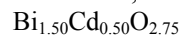
*cI40**(230) Ia-3d – da* **$\text{Cd}_{0.5}\text{Bi}_{1.5}\text{O}_{2.75}$ ht [1]**

Structural features: (Bi,Cd)O₆ octahedra share atoms to form a 3D-framework with disordered vacancies in the O sublattice.

Sillén L.G., Sillén B. (1941) [1]



$a = 0.8472 \text{ nm}$, $V = 0.6081 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$24d$	-4..	$\frac{3}{8}$	0	$\frac{1}{4}$	0.917	tetrahedron Bi ₄
M2	$16a$	-.3.	0	0	0		octahedron O ₆

$\text{M2} = 0.75\text{Bi} + 0.25\text{Cd}$

Experimental: powder, film, X-rays

Remarks: Phase stable at $T > 915 \text{ K}$, homogeneity range $\text{Bi}_{1-x}\text{Cd}_x\text{O}_{1.5-x/2}$, $x = 0.11-0.25$ at 983 K [2]. The structure was later refined in space group *(229) Im-3m* with $\frac{1}{8}$ cell volume [2].

References: [1] Sillén L.G., Sillén B. (1941), *Z. Phys. Chem., Abt. B* 49, 27-33. [2] Graia T., Conflant P., Nowogrocki G., Boivin J.C., Thomas D. (1986), *J. Solid State Chem.* 63, 160-165.

(Mn_{0.88}Mg_{0.06}Cu_{0.06})₉MnAs₆O₁₈(Cl_{0.80}[OH]_{0.20})

cI696

(230) *Ia-3d* – h⁵g⁴d

(Mn,Mg,Cu)₉MnAs₆O₁₈(OH,Cl) [1], magnussonite

Structural features: Single :AsO₃ ψ -tetrahedra share atoms with distorted MnO₈ cubes, MnO₆ octahedra, MnO₆ trigonal prisms and MnO₄ squares to form a 3D-framework; additional Mn (Mn⁺) in octahedral voids surrounded by As electron lone pairs.

Moore P.B., Araki T. (1979) [1]

As₆Cl_{0.80}Cu_{0.51}H_{0.20}Mg_{0.56}Mn_{8.88}O_{18.20}

a = 1.968 nm, *V* = 7.6221 nm³, *Z* = 16

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.03884	0.31841	0.05683		single atom As
O2	96 <i>h</i>	1	0.07014	0.18021	0.2866		non-coplanar triangle AsMn ₂
O3	96 <i>h</i>	1	0.08379	0.30555	0.3227		single atom As
As4	96 <i>h</i>	1	0.1162	0.25088	0.25839		non-coplanar triangle O ₃
Mn5	96 <i>h</i>	1	0.23664	0.2425	0.25073	0.158	
M6	48 <i>g</i>	..2	1/8	0.01737	0.23263	0.5	
M7	48 <i>g</i>	..2	1/8	0.14136	0.10864	0.333	
M8	48 <i>g</i>	..2	1/8	0.61266	0.63734		octahedron O ₆
M9	48 <i>g</i>	..2	1/8	0.73577	0.51423		trigonal prism O ₆
M10	24 <i>d</i>	-4..	3/8	0	1/4		square antiprism O ₈

M6 = 0.66Mn + 0.34Cu; M7 = 0.80Cl + 0.20OH; M8 = 0.90Mn + 0.10Mg; M9 = 0.94Mn + 0.06Mg; M10 = 0.95Mn + 0.05Mg

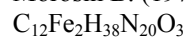
Experimental: single crystal, diffractometer, X-rays, R = 0.082

Remarks: Natural specimen from Långban mine, Värmland, Sweden. 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] Moore P.B., Araki T. (1979), *Am. Mineral.* 64, 390-401.

*cI296* $(230) Ia-3d - h^2gcba$ **(NH₄)₄Fe(CN)₆·1.5H₂O [1]**Structural features: Single Fe(CN)₆ octahedra.

Morosin B. (1978) [1]

 $a = 1.8261 \text{ nm}, V = 6.0894 \text{ nm}^3, Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	96 <i>h</i>	1	0.0975	0.1943	0.2895		single atom C
C2	96 <i>h</i>	1	0.1554	0.2146	0.2755		single atom N
(NH ₄)3	48 <i>g</i>	..2	$\frac{1}{8}$	0.7074	0.5426		non-colinear N ₂
(OH ₂)4	24 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		colinear (NH ₄) ₂
(NH ₄)5	16 <i>b</i>	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		tricapped trigonal prism (OH ₂) ₃ C ₆
Fe6	16 <i>a</i>	-.3.	0	0	0		octahedron C ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.068

Remarks: The atom coordinates of former N3 are interpreted in agreement with [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Morosin B. (1978), Acta Crystallogr. B 34, 3730-3731. [2] Hellner E., Koch E. (1982), Acta Crystallogr. B 38, 376-379.

$\text{Ca}_{15}\text{B}_6\text{C}_{10}\text{N}_6\text{O}$ $cI312$ $(230) Ia-3d - h^2\text{geca}$ **Ca₁₅(CBN)₆(C₂)₂O** [1]

Structural features: C-B-N linear units and C-C dumbbells (triple bond) in substitutional disorder.

Wörle M. et al. (1997) [1]

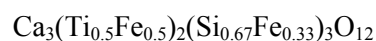
 $\text{B}_6\text{C}_{9.40}\text{Ca}_{15}\text{N}_{6.60}\text{O}_{0.96}$ $a = 1.65684 \text{ nm}$, $V = 4.5482 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	96h	1	0.0226	0.0809	0.3301		single atom B
Ca2	96h	1	0.11899	0.1982	0.29805		tetrahedron ON ₃
B3	48g	..2	$\frac{1}{8}$	0.7203	0.5297		non-colinear N ₂
C4	32e	.3.	0.1059	0.1059	0.1059		single atom C
Ca5	24c	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		coplanar square N ₄
O6	16a	-.3.	0	0	0	0.48	octahedron Ca ₆

 $M1 = 0.55N + 0.45C$

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

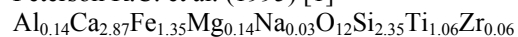
References: [1] Wörle M., Muhr H. J., Meyer H., Nesper R. (1997), J. Alloys Compd. 260, 80-87.


cI256

 (230) *Ia-3d* – *h²dca*
Ca₃(Ti_{0.5}Fe_{0.5})(Si_{0.67}Fe_{0.33})₃O₁₂ [1], schorlomite, garnet family

 Structural features: (Ti,Fe)O₆ octahedra and (Si,Fe)O₄ tetrahedra share atoms to form a 3D-framework; Ca in 8-fold coordination. Splitting of the O site corresponds to occupation of the tetrahedral positions by either Si or Fe.

Peterson R.C. et al. (1995) [1]



$$a = 1.2157 \text{ nm}, V = 1.7967 \text{ nm}^3, Z = 8$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96 <i>h</i>	1	0.0944	0.2021	0.2906	0.783	
O2	96 <i>h</i>	1	0.11	0.198	0.271	0.217	
M3	24 <i>d</i>	-4..	³ / ₈	0	¹ / ₄		tetrahedron O ₄
M4	24 <i>c</i>	2.22	¹ / ₈	0	¹ / ₄		
M5	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

$$\text{M3} = 0.783\text{Si} + 0.217\text{Fe}; \text{M4} = 0.957\text{Ca} + 0.033\text{Mg} + 0.010\text{Na}; \text{M5} = 0.53\text{Ti} + 0.35\text{Fe} + 0.07\text{Al} + 0.03\text{Zr} + 0.02\text{Mg}$$

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

 Remarks: Natural specimen from Ice River alkaline intrusive complex, Yoho National Park, British Columbia.
 Composition $[\text{Ca}_{2.87}\text{Mg}_{0.10}\text{Na}_{0.04}][\text{Ti}_{1.06}\text{Fe}^{3+}_{0.34}\text{Al}_{0.14}\text{Fe}^{2+}_{0.06}\text{Zr}_{0.04}\text{Mg}_{0.04}\text{Mn}_{0.03}\text{V}_{0.01}](\text{Si}_{2.35}\text{Fe}^{3+}_{0.34}\text{Fe}^{2+}_{0.31})\text{O}_{12}$ from XANES and Mössbauer spectroscopy. Short interatomic distances for partly occupied site(s).

 References: [1] Peterson R.C., Locock A.J., Luth R.W. (1995), *Can. Mineral.* 33, 627-631.

Ca₃Al₂(OH)₁₂ [2], hydrogarnet, garnet family, Strukturbericht notation J2₃
Structural features: Single Al(OH)₆ octahedra. See Fig. I.1.

Smrcok L. (1987) [1]

Al₂Ca₃H₁₂O₁₂

$a = 1.25755 \text{ nm}$, $V = 1.9887 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96 <i>h</i>	1	0.1099	0.1973	0.279		single atom Al
Ca2	24 <i>c</i>	2.22	1/8	0	1/4		square antiprism O ₈
Al3	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆
H4	96 <i>h</i>	1	0.0959	0.206	0.3281		

Experimental: powder, diffractometer, X-rays, $R_B = 0.018$

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

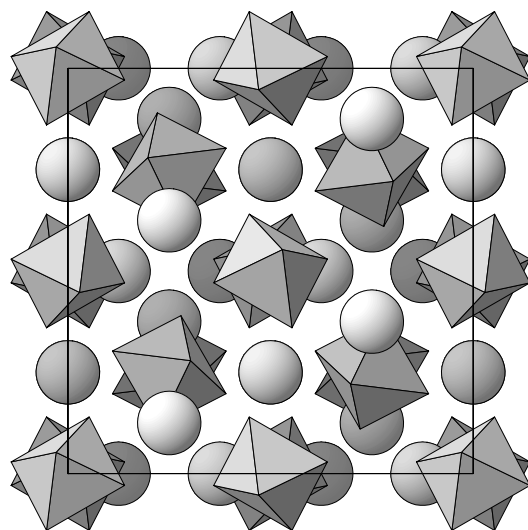


Fig. I.1. **Ca₃Al₂(OH)₁₂**

Arrangement of Al(OH)₆ octahedra and Ca atoms.

References: [1] Smrcok L. (1987), J. Appl. Crystallogr. 20, 320-322. [2] Büsser W., Eitel A. (1936), Z. Kristallogr. 95, 175-188.

Ca₃Al₂Si₃O₁₂ [2], grossular, garnet, Strukturbericht notation S1₄

Structural features: AlO₆ octahedra and SiO₄ tetrahedra share vertices to form a 3D-framework; Ca in 8-fold coordination. See Fig. I.2.

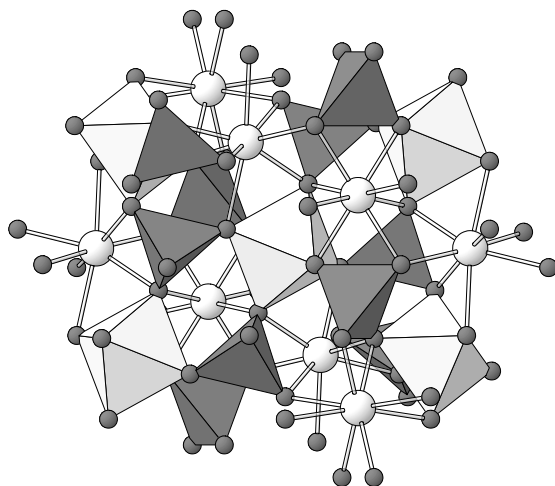


Fig. I.2. **Ca₃Al₂Si₃O₁₂**

Arrangement of SiO₄ tetrahedra (dark), AlO₆ octahedra (light) and CaO₈ polyhedra (Ca atoms large, O atoms small).

Sawada H. (1999) [1]

Al₂Ca₃O₁₂Si₃

$a = 1.18504 \text{ nm}$, $V = 1.6642 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96 <i>h</i>	1	0.09869	0.20477	0.28825		non-colinear SiAl
Si2	24 <i>d</i>	-4..	$\frac{3}{8}$	0	$\frac{1}{4}$		tetrahedron O ₄
Ca3	24 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		square antiprism O ₈
Al4	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, $R = 0.008$

Remarks: Natural specimen from Quebec. Grossular refers to the mineral, garnet to the structure type. Electron density study.

References: [1] Sawada H. (1999), *J. Solid State Chem.* 142, 273-278. [2] Menzer G. (1926), *Z. Kristallogr.* 63, 157-158.

$\text{Ca}_3\text{Mn}_{2.26}[\text{SiO}_4]_{2.42}\text{O}_{2.32}$ *cI208**(230) Ia-3d – hgdca***Ca₃Mn_{2.26}(SiO₄)_{2.42}O_{2.32}** [1], henritermierite dehydratedStructural features: SiO₄ tetrahedra and MnO₆ octahedra share atoms to form a 3D-framework; part of Si is replaced by additional Mn in octahedral coordination (disorder).

Armbruster T. et al. (2001) [1]

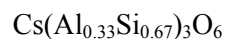
 $\text{Ca}_3\text{Mn}_{2.26}\text{O}_{12}\text{Si}_{2.43}$ $a = 1.21225 \text{ nm}$, $V = 1.7815 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96h	1	0.096	0.2013	0.2873		single atom Si
Mn2	48g	..2	$\frac{1}{8}$	0.688	0.562	0.044	8-vertex polyhedron Si ₂ O ₆
Si3	24d	-4..	$\frac{3}{8}$	0	$\frac{1}{4}$	0.81	square antiprism O ₄ Mn ₄
Ca4	24c	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		square prism (cube) O ₈
Mn5	16a	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.040, T = 293 K

Remarks: Natural specimen from N'Chwaning II mine, Kalahari manganese fields; dehydrated.

References: [1] Armbruster T., Kohler T., Libowitzky E., Friedrich A., Miletich R., Kunz M., Medenbach O., Gutzmer J. (2001), *Am. Mineral.* 86, 147-158.

*cI160**(230) Ia-3d – hgb*

CsAlSi₂O₆ rt [2], pollucite, zeolite ANA-Cs; **KAlSi₂O₆ ht** [3], leucite high, zeolite ANA-K

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; Cs in non-intersecting channels along $\langle 111 \rangle$.

Yanase I. et al. (1997) [1]



$$a = 1.36645 \text{ nm}, V = 2.5514 \text{ nm}^3, Z = 16$$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.03	0.116	0.351		non-colinear Si ₂
M2	48 <i>g</i>	..2	$\frac{1}{8}$	0.6628	0.5872		tetrahedron O ₄
Cs3	16 <i>b</i>	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		icosahedron O ₁₂

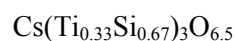
$$\text{M2} = 0.667\text{Si} + 0.333\text{Al}$$

Experimental: powder, diffractometer, X-rays, R = 0.017, T = 273 K

Remarks: Phase stable at T > 270 K.

References: [1] Yanase I., Kobayashi H., Shibasaki Y., Mitamura T. (1997), J. Am. Ceram. Soc. 80, 2693-2695.

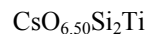
[2] Naray Szabo S. (1938), Z. Kristallogr. 99, 277-282. [3] Wyart M.J. (1940), Bull. Soc. Fr. Mineral. 63, 5-17.

 $cI352$ $(230) Ia-3d - h^3gb$

CsTiSi₂O_{6.5} [2], zeolite ANA(Ti)-Cs

Structural features: (Si,Ti)O₄ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; Cs in non-intersecting channels along $\langle 111 \rangle$, additional O bonded to Cs.

Balmer M.L. et al. (1997) [1]



$$a = 1.38417 \text{ nm}, V = 2.6520 \text{ nm}^3, Z = 16$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96h	1	0.0325	0.1151	0.3542		5-vertex polyhedron Si ₂ O ₃
O2	96h	1	0.044	0.229	0.312	0.06	single atom O
O3	96h	1	0.209	0.295	0.235	0.023	
M4	48g	..2	$\frac{1}{8}$	0.661	0.589		tetrahedron O ₄
Cs5	16b	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		

$$\text{M4} = 0.667\text{Si} + 0.333\text{Ti}$$

Experimental: powder, diffractometer, neutrons, $R_p = 0.057$

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

References: [1] Balmer M.L., Huang Q., Wong Ng W., Roth R.S., Santoro A. (1997), J. Solid State Chem. 130, 97-102. [2] McCready D.E., Balmer M.L., Keefer K.D. (1997), Powder Diffr. 12, 40-46.

$\text{Cs}_3\text{Na}_4(\text{Ga}_{0.29}\text{Si}_{0.71})_{24}\text{O}_{48}$

cI208

(230) *Ia-3d* – hgfb**Cs₆Na₈Ga₁₄Si₃₄O₉₆** [1], zeolite ANA(Ga)-Cs,NaStructural features: (Si,Ga)O₄ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; Na near the centers of 8-rings (split site), Cs in non-intersecting channels along <111>.

Yelon W.B. et al. (1990) [1]

 $\text{Cs}_{2.98}\text{Ga}_{6.94}\text{Na}_{3.96}\text{O}_{48}\text{Si}_{17.06}$ $a = 1.3703 \text{ nm}$, $V = 2.5730 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.0312	0.1154	0.3548		non-colinear Si ₂
M2	48 <i>g</i>	..2	¹ / ₈	0.6631	0.5869		tetrahedron O ₄
Na3	48 <i>f</i>	2..	0.058	0	¹ / ₄	0.165	
Cs4	16 <i>b</i>	.32	¹ / ₈	¹ / ₈	¹ / ₈	0.373	

 $\text{M2} = 0.711\text{Si} + 0.289\text{Ga}$ Experimental: powder, diffractometer, neutrons, $R_B = 0.116$

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

References: [1] Yelon W.B., Xie D., Newsam J.M., Dunn J. (1990), *Zeolites* 10, 553-558.

$\text{CsTi}_2[\text{AsO}_4]_3$ *cI608**(230) Ia-3d - h⁵g²ba***CsTi₂As₃O₁₂** [1]

Structural features: TiO₆ octahedra and AsO₄ tetrahedra share vertices to form a 3D-framework; Cs in large voids interconnected by a 3D-system of channels.

Kwang Hwa Lii (1995) [1]

 $\text{As}_3\text{CsO}_{12}\text{Ti}_2$ $a = 2.0495 \text{ nm}$, $V = 8.6088 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.0547	0.1549	0.2696		non-colinear AsTi
O2	96 <i>h</i>	1	0.068	0.287	0.2617		non-colinear AsTi
O3	96 <i>h</i>	1	0.0928	0.2204	0.3791		non-colinear AsTi
As4	96 <i>h</i>	1	0.09699	0.21891	0.29768		tetrahedron O ₄
O5	96 <i>h</i>	1	0.1742	0.2021	0.2769		non-colinear AsTi
Cs6	48 <i>g</i>	..2	$\frac{1}{8}$	0.01916	0.23084	0.5	14-vertex Frank-Kasper O ₁₂ Cs ₂
Ti7	48 <i>g</i>	..2	$\frac{1}{8}$	0.7145	0.5355		octahedron O ₆
Cs8	16 <i>b</i>	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	0.5	15-vertex Frank-Kasper O ₁₂ Cs ₃
Ti9	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, wR = 0.021, T = 296 K

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

References: [1] Kwang Hwa Lii (1995), Inorg. Chem. 34, 1700-1704.

Hg₃[TeO₆]

*c*1160

(230) *Ia-3d* – hga

Hg₃TeO₆ [1]

Structural features: Single TeO₆ octahedra.

Falqui M.T. (1963) [1]

Hg₃O₆Te

a = 1.3392 nm, *V* = 2.4018 nm³, *Z* = 16

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.11	0.215	0.285		tetrahedron TeHg ₃
Hg2	48 <i>g</i>	..2	¹ / ₈	0.7083	0.5417		octahedron O ₆
Te3	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, Weissenberg and rotation photographs, X-rays, *R* = 0.094

References: [1] Falqui M.T. (1963), Ric. Sci., Parte 2, Sez. A 33, 627-634.

$\text{Hg}_6\text{Cl}_3\text{O}[\text{OH}]$

cI176

(230) *Ia-3d* – hge**Hg₆O(OH)Cl₃** [2], eglestonite

Structural features: Hg-Hg dumbbells are interconnected via O-H···O bridges to form infinite chains in three mutually perpendicular directions.

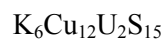
Mereiter K. et al. (1992) [1]

 $\text{Cl}_3\text{HHg}_6\text{O}_2$ $a = 1.6036 \text{ nm}$, $V = 4.1237 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Hg1	96h	1	0.0091	0.17229	0.01331		trigonal bipyramid OHgCl ₃
Cl2	48g	..2	¹ / ₈	0.63648	0.61352		octahedron Hg ₆
O3	32e	.3.	0.0449	0.0449	0.0449		tetrahedron Hg ₃ O
H4	32e	.3.	0.0069	0.0069	0.0069	0.5	

Experimental: powder, diffractometer, neutrons, $R_B = 0.065$ 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 reports on eglestonite with composition Hg₄Cl₂O ([3], [4], [5]).

References: [1] Mereiter K., Zemann J., Hewat A.W. (1992), Am. Mineral. 77, 839-842. [2] Mereiter K., Zemann J. (1976), Tschermaks Mineral. Petrogr. Mitt. 23, 105-115. [3] Hillebrand W.F., Schaller W.T. (1909), U.S. Geol. Surv. Bull. 405, 1-174. [4] Vershovskaya O.V., Chernitsova N.M., Vlasova E.V., Valiyeva A.A., Stepanov I.I. (1979), Dokl. Akad. Nauk SSSR 248, 715-718. [5] Vasiliev V.I., Lavrentiev Y.G. (1986), Dokl. Akad. Nauk SSSR 287, 960-963.

*cI280**(230) Ia-3d - h²gca***K₆Cu₁₂U₂S₁₅** [1]

Structural features: US₆ octahedra and CuS₃ trigonal units share edges and vertices to form a 3D-framework; K in channels.

Sutorik A.C. et al. (2000) [1]

 $a = 1.8642 \text{ nm}$, $V = 6.4785 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	96 <i>h</i>	1	0.0077	0.1427	0.076		non-coplanar triangle S ₃
S2	96 <i>h</i>	1	0.1223	0.2066	0.2884		non-coplanar triangle Cu ₂ U
K3	48 <i>g</i>	..2	¹ / ₈	0.7171	0.5329		14-vertex Frank-Kasper S ₈ Cu ₆
S4	24 <i>c</i>	2.22	¹ / ₈	0	¹ / ₄		tetrahedron Cu ₄
U5	16 <i>a</i>	..3.	0	0	0		icosahedron S ₆ Cu ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.044, T = 296 K

References: [1] Sutorik A.C., Patschke R., Schindler J., Kannewurf C.R., Kanatzidis M.G. (2000), Chem. Eur. J. 6, 1601-1607.

KBi₆IO₉

cI272

(230) *Ia-3d* – hg²fba**KBi₆O₉I** [2]

Structural features: :BiO₅ ψ -octahedra and :BiO₄ square ψ -pyramids share atoms to form a 3D-framework; K and I form non-intersecting infinite chains.

Eggenweiler U. et al. (1998) [1]

Bi₆IKO₉

$a = 1.7254$ nm, $V = 5.1365$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96h	1	0.0982	0.2487	0.3137		non-coplanar triangle Bi ₃
Bi2	48g	..2	$\frac{1}{8}$	0.64331	0.60669		5-vertex polyhedron O ₅
O3	48g	..2	$\frac{1}{8}$	0.7293	0.5207		coplanar triangle Bi ₃
Bi4	48f	2..	0.01199	0	$\frac{1}{4}$		4-vertex polyhedron O ₄
I5	16b	.32	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$		7-capped pentagonal prism O ₉ Bi ₆ K ₂
K6	16a	-.3.	0	0	0		octahedron O ₆

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

References: [1] Eggenweiler U., Keller E., Krämer V., Meyer C.A., Ketterer J. (1998), Z. Kristallogr. 213, 377-381. [2] Eggenweiler U., Keller E., Krämer V. (1997), Z. Kristallogr., New Cryst. Struct. 212, 88.

$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$ *cI176**(230) Ia-3d – hdcba***Li₅La₃Nb₂O₁₂** [1]; **Li₅La₃Ta₂O₁₂** [1]Structural features: NbO₆ octahedra, LiO₄ tetrahedra and LaO₈ polyhedra share atoms to form a garnet-type substructure; additional Li in tetrahedral voids.

Mazza D. (1988) [1]

 $\text{La}_3\text{Li}_5\text{Nb}_2\text{O}_{12}$ $a = 1.2889 \text{ nm}$, $V = 2.1412 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.103	0.202	0.284		non-colinear LiNb
Li2	24 <i>d</i>	-4..	³ / ₈	0	¹ / ₄		tetrahedron O ₄
La3	24 <i>c</i>	2.22	¹ / ₈	0	¹ / ₄		bicapped square antiprism Li ₂ O ₈
Li4	16 <i>b</i>	.32	¹ / ₈	¹ / ₈	¹ / ₈		tricapped trigonal prism La ₃ O ₆
Nb5	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

Experimental: powder, diffractometer, X-rays, R = 0.060

References: [1] Mazza D. (1988), Mater. Lett. 7, 205-207.

$\text{Na}_{0.33}\text{Nb}_2\text{Cl}_5$ *cI384**(230) Ia-3d - h³gf***NaNb₆Cl₁₅ rt** [1]

Structural features: Nb₆Cl₁₈ clusters (Nb₆ octahedron surrounded by a Cl₁₂ cuboctahedron and a Cl₆ octahedron) share vertices of the Cl₆ octahedron to form a 3D-framework; Na in disordered arrangement.

Sägebarth M.E. et al. (1995) [1]

Cl₅Na_{0.32}Nb₂ $a = 2.0417 \text{ nm}$, $V = 8.5109 \text{ nm}^3$, $Z = 48$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cl1	96 <i>h</i>	1	0.02956	0.05073	0.15777		non-colinear Nb ₂
Cl2	96 <i>h</i>	1	0.139	0.23174	0.37429		non-colinear Nb ₂
Nb3	96 <i>h</i>	1	0.17392	0.28285	0.19137		monocapped square prism Cl ₅ Nb ₄
Cl4	48 <i>g</i>	..2	¹ / ₈	0.57191	0.67808		non-colinear Nb ₂
Na5	48 <i>f</i>	2..	0.318	0	¹ / ₄	0.322	tricapped trigonal prism NaCl ₈

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

Remarks: Phase stable at $T > 150 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Sägebarth M.E., Simon A., Imoto H., Weppner W., Kliche G. (1995), *Z. Anorg. Allg. Chem.* 621, 1589-1596.

$\text{Na}_{0.5}\text{Zr}_6\text{CCl}_{15}$ $cI400$ $(230) Ia-3d - h^3g^2a$ **$\text{Na}_{0.5}\text{Zr}_6\text{Cl}_{15}\text{C}$ [1]**

Structural features: $\text{CZr}_6\text{Cl}_{18}$ clusters (a central C atom surrounded by a Ta_6 octahedron, a Cl_{12} cuboctahedron and a Cl_6 octahedron) share vertices of the Cl_6 octahedron to form a 3D-framework; Na in disordered arrangement.

Ziebarth R.P., Corbett J.D. (1988) [1]

 $\text{CCl}_{15}\text{Na}_{0.54}\text{Zr}_6$ $a = 2.1466 \text{ nm}$, $V = 9.8913 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	96h	1	0.0294	0.05022	0.15554		non-coplanar triangle Zr_2Na
Cl2	96h	1	0.14129	0.23116	0.37305		non-coplanar triangle Zr_2Na
Zr3	96h	1	0.1704	0.28455	0.18909		octahedron CCl_5
Cl4	48g	..2	$\frac{1}{8}$	0.57195	0.67805		non-colinear Zr_2
Na5	48g	..2	$\frac{1}{8}$	0.747	0.503	0.18	tetrahedron Cl_4
C6	16a	..3.	0	0	0		octahedron Zr_6

Experimental: single crystal, diffractometer, X-rays, $R = 0.032$ References: [1] Ziebarth R.P., Corbett J.D. (1988), *J. Less-Common Met.* 137, 21-34.

NaAlSi₂O₆·H₂O [2], analcime-1C, zeolite ANA-Na hydrated, Strukturbericht notation S6₁

Structural features: (Si,Al)O₄ tetrahedra share vertices to form an ANA-type zeolite framework with 4-, 6- and 8-rings; Na at the centers of 8-rings, H₂O in non-intersecting channels along <111>. See Fig. I.4.

Ferraris G. et al. (1972) [1]

Al_{7.99}H₁₆Na₈O₅₆Si_{16.01}

$a = 1.373 \text{ nm}$, $V = 2.5883 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	96 <i>h</i>	1	0.03068	0.1156	0.35428		non-colinear Si ₂
M2	48 <i>g</i>	..2	1/8	0.66208	0.58792		tetrahedron O ₄
Na3	24 <i>c</i>	2.22	1/8	0	1/4	0.667	octahedron O ₆
O4	16 <i>b</i>	.32	1/8	1/8	1/8		coplanar triangle Na ₃
H5	96 <i>h</i>	1	0.0548	0.1402	0.1006	0.25	
H6	32 <i>e</i>	.3.	0.0791	0.0791	0.0791	0.25	

M2 = 0.667Si + 0.333Al

Experimental: single crystal, diffractometer, neutrons, R = 0.044

Remarks: Natural specimen from Cyclopean Islands. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the *z*-coordinate of the O site in Wyckoff position 96*h* is misprinted as 0.21932 instead of 0.71932 (checked on interatomic distances).

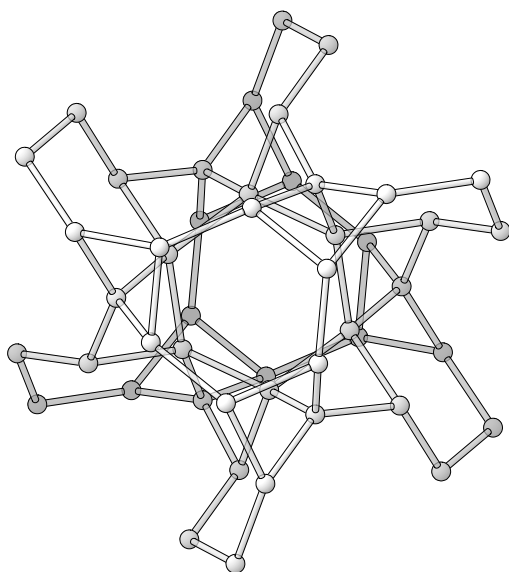


Fig. I.4. **NaAlSi₂O₆·H₂O**

ANA-type (Si,Al) framework.

References: [1] Ferraris G., Jones D.W., Yerkess J. (1972), Z. Kristallogr. 135, 240-252. [2] Taylor W.H. (1930), Z. Kristallogr. 74, 1-19.

Ni_3Ga_4 $cI112$ $(230) Ia-3d - gfa$ **Ni₃Ga₄** [1]

Structural features: Vacancy derivative of CsCl, which is an ordering variant of W (b.c.c.), with 25% of the Ni positions vacant, $[\text{Ni}_3\Box][\text{Ga}_4]$.

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

 Ga_4Ni_3 $a = 1.1411 \text{ nm}$, $V = 1.4858 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	48g	..2	$\frac{1}{8}$	0.625	0.625		anticuboctahedron Ga_8Ni_4
Ga2	48f	2..	0.0	0	$\frac{1}{4}$		anticuboctahedron Ni_6Ga_6
Ga3	16a	.-3.	0	0	0		cuboctahedron Ni_6Ga_6

Experimental: powder, Guinier film, X-rays

References: [1] Ellner M., Best K.J., Jacobi H., Schubert K. (1969), J. Less-Common Met. 19, 294-296.

RhBi₄*cI120**(230) Ia-3d – hc***RhBi₄ α** [2]

Structural features: Distorted RhBi₈ cubes share atoms to form a 3D-framework. Atom arrangement similar to the substructure formed by Ca and O in garnet (Ca₃Al₂Si₃O₁₂).

Glagoleva V.P., Zhdanov G.S. (1956) [1]

Bi₄Rh

$a = 1.4928$ nm, $V = 3.3266$ nm³, $Z = 24$

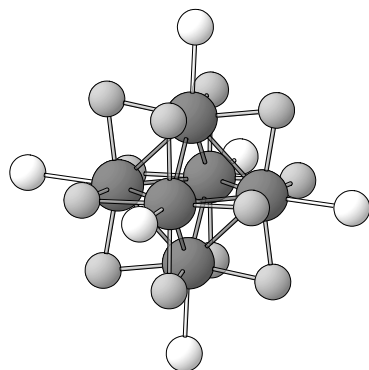
site	Wyck.	sym.	x	y	z	occ.	atomic environment
Bi1	96 <i>h</i>	1	0.097	0.186	0.274		non-colinear Rh ₂
Rh2	24 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		square prism (cube) Bi ₈

Experimental: single crystal, oscillation photographs, X-rays

References: [1] Glagoleva V.P., Zhdanov G.S. (1956), Sov. Phys. JETP (Engl. Transl.) 3, 155-158. [2] Zhuralev N.N., Zhdanov G.S. (1955), Zh. Eksp. Teor. Fiz. 28, 228-236.

Ta₆Cl₁₅ [2]

Structural features: Ta₆Cl₁₈ clusters (Ta₆ octahedron surrounded by a Cl₁₂ cuboctahedron and a Cl₆ octahedron) share vertices of the Cl₆ octahedron to form a 3D-framework. See Fig. I.5.

Fig. I.5. **Ta₆Cl₁₅**

24-atom cluster: Ta₆ octahedron + Cl₁₂ cuboctahedron + Cl₆ octahedron.

Von Schnering H.G. et al. (1999) [1]

Cl₅Ta₂

$a = 2.0326$ nm, $V = 8.3976$ nm³, $Z = 48$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	96 <i>h</i>	1	0.0294	0.0505	0.1577		non-colinear Ta ₂
Cl2	96 <i>h</i>	1	0.1395	0.2316	0.3741		non-colinear Ta ₂
Ta3	96 <i>h</i>	1	0.17391	0.28305	0.1918		monocapped square prism Cl ₅ Ta ₄
Cl4	48 <i>g</i>	..2	$\frac{1}{8}$	0.5718	0.6782		non-colinear Ta ₂

Experimental: single crystal, diffractometer, X-rays, wR = 0.027

References: [1] Von Schnering H.G., Vu D., Jin S.L., Peters K. (1999), Z. Kristallogr., New Cryst. Struct. 214, 15-16. [2] Bauer D., Von Schnering H.G. (1968), Z. Anorg. Allg. Chem. 361, 259-276.

Y₃Al₅O₁₂ [2], YAG, garnet family

Structural features: AlO₆ octahedra and AlO₄ tetrahedra share vertices to form a 3D-framework; Y in 8-fold coordination. See Fig. I.3.

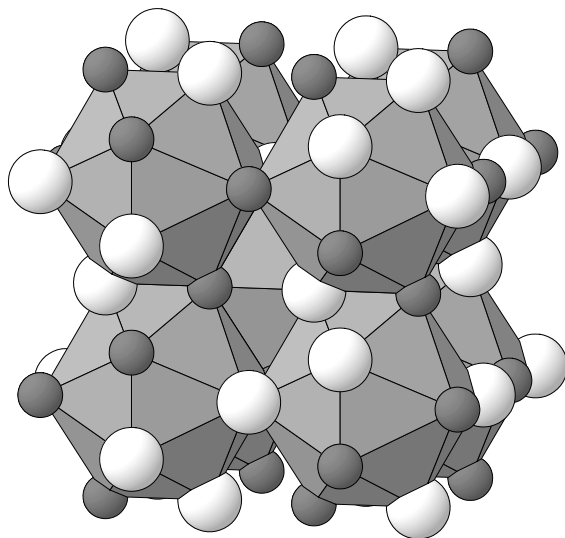


Fig. I.3. **Y₃Al₅O₁₂**

Arrangement of Al(Y₆Al₆) icosahedra
(Y atoms light, Al atoms dark).

Nakatsuka A. et al. (1999) [1]

Al₅O₁₂Y₃

$a = 1.20062 \text{ nm}$, $V = 1.7307 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	96 <i>h</i>	1	0.1002	0.1989	0.2818		non-colinear Al ₂
Al2	24 <i>d</i>	-4..	$\frac{3}{8}$	0	$\frac{1}{4}$		tetrahedron O ₄
Y3	24 <i>c</i>	2.22	$\frac{1}{8}$	0	$\frac{1}{4}$		square antiprism O ₈
Al4	16 <i>a</i>	-.3.	0	0	0		octahedron O ₆

Experimental: single crystal, diffractometer, X-rays, $wR = 0.026$, $T = 296 \text{ K}$

References: [1] Nakatsuka A., Yoshiasa A., Yamanaka T. (1999), Acta Crystallogr. B 55, 266-272. [2] Yoder H.S., Keith M.L. (1950), Geol. Soc. Am. Bull. 61, 1516-1517.

ZnNi₃Ga₃

cI112

(230) *Ia-3d* – gfa

Ni₃ZnGa₃ [1]

Structural features: Substitution variant of Ni₃Ga₄, which is a vacancy derivative of CsCl with 25% of the Ni positions vacant.

Sarah N. et al. (1981) [1]

Ga₃Ni₃Zn

$a = 1.14302$ nm, $V = 1.4933$ nm³, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	48g	..2	$\frac{1}{8}$	0.6334	0.6166		anticuboctahedron Ga ₆ Zn ₂ Ni ₄
Ga2	48f	2..	0.0124	0	$\frac{1}{4}$		cuboctahedron Ni ₆ Ga ₄ Zn ₂
Zn3	16a	-.3.	0	0	0		cuboctahedron Ni ₆ Ga ₆

Experimental: single crystal, diffractometer, X-rays, R = 0.027

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

References: [1] Sarah N., Rajasekharan T., Schubert K. (1981), *Z. Metallkd.* 72, 732-735.

Zr_6NCl_{15}

cI352

(230) $Ia-3d - h^3ga$ **Zr₆Cl₁₅N** [1]

Structural features: NZr₆Cl₁₈ clusters (a central N atom surrounded by a Zr₆ octahedron, a Cl₁₂ cuboctahedron and a Cl₆ octahedron) share vertices of the Cl₆ octahedron to form a 3D-framework.

Ziebarth R.P., Corbett J.D. (1988) [1]

Cl₁₅NZr₆ $a = 2.11712 \text{ nm}$, $V = 9.4893 \text{ nm}^3$, $Z = 16$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	96h	1	0.0291	0.0511	0.1569		non-colinear Zr ₂
Cl2	96h	1	0.1403	0.2305	0.3736		non-colinear Zr ₂
Zr3	96h	1	0.1601	0.28453	0.18857		octahedron Cl ₅ N
Cl4	48g	..2	¹ / ₈	0.5707	0.6793		non-colinear Zr ₂
N5	16a	-.3.	0	0	0		octahedron Zr ₆

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

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

References: [1] Ziebarth R.P., Corbett J.D. (1988), J. Less-Common Met. 137, 21-34.