	24h	$m.m$2	0	0.329	0.329		
D3	16f	.3m	0.123	0.123	0.123	0.919	single atom Al
Tb4	12e	4$m.m$	0.293	0	0		square antiprism D_8
D5	12d	-4m.2	$^1/_4$	0	$^1/_2$	0.204	
M6	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		colinear D_2

M2 = 0.96Ni + 0.04Al; M6 = 0.89Al + 0.11Ni
Experimental: powder, diffractometer, neutrons, $R_B = 0.083$

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

References: [1] Yartys' V.A., Pavlenko V.V., Khidirov I. (1992), Russ. J. Inorg. Chem. 37, 12-16 (Zh. Neorg. Khim. 37, 25-31). [2] Yartys' V.A., Pavlenko V.V., Khidirov I. (1992), Sov. J. Coord. Chem. 18, 371-377 (Koord. Khim. 18, 428-435).

$Th_6Br_{15}H_7$		$cI58$	(229) $Im\text{-}3m$ – hfeb

$Th_6Br_{15}H_7$ [1]

Structural features: Th_6Br_{18} clusters (Th_6 octahedron surrounded by a Br_{12} cuboctahedron and a Br_6 octahedron) share vertices of the Br_6 octahedron to form a 3D-framework. Part of the Th_6 octahedron faces are capped by H atoms (disorder).

Simon A. et al. (1991) [1]
$Br_{15}D_{7.04}Th_6$
$a = 1.13761$ nm, $V = 1.4722$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Br1	24h	$m.m2$	0	0.2582	0.2582		4-vertex polyhedron D_2Th_2
D2	16f	$.3m$	0.0901	0.0901	0.0901	0.88	non-coplanar triangle D_3
Th3	12e	$4m.m$	0.24	0	0		non-coplanar square D_4
Br4	6b	$4/mm.m$	0	$^1/_2$	$^1/_2$		colinear Th_2

Experimental: powder, diffractometer, neutrons, wR$_p$ = 0.075

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

References: [1] Simon A., Böttcher F., Cockcroft J.K. (1991), Angew. Chem. 103, 79-80. [2] Böttcher F., Simon A., Kremer R.K., Buchkremer Hermanns H., Cockcroft J.K. (1991), Z. Anorg. Allg. Chem. 598/599, 25-44.

Tl$_7$Sb$_2$		cI54	(229) Im-3m – hfea

Tl$_7$Sb$_2$ [2], Strukturbericht notation L2$_2$
Structural features: 27-atom nested polyhedra units consisting of a central Tl atom surrounded by a Tl$_8$ cube, a Sb$_6$ octahedron and a Tl$_{12}$ cuboctahedron.

Stokhuyzen R. et al. (1977) [1]
Sb$_2$Tl$_7$
a = 1.1618 nm, V = 1.5682 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Tl1	24h	$m.m$2	0	0.3497	0.3497		rhombic dodecahedron Sb$_4$Tl$_{10}$
Tl2	16f	.3m	0.1704	0.1704	0.1704		rhombic dodecahedron Tl$_{11}$Sb$_3$
Sb3	12e	4$m.m$	0.3138	0	0		rhombic dodecahedron Tl$_{13}$Sb
Tl4	2a	m-3m	0	0	0		rhombic dodecahedron Tl$_8$Sb$_6$

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

Remarks: Space group (217) I-43m was tested and rejected.
References: [1] Stokhuyzen R., Chieh C., Pearson W.B. (1977), Can. J. Chem. 55, 1120-1122. [2] (1931), Strukturberichte 1, 488.

$U_4(Re_{0.17}Si_{0.83})_{13}$	$cI34$	(229) $Im\text{-}3m$ – edca

$U_4(Si,Re)_{13}$ [1]

Structural features: Close-packed U(Si,Re)$_3$ layers in c stacking (Cu$_3$Au-type substructure), additional (Si,Re) in octahedral voids.

Akselrud L.G. et al. (1978) [1]
$Re_{2.21}Si_{10.79}U_4$
$a = 0.8192$ nm, $V = 0.5498$ nm^3, $Z = 2$

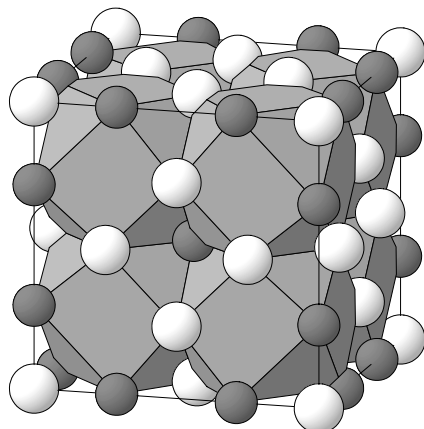| site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	12e	4m.m	0.302	0	0		tricapped trigonal prism Si$_5$U$_4$
M2	12d	-4m.2	$^1/_4$	0	$^1/_2$		cuboctahedron Si$_8$U$_4$
U3	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron Si$_{12}$
M4	2a	m-3m	0	0	0		octahedron Si$_6$

M1 = 0.83Si + 0.17Re; M2 = 0.83Si + 0.17Re; M4 = 0.83Si + 0.17Re
Experimental: powder, diffractometer, X-rays

References: [1] Akselrud L.G., Yarmolyuk Y.P., Gladyshevskii E.I. (1978), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1978, 359-362.

U$_4$Re$_7$Si$_6$ [1]

Structural features: Close-packed U$_2$Re$_3$Si$_3$ layers in c stacking (ordered Cu$_3$Au-type substructure), additional Re in octahedral voids. Ordering variant of pseudo-binary U$_4$(Si,Re)$_{13}$. See Fig. I.8.

Fig. I.8. **U$_4$Re$_7$Si$_6$**

Arrangement of U(Re$_6$Si$_6$) cubocta-hedra (Re atoms light, Si atoms dark) and additional Re atoms (at the origin).

Akselrud L.G. et al. (1978) [1]
Re$_7$Si$_6$U$_4$
a = 0.8224 nm, V = 0.5562 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	12e	4m.m	0.29	0	0		tricapped trigonal prism Re$_5$U$_4$
Re2	12d	-4m.2	$^1/_4$	0	$^1/_2$		cuboctahedron Si$_4$Re$_4$U$_4$
U3	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron Re$_6$Si$_6$
Re4	2a	m-3m	0	0	0		octahedron Si$_6$

Experimental: powder, diffractometer, X-rays, R = 0.105
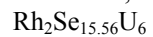
Remarks: Space group (217) *I*-43*m* was tested and rejected.

References: [1] Akselrud L.G., Yarmolyuk Y.P., Gladyshevskii E.I. (1978), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1978, 359-362.

$U_6Rh_2Se_{15.5}$		$cI98$	(229) Im-$3m$ – khdcb

$U_6Rh_2Se_{15.5}$ [1]

Structural features: $RhSe_6$ octahedra and USe_6Se_2 bicapped trigonal prisms share atoms to form a 3D-framework; additional Se (partial disorder) in intersecting channels.

Daoudi A., Noel H. (1996) [1]
$Rh_2Se_{15.56}U_6$
$a = 1.3737$ nm, $V = 2.5922$ nm^3, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Se1	48k	..m	0.1287	0.1287	0.3101		4-vertex polyhedron RhU_3
U2	24h	$m.m$2	0	0.2966	0.2966		square antiprism Se_8
Se3	12d	-4m.2	$^1/_4$	0	$^1/_2$		14-vertex Frank-Kasper U_4Se_{10}
Rh4	8c	.-3m	$^1/_4$	$^1/_4$	$^1/_4$		octahedron Se_6
Se5	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$	0.37	16-vertex polyhedron $Se_{12}U_4$

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

References: [1] Daoudi A., Noel H. (1996), J. Alloys Compd. 233, 169-173.

$V_{18}Fe_3[VO_4]_{0.5}[SO_4]_{0.5}O_{42}[H_2O]_{36}$	$cI240$	(229) Im-$3m$ – k^{2}jh^{2}fe^{2}ba

[Fe$_3$V$_{18}$O$_{42}$(H$_2$O)$_{12}$((V,S)O$_4$)]·24H$_2$O [1]

Structural features: $(S,V)_{18}O_{46}$ units consisting of eighteen VO_5 square pyramids sharing edges and vertices around a $(S,V)O_4$ tetrahedron (orientational disorder) are loosely interconnected via $Fe(H_2O)_4$ units to form two interpenetrating 3D-frameworks.
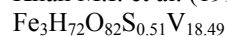
Khan M.I. et al. (1999) [1]
$Fe_3H_{72}O_{82}S_{0.51}V_{18.49}$
$a = 1.54679$ nm, $V = 3.7008$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48k	..m	0.0824	0.0824	0.2113		non-coplanar triangle V$_3$
(OH$_2$)2	48k	..m	0.1612	0.1612	0.3552		
(OH$_2$)3	48j	m..	0	0.3849	0.4294	0.5	
V4	24h	$m.m2$	0	0.16645	0.16645		
O5	24h	$m.m2$	0	0.239	0.239		
O6	16f	.3m	0.0574	0.0574	0.0574	0.5	
V7	12e	4$m.m$	0.25815	0	0		square pyramid O$_5$
O8	12e	4$m.m$	0.3639	0	0		colinear VFe
Fe9	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		
M10	2a	m-3m	0	0	0		square prism (cube) O$_8$

M10 = 0.51S + 0.49V
Experimental: single crystal, diffractometer, X-rays, R = 0.045

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] Khan M.I., Yohannes E., Doedens R.J. (1999), Angew. Chem. Int. Ed. 38, 1292-1294.

| VH$_{0.5}$ | | *cI*14 | (229) *Im-3m* – da |

VH$_{0.5}$ [1], (VH) α; AgI α [2]

Structural features: Filled-up derivative of W (prototype for a body-centered cubic atom arrangement) with H in tetrahedral voids.

Westlake D.G. et al. (1973) [1]

D$_{0.50}$V

$a = 0.314$ nm, $V = 0.0310$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
D1	12*d*	-4*m*.2	$^1/_4$	0	$^1/_2$	0.083	tetrahedron D$_4$
V2	2*a*	*m*-3*m*	0	0	0		24-vertex polyhedron D$_{24}$

Experimental: powder, diffractometer, neutrons, T = 425 K

Remarks: Cell parameter taken from figure. Partial occupation of the octahedral site in Wyckoff position 6*b* by H could not be excluded. So-called (VH) α' crystallizes in the same structure type, but contains more H.

References: [1] Westlake D.G., Mueller M.H., Knott H.W. (1973), J. Appl. Crystallogr. 6, 206-216. [2] Wright A.F., Fender B.E.F. (1977), J. Phys. C: Solid State Phys. 10, 2261-2267.

W [2], b.c.c. (body-centered cubic), Strukturbericht notation A2; Fe α [3]
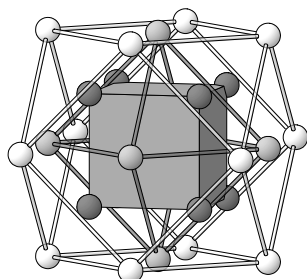Structural features: Infinite 3D-framework of fused WW$_8$ cubes. See Fig. I.6.

Fig. I.6. **W**

27-atom (W-type) nested polyhedra unit: W central atom + W$_8$ cube + W$_6$ octahedron + W$_{12}$ cuboctahedron.

Hartmann H. et al. (1931) [1]
W
a = 0.315 nm, V = 0.0313 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
W1	2*a*	*m*-3*m*	0	0	0		rhombic dodecahedron W$_{14}$

Experimental: powder, film, X-rays

Remarks: According to [4] ferromagnetic Fe α has tetragonal symmetry.

References: [1] Hartmann H., Ebert F., Bretschneider O. (1931), Z. Anorg. Allg. Chem. 198, 116-140. [2] (1931), Strukturberichte 1, 15, 61. [3] (1931), Strukturberichte 1, 16, 66. [4] Izyumov Yu.A., Naish V.E., Ozerov R.P. (1991), Neutron Diffraction of Magnetic Materials, New York: Consultants Bureau, 1991, p. 50.

| $Y_3Fe_{62}B_{14}$ | | $cI158$ | (229) Im-$3m$ – kjf^{2}edb |

$Y_3Fe_{62}B_{14}$ [1]
Structural features: Distorted Fe(Fe$_{11}$Y) icosahedra interpenetrate to form a 3D-framework.

De Mooij D.B. et al. (1987) [1]
B$_{14}$Fe$_{62}$Y$_3$
$a = 1.236$ nm, $V = 1.8882$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	48k	..m	0.156	0.156	0.4		icosahedron Fe$_{11}$Y
Fe2	48j	m..	0	0.148	0.291		14-vertex Frank-Kasper B$_3$Fe$_{10}$Y
B3	16f	.3m	0.083	0.083	0.083		7-vertex polyhedron B$_6$Fe
Fe4	16f	.3m	0.191	0.191	0.191		14-vertex Frank-Kasper BFe$_{13}$
B5	12e	4m.m	0.21	0	0		square antiprism Fe$_4$B$_4$
Fe6	12d	-4m.2	$^1/_4$	0	$^1/_2$		14-vertex Frank-Kasper Fe$_{12}$Y$_2$
Y7	6b	4/mm.m	0	$^1/_2$	$^1/_2$		22-vertex polyhedron Fe$_{20}$B$_2$

Experimental: powder, diffractometer, X-rays, R$_B$ = 0.150

Remarks: Metastable phase.

References: [1] De Mooij D.B., Daams J.L.C., Buschow K.H.J. (1987), Philips J. Res. 42, 339-349.

Y$_4$PdGa$_{12}$		*cI*34	(229) *Im*-3*m* – edca

Y$_4$PdGa$_{12}$ [1]

Structural features: Close-packed YGa$_3$ layers in c stacking (Cu$_3$Au-type substructure), Pd in octahedral voids. Ordered variant of pseudo-binary U$_4$(Si,Re)$_{13}$.

Vasilechko L.O. et al. (1988) [1]
Ga$_{12}$PdY$_4$
a = 0.8598 nm, V = 0.6356 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	12*e*	4*m.m*	0.296	0	0		tricapped trigonal prism PdGa$_4$Y$_4$
Ga2	12*d*	-4*m.2*	$^1/_4$	0	$^1/_2$		cuboctahedron Ga$_8$Y$_4$
Y3	8*c*	.-3*m*	$^1/_4$	$^1/_4$	$^1/_4$		cuboctahedron Ga$_{12}$
Pd4	2*a*	*m*-3*m*	0	0	0		octahedron Ga$_6$

Experimental: powder, diffractometer, X-rays, R$_B$ = 0.075

References: [1] Vasilechko L.O., Noga A.S., Grin Y.N., Koterlin M.D., Yarmolyuk Y.P. (1988), Russ. Metall. 1988(5), 216-220 (Izv. Akad. Nauk SSSR, Met. 1988(5) 216-220).

$Yb_{11}Ni_{60}C_6$		$cI154$	(229) $Im\text{-}3m$ – kjfe^{2}db

$Yb_{11}Ni_{60}C_6$ [2]; $Tm_{11}Ni_{60}C_6$ [3]
Structural features: C in $YbNi_5$ octahedral voids.

Moss M.A., Jeitschko W. (1992) [1]
$C_6Ni_{60}Yb_{11}$
$a = 1.2441$ nm, $V = 1.9256$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	48k	..m	0.32644	0.32644	0.09298		pseudo Frank-Kasper Ni_9Yb_3C
Ni2	48j	m..	0	0.14866	0.31742		single atom C
Yb3	16f	.3m	0.16817	0.16817	0.16817		19-vertex polyhedron $Ni_{15}C_3Yb$
Ni4	12e	4$m.m$	0.1446	0	0		single atom C
C5	12e	4$m.m$	0.2944	0	0		square pyramid Ni_5
Ni6	12d	-4m.2	$^1/_4$	0	$^1/_2$		14-vertex Frank-Kasper $Ni_{12}Yb_2$
Yb7	6b	4/$mm.m$	0	$^1/_2$	$^1/_2$		22-vertex polyhedron C_2Ni_{20}

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

Remarks: Refinement of the site occupancies showed no significant deviation from unity. Data for $Tm_{11}Ni_{60}C_6$ also reported in [4]. A report on so-called $Y_5Ni_{29}C_3$ [5] is superseded (see [1]).

References: [1] Moss M.A., Jeitschko W. (1992), J. Alloys Compd. 182, 157-164. [2] Putyatin A.A. (1987), Moscow Univ. Chem. Bull. (Engl. Transl.) 42, 108-113. [3] Khalili M.M., Bodak O.I., Marusin E.P., Pecharskaya A.O. (1990), Sov. Phys. Crystallogr. (Engl. Transl.) 35, 812-813. [4] Pecharskaya A.O., Bodak O.I., Marusin E.P., Halili M.M. (1989), XII Eur. Crystallogr. Meet., Moscow, 1989, Coll. Abs. 2, 127. [5] Stadelmaier H.H., Kim S.B. (1984), Z. Metallkd. 75, 381-383.