

Space group (218) $P\bar{4}3n$ 218
 $cP16$

$\text{Li}_{0.64}\text{Pt}_3\text{O}_4$	$cP16$	(218) $P\bar{4}3n$ – eda
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 $\text{Li}_{0.64}\text{Pt}_3\text{O}_4$ [2]; $\text{Ni}_{0.25}\text{Pt}_3\text{O}_4$ (see remark)Structural features: Mutually perpendicular PtO_4 squares (distorted) share vertices to form a 3D-framework; Li in tetrahedral voids.

Schwartz K.B. et al. (1982) [1]

 $\text{Li}_{0.64}\text{O}_4\text{Pt}_3$ $a = 0.56242 \text{ nm}$, $V = 0.1779 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$8e$.3.	0.2283	0.2283	0.2283		tetrahedron Pt_3Li
Pt2	$6d$	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Li3	$2a$	23.	0	0	0	0.64	tetrahedron O_4

Transformation from published data: $-x, -y, -z$ Experimental: powder, diffractometer, neutrons, $R_B = 0.037$ Remarks: A similar model was tested for $\text{Ni}_{0.25}\text{Pt}_3\text{O}_4$ in [3] but rejected in favor of space group (223) $Pm\bar{3}n$.

References: [1] Schwartz K.B., Parise J.B., Prewitt C.T., Shannon R.D. (1982), Acta Crystallogr. B 38, 2109-2116. [2] Schwartz K.B., Parise J.B., Shannon R.D. (1981), Acta Crystallogr. A 37, C172b. [3] Cahen D., Ibers J.A., Shannon R.D. (1972), Inorg. Chem. 11, 2311-2315.

218
 $cP16$

$\text{Ag}_3[\text{PO}_4]$	$cP16$	(218) $P\bar{4}3n$ – eda
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 Ag_3PO_4 form I [2], Strukturbericht notation $\text{H}2_1$ Structural features: Ag atoms and single PO_4 tetrahedra in a Cr_3Si -type arrangement. PO_4 tetrahedra in Ag_{12} icosahedra.

Masse R. et al. (1976) [1]

 $\text{Ag}_3\text{O}_4\text{P}$ $a = 0.6026 \text{ nm}$, $V = 0.2188 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$8e$.3.	0.1486	0.1486	0.1486		single atom P
Ag2	$6d$	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
P3	$2a$	23.	0	0	0		tetrahedron O_4

Experimental: single crystal, diffractometer, X-rays, $R = 0.042$ Remarks: Phase stable at $T < 793 \text{ K}$.

References: [1] Masse R., Tordjman I., Durif A. (1976), Z. Kristallogr. 144, 76-81. [2] Wyckoff R.W.G. (1931), Z. Kristallogr. 62, 529-539.

218
cP22

$\text{Ag}_3[\text{PO}_4]$	<i>cP22</i>	(218) <i>P</i> -43 <i>n</i> – hea
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Ag₃PO₄ form I [2]

Structural features: Ag atoms (split site) and single PO₄ tetrahedra in a Cr₃Si-type arrangement. PO₄ tetrahedra in Ag₁₂ icosahedra.

Deschizeaux Cheruy M.N. et al. (1982) [1]

Ag₃O₄P

$a = 0.6023 \text{ nm}$, $V = 0.2185 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	12 <i>h</i>	2..	0.2347	0	$\frac{1}{2}$	0.5	
O2	8 <i>e</i>	.3.	0.1484	0.1484	0.1484		single atom P
P3	2 <i>a</i>	23.	0	0	0		tetrahedron O ₄

Experimental: single crystal, diffractometer, X-rays, $wR = 0.010$, $T = 290 \text{ K}$

Remarks: Phase stable at $T < 793 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Deschizeaux Cheruy M.N., Aubert J.J., Joubert J.C., Capponi J.J., Vincent H. (1982), Solid State Ionics 7, 171-176. [2] Ng H.N., Calvo C., Faggiani R. (1978), Acta Crystallogr. B 34, 898-899.

218
cP28

$\text{Ag}_3[\text{PO}_4]$	<i>cP28</i>	(218) <i>P</i> -43 <i>n</i> – heca
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Ag₃PO₄ form I [1]

Structural features: Ag atoms (ideal and split site) and single PO₄ tetrahedra in a Cr₃Si-type arrangement.

Newsam J.M. et al. (1980) [1]

Ag₃O₄P

$a = 0.60095 \text{ nm}$, $V = 0.2170 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	12 <i>h</i>	2..	0.2375	0	$\frac{1}{2}$	0.498	
O2	8 <i>e</i>	.3.	0.1489	0.1489	0.1489		single atom P
Ag3	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	0.005	tetrahedron Ag ₄
P4	2 <i>a</i>	23.	0	0	0		tetrahedron O ₄

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.019$

Remarks: Phase stable at $T < 793 \text{ K}$. Short interatomic distances for partly occupied site(s).

References: [1] Newsam J.M., Cheetham A.K., Tofield B.C. (1980), Solid State Ionics 1, 377-393.

218
cP40

$\text{Os}(\text{O}_{0.5}\text{F}_{0.5})_4$	<i>cP40</i>	(218) <i>P</i> -43 <i>n</i> – ieda
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OsO₂F₂ cubic [1]

Structural features: Close-packed (O,F) layers in c stacking, Os in tetrahedral voids. Single Os(O,F)₄ tetrahedra.

Burbank R.D. (1974) [1]

$\text{F}_2\text{O}_2\text{Os}$

$a = 0.8595 \text{ nm}$, $V = 0.6349 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	$24i$	1	0.125	0.375	0.375		single atom Os
M2	$8e$.3.	0.125	0.125	0.125		single atom Os
Os3	$6d$	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron F_4
Os4	$2a$	23.	0	0	0		tetrahedron F_4

$\text{M1} = 0.5\text{F} + 0.5\text{O}$; $\text{M2} = 0.5\text{F} + 0.5\text{O}$

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

Experimental: single crystal, precession photographs, X-rays

Remarks: The composition could not be determined with accuracy; the author states that the correct formula may also be OsO_3F . Space group (195) $P23$ could not be excluded.

References: [1] Burbank R.D. (1974), J. Appl. Crystallogr. 7, 41-44.

218
cP44

$\text{Na}_6\text{Al}_6[\text{SiO}_4]_6$	<i>cP44</i>	(218) $P\text{-}43n - \text{iedc}$
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$\text{Na}_6\text{Al}_6\text{Si}_6\text{O}_{24}$ [1], zeolite SOD

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); Na near the centers of 6-rings.

Felsche J. et al. (1986) [1]

$\text{Al}_6\text{Na}_6\text{O}_{24}\text{Si}_6$

$a = 0.9122 \text{ nm}$, $V = 0.7590 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$24i$	1	0.145	0.155	0.489		non-colinear SiAl
Na2	$8e$.3.	0.235	0.235	0.235	0.75	octahedron O_6
Al3	$6d$	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Si4	$6c$	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.069$, $T = 673 \text{ K}$

References: [1] Felsche J., Luger S., Baerlocher C. (1986), Zeolites 6, 367-372.

218
cP46

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6\text{Cl}_2$	<i>cP46</i>	(218) $P\text{-}43n - \text{iedca}$
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$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}\text{Cl}_2$ [2], sodalite, zeolite SOD-Cl, Strukturbericht notation S6_2

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by Cl; Na above the centers of 6-rings. See Fig. II.1.

Wartchow R. (1997) [1]

$\text{Al}_6\text{Cl}_2\text{Na}_8\text{O}_{24}\text{Si}_6$

$a = 0.8873 \text{ nm}$, $V = 0.6986 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.13935	0.14949	0.4385		non-colinear SiAl
Na2	8e	.3.	0.1777	0.1777	0.1777		non-coplanar triangle O ₃
Al3	6d	-4..	1/4	0	1/2		tetrahedron O ₄
Si4	6c	-4..	1/4	1/2	0		tetrahedron O ₄
Cl5	2a	23.	0	0	0		tetrahedron Na ₄

Experimental: single crystal, diffractometer, X-rays, R = 0.018, T = 298 K

Remarks: Natural specimen of not specified origin.

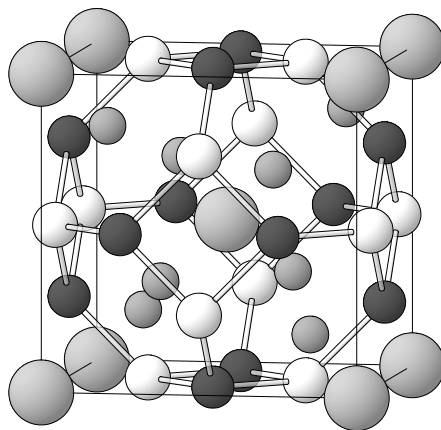


Fig. II.1. **Na₈Al₆Si₆O₂₄Cl₂**

SOD-type (Si,Al) framework (Si atoms dark, Al atoms light), Na (small) and Cl (large) atoms.

References: [1] Wartchow R. (1997), Z. Kristallogr., New Cryst. Struct. 212, 80. [2] Pauling L. (1930), Z. Kristallogr. 74, 213-225.

218
cP52

Na ₈ Al ₆ [GeO ₄] ₆ [OH] ₂	cP52	(218) <i>P</i> -43n – ie ² dc
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Na₈Al₆Ge₆O₂₄(OH)₂ [1], zeolite SOD(Ge)-OH; Na₆Al₆Si₆O₂₄·8H₂O [2], hydrosodalite, zeolite SOD-H₂O; Pb₂Al₆Si₆O₂₄(OH)₂·2H₂O [3]

Structural features: AlO₄ and GeO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); OH near the cage centers (disorder), Na above the centers of 6-rings.

Belokoneva E.L. et al. (1982) [1]

Al₆Ge₆H₂Na₈O₂₆

a = 0.9029 nm, *V* = 0.7361 nm³, *Z* = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.0693	0.3552	0.3565		non-colinear GeAl
(OH)2	8e	.3.	0.0738	0.0738	0.0738	0.25	non-coplanar triangle (OH) ₃
Na3	8e	.3.	0.3313	0.3313	0.3313		octahedron O ₃ (OH) ₃
Al4	6d	-4..	1/4	0	1/2		tetrahedron O ₄
Ge5	6c	-4..	1/4	1/2	0		tetrahedron O ₄

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

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

Remarks: The general formula of hydrosodalite is $\text{Na}_{6+x}\text{Al}_6\text{Si}_6\text{O}_{24}(\text{OH})_x\cdot n\text{H}_2\text{O}$. 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] Belokoneva E.L., Dem'yanets L.N., Uvarova T.G., Belov N.V. (1982), Sov. Phys. Crystallogr. (Engl. Transl.) 27, 597-598. [2] Felsche J., Luger S., Baerlocher C. (1986), Zeolites 6, 367-372. [3] Eiden Abmann S., Schneider A.M., Behrens P., Wiebcke M., Engelhardt G., Felsche J. (2000), Chem. Eur. J. 6, 292-297.

218
cP52

$\text{Na}_6\text{Al}_6[\text{SiO}_4]_6[\text{H}_2\text{O}]_8$	cP52	(218) $P\text{-}43n - \text{ie}^2\text{dc}$
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$\text{Na}_6\text{Al}_6\text{Si}_6\text{O}_{24}\cdot 8\text{H}_2\text{O}$ [2]

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); Na and H_2O above the centers of 6-rings ($\text{Na}_3\Box[\text{OH}_2]_4$ defect cubane-like units).

Felsche J. et al. (1987) [1]

$\text{Al}_6\text{D}_{15.84}\text{Na}_6\text{O}_{32}\text{Si}_6$

$a = 0.8816 \text{ nm}$, $V = 0.6852 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.0687	0.3545	0.3637		non-colinear SiAl
O2	8e	.3.	0.1227	0.1227	0.1227		non-coplanar triangle Na_3
Na3	8e	.3.	0.349	0.349	0.349	0.75	octahedron O_6
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4
D6	24i	1	0.06	0.127	0.224	0.33	
D7	24i	1	0.121	0.214	0.202	0.33	

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

Experimental: powder, diffractometer, neutrons, $R_p = 0.156$, $T = 10.0 \text{ K}$

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

References: [1] Felsche J., Luger S., Fischer P. (1987), Acta Crystallogr. C 43, 809-811. [2] Felsche J., Luger S., Baerlocher C. (1986), Zeolites 6, 367-372.

218
cP54

$\text{Ge}_{19}\text{P}_4\text{I}_4$	cP54	(218) $P\text{-}43n - \text{ie}^2\text{dca}$
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$\text{Ge}_{38}\text{P}_8\text{I}_8$ [2], clathrate I; $\text{Na}_4(\text{Ge}, \text{Al})_{23}$ [3]

Structural features: Ge and P form a tetrahedral framework with 20- (pentagonal dodecahedra) and 24-vertex polyhedra centered by I.

Menke H., Von Schnering H.G. (1973) [1]

$\text{Ge}_{19}\text{I}_4\text{P}_4$

$a = 1.05067 \text{ nm}$, $V = 1.1598 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ge1	24i	1	0.0009	0.1186	0.3072		tetrahedron PGe_3
P2	8e	.3.	0.1848	0.1848	0.1848		tetrahedron Ge_4

Ge3	8e	.3.	0.3158	0.3158	0.3158	tetrahedron PGe ₃
I4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$	24-vertex polyhedron Ge ₂₀ P ₄
Ge5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	tetrahedron Ge ₄
I6	2a	23.	0	0	0	20-vertex polyhedron Ge ₁₆ P ₄

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

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

Remarks: The same data are quoted in [4] and compared with calculated values. Correct symmetry for Na₄(Ge,Al)₂₃ [3] is space group (223) $Pm\bar{3}n$ if the atom sites in Wyckoff position 8e have the same Ge/Al distribution.

References: [1] Menke H., Von Schnering H.G. (1973), Z. Anorg. Allg. Chem. 395, 223-238. [2] Von Schnering H.G., Menke H. (1972), Angew. Chem. 84, 30-31. [3] Westerhaus W., Schuster H.U. (1977), Z. Naturforsch. B 32, 1365-1367. [4] Yang Q.B., Andersson S. (1987), Acta Crystallogr. B 43, 1-14.

218
cP54

H₂Na_{7.1}Al₆Si_{5.5}Cl_{0.4}O₂₄[OH]_{0.7} cP54 (218) $P\bar{4}3n - ie^2dca$

Na_{7.1}H₂Al₆Si_{5.5}O₂₄(OH)Cl [1], hydrosodalite, zeolite SOD-OH,Cl

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by Cl; Na and OH near the centers of 6-rings (split site), part of Si replaced by four H (O₄H₄ units).

Bukin V.I., Makarov Ye.S. (1967) [1]

Al₆Cl_{0.40}H_{2.34}Na_{7.10}O_{24.35}Si_{5.50}

$a = 0.8887$ nm, $V = 0.7019$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.1374	0.1507	0.4395		non-colinear SiAl
O2	8e	.3.	0.1703	0.1703	0.1703	0.044	
Na3	8e	.3.	0.1793	0.1793	0.1793	0.888	
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	0.917	tetrahedron O ₄
Cl6	2a	23.	0	0	0	0.2	tetrahedron O ₄
H7	24i	1	0.04	0.3251	0.3796	0.083	
H8	8e	.3.	0.239	0.239	0.239	0.044	

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

Experimental: single crystal, diffractometer, neutrons, R = 0.075

Remarks: Nominal composition of the sample Na₆Al₆Si_{5.5}(H₄)_{0.5}O₂₄·0.4NaCl·0.7NaOH; the 0.7 H₂O per unit cell detected by the chemical analysis were not located. Ambiguous data: coordinates of the centrosymmetric counterparts of sites O2 and H2 are added to table 1 ("or"), however, in the summary OH groups are stated to substitute for Na (no counterpart). 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] Bukin V.I., Makarov Ye.S. (1967), Geochem. Int. 4, 19-28.

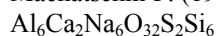
218
cP54

(Na_{0.75}Ca_{0.25})₈Al₆[SiO₄]₆[SO₄]₂ cP54 (218) $P\bar{4}3n - ie^2dca$

Na₂(Ca,K)₂Al₆Si₆O₂₄(SO₄)₂ [1], h a yne, Strukturbericht notation S6₉, zeolite SOD-SO₄

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO_4 tetrahedra; (Na,Ca) near the centers of 6-rings.

Machatschki F. (1934) [1]



$$a = 0.91 \text{ nm}, V = 0.7536 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.025	0.353	0.364		non-colinear SiAl
O2	8e	.3.	0.1	0.1	0.1		single atom S
M3	8e	.3.	0.278	0.278	0.278		non-coplanar triangle O_3
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4
S6	2a	23.	0	0	0		tetrahedron O_4

$$\text{M3} = 0.75\text{Na} + 0.25\text{Ca}$$

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

Experimental: powder, film, X-rays

Remarks: Natural specimen from Niedermendig, Laacher See. 32.5 wt.% SiO_2 , 28.4 wt.% Al_2O_3 , 8.8 wt.% CaO , and 12.2 wt.% SO_3 from chemical analysis, undetermined amounts of Na_2O , trace amounts of Cl.

References: [1] Machatschki F. (1934), Zentralbl. Mineral. Geol. Palaeontol. 1934, 136-144.

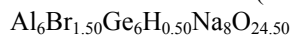
218
cP54

$\text{Na}_8\text{Al}_6\text{Ge}_6\text{Br}_{1.5}\text{O}_{24}[\text{OH}]_{0.5}$	cP54	(218) $P\text{-}43n - \text{ie}^2\text{dca}$
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$\text{Na}_8[\text{AlGeO}_4]_6(\text{Br}_{1.5}\text{OH}_{0.5})$ [1], zeolite SOD(Ge)-Br,OH

Structural features: AlO_4 and GeO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by Br or OH (the latter considerably displaced from the polyhedron center into a split site); Na above the centers of 6-rings.

Belokoneva E.L. et al. (1985) [1]



$$a = 0.90895 \text{ nm}, V = 0.7510 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.068	0.355	0.356		non-colinear GeAl
(OH)2	8e	.3.	0.087	0.087	0.087	0.063	single atom Br
Na3	8e	.3.	0.3212	0.3212	0.3212		7-vertex polyhedron $\text{O}_3(\text{OH})_3\text{Br}$
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Ge5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4
Br6	2a	23.	0	0	0	0.75	tetrahedron $(\text{OH})_4$

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.051$

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] Belokoneva E.L., Uvarova T.G., Dem'yanets L.N. (1985), Sov. Phys. Crystallogr. (Engl. Transl.) 30, 465-466.

218
cP58

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6\text{S}_{2.5}[\text{H}_2\text{O}]_{0.6}$	<i>cP58</i>	(218) <i>P-43n</i> – ifedca
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 $\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{S}_2)\text{S}_{0.5}\cdot x\text{H}_2\text{O}$ [1], lazurite-1C, ultramarine, zeolite SOD-S, S_2 Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by S_2 , $(\text{S}_2)^{2-}$ (orientational disorder), S^{2-} and H_2O (substitutional disorder); Na near the centers of 6-rings.

Podschus E. et al. (1936) [1]

 $\text{Al}_6\text{H}_{1.20}\text{Na}_8\text{O}_{24.60}\text{S}_{2.50}\text{Si}_6$ $a = 0.906 \text{ nm}$, $V = 0.7437 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.136	0.147	0.475	0.183	non-collinear SiAl
S2	12f	2..	0.11	0	0		
Na3	8e	.3.	0.217	0.217	0.217	0.45	non-coplanar triangle O_3
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	0.45	tetrahedron O_4
M6	2a	23.	0	0	0		

 $\text{M6} = 0.667\text{OH}_2 + 0.333\text{S}$ Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

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

Remarks: Approximate composition, the authors state that part of the sulfur dumbbells may be $(\text{S}_2)^{2-}$. Composition $\text{Na}_{6.63}\text{Al}_{5.87}\text{Si}_{6.13}\text{S}_{2.45}\text{O}_{24}\cdot 0.6\text{H}_2\text{O}$ from density considerations. 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] Podschus E., Hofmann U., Leschewski K. (1936), Z. Anorg. Allg. Chem. 228, 305-333.

218
cP60

$\text{Na}_{4.15}\text{Li}_{3.85}\text{Al}_6[\text{SiO}_4]_6\text{Cl}_2$	<i>cP60</i>	(218) <i>P-43n</i> – ie ³ dc
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 $\text{Na}_{4.15}\text{Li}_{3.85}\text{Al}_6\text{Si}_6\text{O}_{24}\text{Cl}_2$ [1], zeolite SOD-ClStructural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); Cl near the cage centers, Na and Li near the centers of 6-rings (split site).

Weller M.T., Wong G. (1989) [1]

 $\text{Al}_6\text{Cl}_2\text{Li}_{3.85}\text{Na}_{4.15}\text{O}_{24}\text{Si}_6$ $a = 0.87101 \text{ nm}$, $V = 0.6608 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.1372	0.1475	0.4256	0.25	non-collinear SiAl
Cl2	8e	.3.	0.0242	0.0242	0.0242		
Na3	8e	.3.	0.1675	0.1675	0.1675	0.481	
Li4	8e	.3.	0.1879	0.1879	0.1879		
Al5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$	0.481	tetrahedron O_4
Si6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4

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

Experimental: powder, diffractometer, neutrons, $R_B = 0.070$

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

References: [1] Weller M.T., Wong G. (1989), Solid State Ionics 32/33, 430-435.

218
cP60

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6[\text{BrO}_3]_2$	<i>cP60</i>	(218) <i>P</i> -43 <i>n</i> – <i>ie</i> ³ <i>dc</i>
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$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{BrO}_3)_{1.77}(\text{OH})_{0.23}$ [1], zeolite SOD- BrO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); BrO_3 ψ -tetrahedra near the cage centers (orientational disorder), Na near the centers of 6-rings.

Mead P.J., Weller M.T. (1995) [1]

$\text{Al}_6\text{Br}_2\text{Na}_8\text{O}_{30}\text{Si}_6$

$a = 0.90435 \text{ nm}$, $V = 0.7396 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.1424	0.1501	0.4537		non-collinear AlSi
Br2	8 <i>e</i>	.3.	0.0689	0.0689	0.0689	0.25	non-coplanar triangle O ₃
Na3	8 <i>e</i>	.3.	0.1951	0.1951	0.1951		tetrahedron BrO ₃
O4	8 <i>e</i>	.3.	0.4129	0.4129	0.4129	0.75	non-coplanar triangle Br ₃
Si5	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Al6	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

Experimental: powder, diffractometer, X-rays, $R_B = 0.068$, $T = 300 \text{ K}$

Remarks: Partial substitution of OH for BrO_3 was ignored in the refinement. Short interatomic distances: $d(\text{Br-O}) = 0.143 \text{ nm}$, $d(\text{Na-Br}) = 0.198 \text{ nm}$. A slightly different model for the arrangement of BrO_3 was proposed for the refinement on diffraction data collected at 4 K.

References: [1] Mead P.J., Weller M.T. (1995), Zeolites 15, 561-568.

218
cP64

KGe	<i>cP64</i>	(218) <i>P</i> -43 <i>n</i> – <i>i</i> ² <i>e</i> ²
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KGe [2]

Structural features: Single empty Ge₄ tetrahedra. See Fig. II.2.

Busmann E. (1961) [1]

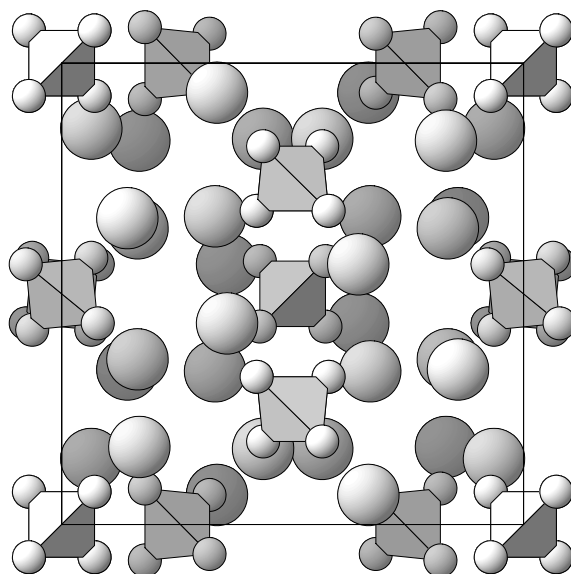
GeK

$a = 1.278 \text{ nm}$, $V = 2.0873 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
K1	24 <i>i</i>	1	0.064	0.142	0.336		7-capped pentagonal prism Ge ₈ K ₉
Ge2	24 <i>i</i>	1	0.064	0.422	0.32		tricapped trigonal prism Ge ₃ K ₆
Ge3	8 <i>e</i>	.3.	0.071	0.071	0.071		tricapped trigonal prism Ge ₃ K ₆
K4	8 <i>e</i>	.3.	0.332	0.332	0.332		pseudo Frank-Kasper Ge ₉ K ₉

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

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.076$

Fig. II.2. **KGe**

Arrangement of Ge_4 tetrahedra (Ge atoms small) and K atoms (large).

References: [1] Busmann E. (1961), Z. Anorg. Allg. Chem. 313, 90-106. [2] Busmann E. (1960), Naturwissenschaften 47, 82.

218
cP66

$\text{Cu}_{13}(\text{Fe}_{0.5}\text{Ge}_{0.5})_4\text{S}_{16}$	cP66	(218) <i>P</i> -43n – ife ² dca
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$\text{Cu}_{26}\text{Fe}_4\text{Ge}_4\text{S}_{32}$ [1], germanite

Structural features: Close-packed S layers in c stacking; (Fe,Ge) and Cu in tetrahedral voids. Single (Fe,Ge) S_4 tetrahedra.

Tettenhorst R.T., Corbato C.E. (1984) [1]

$\text{Cu}_{13}\text{Fe}_2\text{Ge}_2\text{S}_{16}$

$a = 1.05862 \text{ nm}$, $V = 1.1864 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	24i	1	0.121	0.364	0.379		tetrahedron Cu_3Fe
Cu2	12f	2..	0.257	0	0		tetrahedron S_4
S3	8e	.3.	0.121	0.121	0.121		trigonal bipyramid FeCu_4
M4	8e	.3.	0.24	0.24	0.24		tetrahedron S_4
Cu5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron S_4
Cu6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S_4
Cu7	2a	23.	0	0	0		fourcapped trigonal prism S_4Cu_6

$\text{M4} = 0.5\text{Fe} + 0.5\text{Ge}$

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

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

Remarks: Natural specimen from Tsumeb, southwestern Africa. Composition $\text{Cu}_{23.44}\text{Zn}_{1.62}\text{Fe}_{3.92}\text{Ge}_{4.24}\text{As}_{2.14}\text{S}_{32}$ from electron microprobe analysis.

References: [1] Tettenhorst R.T., Corbato C.E. (1984), Am. Mineral. 69, 943-947.

218
cP66

$\text{Cu}_{13}\text{V}(\text{Sn}_{0.33}\text{As}_{0.67})_3\text{S}_{16}$	<i>cP66</i>	(218) <i>P</i> -43 <i>n</i> – ife ² dca
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Cu_{12+x}VS_nAs_{3-x}S₁₆ [1], colusiteStructural features: Close-packed S layers in c stacking; Cu, V and (As,Sn) in tetrahedral voids. VS₄ tetrahedra share all six edges with CuS₄ tetrahedra.

Spry P.G. et al. (1994) [1]

As_{1.92}Cu₁₃S₁₆Sn_{1.08}V $a = 1.0621 \text{ nm}$, $V = 1.1981 \text{ nm}^3$, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	24 <i>i</i>	1	0.122	0.3704	0.3734		tetrahedron AsCu ₃
Cu2	12 <i>f</i>	2..	0.257	0	0		tetrahedron S ₄
S3	8 <i>e</i>	.3.	0.1192	0.1192	0.1192		trigonal bipyramid VCu ₄
Cu4	8 <i>e</i>	.3.	0.2495	0.2495	0.2495		tetrahedron S ₄
Cu5	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron S ₄
M6	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron S ₄
V7	2 <i>a</i>	23.	0	0	0		fourcapped trigonal prism S ₄ Cu ₆

M6 = 0.64As + 0.36Sn

Experimental: single crystal, diffractometer, X-rays, wR = 0.043, T = 298 K

Remarks: Natural specimen from Carrara area, Lorano, Italy. Composition Cu_{26.46}V_{2.07}Ge_{0.52}Sn_{1.89}As_{3.99}Sb_{0.26}S₃₂ from electron microprobe analysis. The authors state that partial substitution of Sn for As is compensated for by vacancies on the Cu site in Wyckoff position 8*e*. Supersedes a structure proposal in space group (215) *P*-43*m* [2]. A report on colusite with sphalerite-type structure [3] is also superseded (see [4]). The correct space group was stated in [5].

References: [1] Spry P.G., Merlino S., Wang S., Zhang X., Buseck P.R. (1994), Am. Mineral. 79, 750-762. [2] Dangel P.N., Wuensch B.J. (1970), Am. Mineral. 55, 1787-1791. [3] Zachariasen W.H. (1933), Am. Mineral. 18, 534-537. [4] Murdoch J. (1953), Am. Mineral. 38, 794-801. [5] Orlandi P., Merlino S., Duchi G., Vezzolini G. (1981), Can. Mineral. 19, 423-427.

218
cP68

$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}[\text{OH}]_2[\text{H}_2\text{O}]_2$	<i>cP68</i>	(218) <i>P</i> -43 <i>n</i> – i ² edc
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Na₈Al₆Si₆O₂₄(OH)₂·2H₂O rt [2], zeolite SOD-OHStructural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); OH and OH₂ near the cage centers (disorder), Na above the centers of 6-rings.

Wiebcke M. et al. (1992) [1]

Al₆D₆Na₈O_{28.01}Si₆ $a = 0.886 \text{ nm}$, $V = 0.6955 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.059	0.061	0.114	0.167	
O2	24 <i>i</i>	1	0.0618	0.3501	0.3609		non-colinear SiAl
Na3	8 <i>e</i>	.3.	0.3241	0.3241	0.3241		
Al4	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si5	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
D6	12 <i>f</i>	2..	0.061	0	0	0.167	

D7 8e .3. 0.1339 0.1339 0.1339 0.5

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

Experimental: powder, diffractometer, neutrons, $R = 0.047$, $T = 173$ K

Remarks: Phase stable at $T > 150$ K. 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] Wiebcke M., Engelhardt G., Felsche J., Kempa P.B., Sieger P., Schefer J., Fischer P. (1992), J. Phys. Chem. 96, 392-397. [2] Hassan I., Grundy H.D. (1983), Acta Crystallogr. C 39, 3-5.

218
cP68

$K_{4.7}Na_{3.3}Al_6[SiO_4]_6[BrO_3]_2$

cP68

(218) $P-43n - ie^4dc$

$K_{4.7}Na_{3.3}Al_6Si_6O_{24}(BrO_3)_{1.77}(OH)_{0.23}$ [1], zeolite SOD- BrO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); $:BrO_3$ ψ -tetrahedra near cage centers (orientational disorder), K near and Na above the centers of 6-rings (split site).

Mead P.J., Weller M.T. (1995) [1]

$Al_6Br_2K_{4.70}Na_{3.30}O_{30}Si_6$

$a = 0.92549$ nm, $V = 0.7927$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.1463	0.1522	0.4887		non-collinear AlSi
Br2	8e	.3.	0.0991	0.0991	0.0991	0.25	
Na3	8e	.3.	0.1822	0.1822	0.1822	0.412	
K4	8e	.3.	0.2694	0.2694	0.2694	0.588	
O5	8e	.3.	0.4276	0.4276	0.4276	0.75	non-coplanar triangle Br_3
Si6	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4
Al7	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O_4

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_B = 0.066$, $T = 300$ K

Remarks: Partial substitution of OH for BrO_3 was ignored in the refinement. We assigned partial occupancies in agreement with the nominal composition, ignoring OH. Short interatomic distances for partly occupied site(s). Other short interatomic distances: $d(Na-Br) = 0.133$ nm.

References: [1] Mead P.J., Weller M.T. (1995), Zeolites 15, 561-568.

218
cP68

$Na_8Al_6[SiO_4]_6[CN]_2$

cP68

(218) $P-43n - if^2edc$

$Na_8Al_6Si_6O_{24}(CN)_2$ [1], zeolite SOD-CN

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); CN units near the cage centers (orientational disorder), Na above the centers of 6-rings.

Gesing T.M., Buhl J.C. (2003) [1]

$Al_6C_2N_2Na_8O_{24}Si_6$

$a = 0.89192$ nm, $V = 0.7095$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.1396	0.15043	0.4404		non-collinear SiAl

C2	12f	2..	0.048	0	0	0.167	
N3	12f	2..	0.087	0	0	0.167	
Na4	8e	.3.	0.1832	0.1832	0.1832		
Al5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

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

Experimental: powder, diffractometer, X-rays, $R_B = 0.020$

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

References: [1] Gesing T.M., Buhl J.C. (2003), Z. Kristallogr., New Cryst. Struct. 218, 275.

218
cP70

Na₈Al₆[SiO₄]₆[NO₂]₂

cP70

(218) *P*-43*n* – i²edca

Na₈Al₆Si₆O₂₄(NO₂)₂ [1], zeolite SOD-NO₂

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by NO₂ non-linear units (orientational disorder); Na above the centers of 6-rings.

Kempa P.B. et al. (1991) [1]

Al₆N₂Na₈O_{28.01}Si₆

$a = 0.893$ nm, $V = 0.7121$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24i	1	0.046	0.048	0.113	0.167	
O2	24i	1	0.0584	0.3489	0.3589		non-colinear SiAl
Na3	8e	.3.	0.3138	0.3138	0.3138		
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
N6	2a	23.	0	0	0		

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

Experimental: powder, diffractometer, X-rays, $R = 0.033$, $T = 295$ K

Remarks: Short interatomic distances for partly occupied site(s). A related model with the N site split into Wyckoff position 24i gave a similar agreement. In table 2 of [1] the occupancy of former O(2) is misprinted as 1.167 instead of 0.167 (given in the text).

References: [1] Kempa P.B., Engelhardt G., Buhl J.C., Felsche J., Harvey G., Baerlocher C. (1991), Zeolites 11, 558-562.

218
cP70

Na₈Al₆[SiO₄]₆[ClO₄]₂

cP70

(218) *P*-43*n* – i²edca

Na₈Al₆Si₆O₂₄(ClO₄)₂ [1], zeolite SOD-ClO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by ClO₄ tetrahedra (orientational disorder); Na above the centers of 6-rings.

Brenchley M.E., Weller M.T. (1994) [1]

Al₆Cl₂Na₈O_{31.99}Si₆

$a = 0.90922$ nm, $V = 0.7516$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.0034	0.0734	0.1327	0.333	non-colinear SiAl
O2	24i	1	0.144	0.1517	0.4599		
Na3	8e	.3.	0.2141	0.2141	0.2141		
Al4	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si5	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
Cl6	2a	23.	0	0	0		

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

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_B = 0.014$, $T = 300$ K

References: [1] Brenchley M.E., Weller M.T. (1994), Zeolites 14, 682-686.

218
cP72

Ba ₄ SiAs ₄	cP72	(218) $P-43n - i^2e^2da$
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Ba₄SiAs₄ [2]; Ca₄SiP₄ [3]

Structural features: Close-packed As layers in c stacking; Ba in octahedral, Si in tetrahedral voids. Single SiAs₄ tetrahedra. See Fig. II.3.

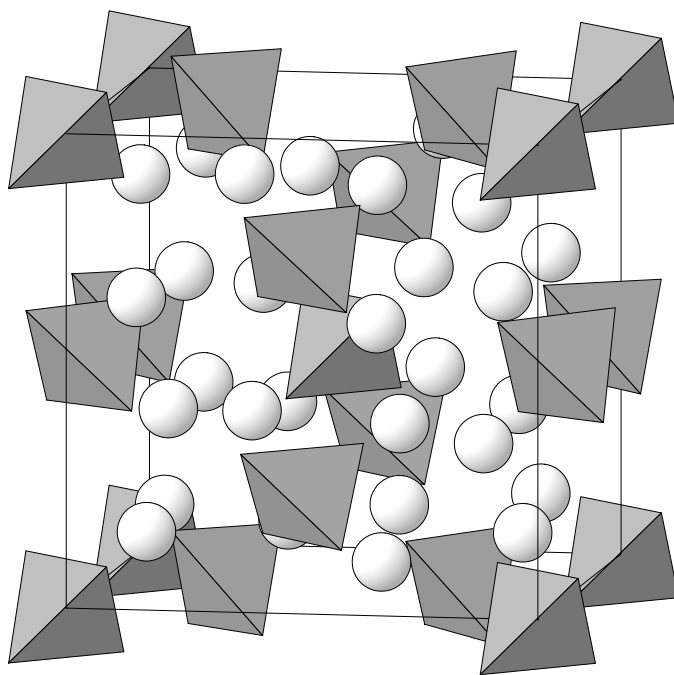


Fig. II.3. **Ba₄SiAs₄**

Arrangement of SiAs₄ tetrahedra and Ba atoms.

Eisenmann B. et al. (1981) [1]

As₄Ba₄Si

$a = 1.3307$ nm, $V = 2.3564$ nm³, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	24i	1	0.0948	0.1318	0.3549		7-vertex polyhedron SiAs ₆
As2	24i	1	0.1029	0.388	0.3479		single atom Si
As3	8e	.3.	0.1038	0.1038	0.1038		single atom Si
Ba4	8e	.3.	0.3554	0.3554	0.3554		7-vertex polyhedron SiAs ₆

Si5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$	tetrahedron As ₄
Si6	2a	23.	0	0	0	tetrahedron As ₄

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.094$

References: [1] Eisenmann B., Jordan H., Schäfer H. (1981), Z. Anorg. Allg. Chem. 475, 74-80. [2] Eisenmann B., Jordan H., Schäfer H. (1981), Angew. Chem. 93, 211. [3] Eisenmann B., Jordan H., Schäfer H. (1982), Mater. Res. Bull. 17, 95-99.

218
cP72

HBO ₂	cP72	(218) $P-43n - i^3$
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HBO₂ γ [2]

Structural features: B(O₂[OH]₂) tetrahedra share vertices to form a 3D-framework stabilized by hydrogen bonds.

Freyhardt C.C. et al. (2000) [1]

BHO₂

$a = 0.88811$ nm, $V = 0.7005$ nm³, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.08016	0.30015	0.16772		non-colinear B ₂
B2	24i	1	0.0811	0.21733	0.30853		tetrahedron O ₄
O3	24i	1	0.14509	0.32221	0.42596		non-colinear B ₂
H4	24i	1	0.1707	0.4275	0.392		

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

Experimental: single crystal, diffractometer, X-rays, $R = 0.019$

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

References: [1] Freyhardt C.C., Wiebcke M., Felsche J. (2000), Acta Crystallogr. A 56, 276-278. [2] Zachariasen W.H. (1963), Acta Crystallogr. 16, 380-384.

218
cP76

Na ₈ Al ₆ [SiO ₄] ₆ [NO ₂] ₂	cP76	(218) $P-43n - i^2e^2dc$
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Na₈Al₆Si₆O₂₄(NO₂)₂ [1], zeolite SOD-NO₂

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); NO₂ non-linear units near the cage centers (orientational disorder), Na above the centers of 6-rings.

Sieger P. et al. (1991) [1]

Al₆N₂Na₈O_{28.01}Si₆

$a = 0.8923$ nm, $V = 0.7104$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.14008	0.15032	0.4428		non-colinear SiAl
O2	24i	1	0.3945	0.455	0.46	0.167	
N3	8e	.3.	0.025	0.025	0.025	0.25	
Na4	8e	.3.	0.1854	0.1854	0.1854		

Al5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$	tetrahedron O ₄
Si6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	tetrahedron O ₄

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

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

References: [1] Sieger P., Wiebcke M., Felsche J., Buhl J.C. (1991), Acta Crystallogr. C 47, 498-501.

218
cP76

Na ₈ Al ₆ [SiO ₄] ₆ [ClO ₃] ₂	cP76	(218) <i>P</i> -43 <i>n</i> – i ² e ² dc
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Na₈Al₆Si₆O₂₄(ClO₃)_{1.91}(OH)_{0.09} [1], zeolite SOD-ClO₃

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); :ClO₃ ψ-tetrahedra near the cage centers (orientational disorder), Na above the centers of 6-rings.

Mead P.J., Weller M.T. (1995) [1]

Al₆Cl₂Na₈O₃₀Si₆

a = 0.90222 nm, *V* = 0.7344 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24i	1	0.1413	0.1497	0.4508		non-collinear AlSi
O2	24i	1	0.3747	0.438	0.427	0.25	
Cl3	8e	.3.	0.0442	0.0442	0.0442	0.25	
Na4	8e	.3.	0.193	0.193	0.193		tetrahedron ClO ₃
Si5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Al6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

Experimental: powder, diffractometer, X-rays, R_B = 0.048, T = 300 K

Remarks: Partial substitution of OH for ClO₃ was ignored in the refinement. Short interatomic distances for partly occupied site(s).

References: [1] Mead P.J., Weller M.T. (1995), Zeolites 15, 561-568.

218
cP76

KNa _{4.5} Ca ₂ Al ₆ [SiO ₄] ₆ [SO ₄] _{1.5} [OH] _{0.5}	cP76	(218) <i>P</i> -43 <i>n</i> – ie ⁵ dc
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KNa_{4.5}Ca₂Al₆Si₆O₂₄(SO₄)_{1.5}(OH)_{0.5} [1], hauyne, zeolite SOD-SO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); SO₄ tetrahedra near the cage centers (orientational disorder), Na near, Ca and K above the centers of 6-rings (split site).

Hassan I., Grundy H.D. (1991) [1]

Al₆Ca_{2.40}K_{1.60}Na_{4.32}O₃₀S_{1.52}Si₆

a = 0.91164 nm, *V* = 0.7577 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24i	1	0.1443	0.1559	0.4681		non-collinear SiAl
O2	8e	.3.	0.0972	0.0972	0.0972	0.75	
K3	8e	.3.	0.1636	0.1636	0.1636	0.2	
Ca4	8e	.3.	0.2008	0.2008	0.2008	0.3	
Na5	8e	.3.	0.2374	0.2374	0.2374	0.54	

S6	8e	.3.	0.4657	0.4657	0.4657	0.19	
Al7	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si8	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

Experimental: single crystal, diffractometer, X-rays, wR = 0.033, T = 293 K

Remarks: Natural specimen from Valle Biachella, Sacrofano, Italy. Composition (Na_{4.35}Ca_{2.28}K_{0.95})Al₆Si₆O₂₄(SO₄)_{2.03} from chemical analysis. OH was not located, however, the authors state that OH may be a significant component of haüyne. 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] Hassan I., Grundy H.D. (1991), Can. Mineral. 29, 123-130.

218
cP78

K _{1.4} Na _{4.4} Ca _{1.9} Al ₆ Si ₆ [SO ₄] _{1.8} O ₂₄	cP78	(218) <i>P</i> -43 <i>n</i> – ie ⁵ dca
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K_{1.4}Na_{4.4}Ca_{1.9}Al₆Si₆O₂₄(SO₄)_{1.8} [1], haüyne, zeolite SOD-SO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO₄ tetrahedra (orientational disorder); (Ca,Na) near, additional Na and K above the centers of 6-rings (partial disorder).

Evsyunin V.G. et al. (1996) [1]

Al₆Ca_{1.89}K_{1.39}Na_{4.40}O_{31.20}S_{1.84}Si₆

a = 0.9118 nm, *V* = 0.7581 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24i	1	0.1442	0.1543	0.4673		non-collinear SiAl
O2	8e	.3.	0.091	0.091	0.091	0.44	
M3	8e	.3.	0.1729	0.1729	0.1729	0.29	
Na4	8e	.3.	0.2031	0.2031	0.2031	0.24	
M5	8e	.3.	0.2341	0.2341	0.2341	0.43	single atom S tetrahedron O ₄ tetrahedron O ₄ square prism (cube) O ₈
O6	8e	.3.	0.406	0.406	0.406	0.46	
Al7	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		
Si8	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		
S9	2a	23.	0	0	0	0.92	

M3 = 0.6K + 0.4Na; M5 = 0.55Ca + 0.45Na

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

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

Remarks: Natural specimen from Arissi, Italy. Composition (Na_{4.52}K_{1.42}Ca_{1.89})[Al_{6.08}Si_{5.92}O₂₄](SO₄)_{1.78}Cl_{0.07} from electron microprobe analysis. We adjusted the charge balance in the chemical formula given in [1] by changing the Na index from 4.5 to 4.4. Short interatomic distances for partly occupied site(s).

References: [1] Evsyunin V.G., Sapozhnikov A.N., Pastsvetaeva R.K., Kashaev A.A. (1996), Kristallografiya 41, 659-662.

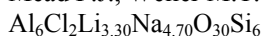
218
cP84

Na _{4.7} Li _{3.3} Al ₆ [SiO ₄] ₆ [ClO ₃] ₂	cP84	(218) <i>P</i> -43 <i>n</i> – i ² e ³ dc
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Na_{4.7}Li_{3.3}Al₆Si₆O₂₄(ClO₃)_{1.91}(OH)_{0.09} [1], zeolite SOD-ClO₃

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); ClO_3 ψ -tetrahedra near the cage centers (orientational disorder), Na and Li opposite 6-rings (split site).

Mead P.J., Weller M.T. (1995) [1]



$$a = 0.88505 \text{ nm}, V = 0.6933 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.1412	0.1469	0.4365		non-colinear AlSi
O2	24i	1	0.3726	0.4185	0.4185	0.25	
Cl3	8e	.3.	0.0381	0.0381	0.0381	0.25	
Li4	8e	.3.	0.111	0.111	0.111	0.412	
Na5	8e	.3.	0.1766	0.1766	0.1766	0.588	
Si6	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Al7	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_B = 0.061$, $T = 300 \text{ K}$

Remarks: Partial substitution of OH for ClO_3 was ignored in the refinement. We assigned partial occupancies in agreement with the nominal composition, ignoring OH. Short interatomic distances for partly occupied site(s).

References: [1] Mead P.J., Weller M.T. (1995), Zeolites 15, 561-568.

218
cP92



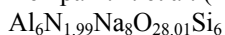
cP92

(218) $P-43n - i^3\text{edc}$

$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{NO}_2)_2$ [1], zeolite SOD- NO_2

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); NO_2 non-linear units near the cage centers (orientational disorder), Na above the centers of 6-rings.

Kempa P.B. et al. (1991) [1]



$$a = 0.893 \text{ nm}, V = 0.7121 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24i	1	0.018	0.018	0.046	0.083	non-colinear SiAl
O2	24i	1	0.1411	0.1511	0.4416		
O3	24i	1	0.387	0.452	0.454	0.167	
Na4	8e	.3.	0.1862	0.1862	0.1862		
Al5	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si6	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

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

Remarks: Short interatomic distances for partly occupied site(s). A related model with N in Wyckoff position 2a gave a similar agreement. In table 2 of [1] the occupancy of former O(2) is misprinted as 1.167 instead of 0.167 (given in the text).

References: [1] Kempa P.B., Engelhardt G., Buhl J.C., Felsche J., Harvey G., Baerlocher C. (1991), Zeolites 11, 558-562.

218
cP94

$\text{Na}_8\text{CaAl}_6[\text{SiO}_4]_6\text{S}_{0.44}[\text{SO}_4]_{1.56}$	<i>cP94</i>	$(218) P\text{-}43n - i^2e^4dca$
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 $\text{Na}_8\text{Ca}_{0.5}\text{Al}_6\text{Si}_6\text{O}_{24}(\text{SO}_4)_{1.56}\text{S}_{0.44}$ [1], lazurite-1C, zeolite SOD- SO_4 ,S

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO_4 tetrahedra (orientational disorder) or S^{2-} (substitutional disorder); Na above the centers of 6-rings (split site).

Hassan I. et al. (1985) [1]

 $\text{Al}_6\text{Na}_{8.56}\text{O}_{30.24}\text{S}_2\text{Si}_6$ $a = 0.9105 \text{ nm}$, $V = 0.7548 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.045	0.353	0.367	0.5	
O2	24 <i>i</i>	1	0.157	0.158	0.474	0.5	
O3	8 <i>e</i>	.3.	0.098	0.098	0.098	0.78	
Na4	8 <i>e</i>	.3.	0.178	0.178	0.178	0.35	
Na5	8 <i>e</i>	.3.	0.231	0.231	0.231	0.5	
Na6	8 <i>e</i>	.3.	0.305	0.305	0.305	0.22	
Al7	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		
Si8	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		
S9	2 <i>a</i>	23.	0	0	0		tetrahedron O_4

Experimental: single crystal, diffractometer, X-rays, $wR = 0.059$

Remarks: Natural specimen from Sary-Sang, Afghanistan. Composition $\text{Fe}_{0.04}\text{Mg}_{0.71}\text{Ca}_{1.65}\text{Na}_{5.88}\text{K}_{0.25}\text{Si}_{6.04}\text{Al}_{5.96}\text{O}_x(\text{SO}_4)_{1.26}\text{S}_{0.66}\text{Cl}_{0.26}$ from chemical analysis. The ideal formula of lazurite is given as $\text{Na}_6\text{Ca}_2(\text{Al}_6\text{Si}_6\text{O}_{24})\text{S}_2$; we adjusted the charge balance in the empirical formula reproduced above by replacing $\text{Na}_{8.56}$ by $\text{Na}_8\text{Ca}_{0.5}$. Ca not located. Short interatomic distances for partly occupied site(s). Additional reflections indicate a possible superstructure.

References: [1] Hassan I., Peterson C., Grundy H.D. (1985), Acta Crystallogr. C 41, 827-832.

218
cP94

$\text{KNa}_5\text{Ca}_{1.5}\text{Al}_6[\text{SiO}_4]_6[\text{SO}_4]_{1.5}$	<i>cP94</i>	$(218) P\text{-}43n - i^2e^4dca$
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 $\text{KNa}_5\text{Ca}_{1.5}\text{Al}_6\text{Si}_6\text{O}_{24}(\text{SO}_4)_{1.5}$ [1], h  y  ne, zeolite SOD- SO_4

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a distorted SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO_4 tetrahedra (orientational disorder); Na, Ca and K near and above the centers of 6-rings (split site).

L  hn J., Schulz H. (1968) [1]

 $\text{Al}_6\text{Ca}_{2.28}\text{K}_{0.81}\text{Na}_{5.09}\text{O}_{26.74}\text{S}_{1.50}\text{Si}_6$ $a = 0.9116 \text{ nm}$, $V = 0.7576 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.145	0.152	0.467	0.495	
O2	24 <i>i</i>	1	0.145	0.467	0.152	0.495	
O3	8 <i>e</i>	.3.	0.097	0.097	0.097	0.156	
M4	8 <i>e</i>	.3.	0.182	0.182	0.182	0.538	
M5	8 <i>e</i>	.3.	0.231	0.231	0.231	0.484	
O6	8 <i>e</i>	.3.	0.403	0.403	0.403	0.217	4-vertex polyhedron SO_3
Si7	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O_4

Al8	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0	tetrahedron O ₄
S9	2a	23.	0	0	0	0.75 square prism (cube) O ₈

M4 = 0.634Na + 0.188K + 0.178Ca; M5 = 0.610Na + 0.390Ca

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

Remarks: Natural specimen from Mte. Somma, Italy. We adjusted the charge balance in the chemical formula given in [1] by changing the Ca index from 2 to 1.5. Short interatomic distances for partly occupied site(s). In table 4 of [1] the *x*-coordinate of former O(4) is misprinted as 0.097 instead of -0.097 (given on page 206).

References: [1] Löhn J., Schulz H. (1968), Neues Jahrb. Mineral., Abh. 109, 201-210.

218
cP96

Li ₇ MnN ₄	cP96	(218) <i>P</i> -43 <i>n</i> – i ² fe ² dcb
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Li₇MnN₄ [2]; Li₇PN₄ [3]; Li₇VN₄ [5]

Structural features: "Close-packed" N layers in c stacking, Li and Mn occupy all tetrahedral voids. Single MnN₄ tetrahedra. Substitution derivative of CaF₂.

Niewa R. et al. (2001) [1]

Li₇MnN₄

a = 0.956 nm, *V* = 0.8737 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	24i	1	0.106	0.38273	0.3571		square prism (cube) MnLi ₇
Li2	24i	1	0.2502	0.2623	0.4814		fourcapped trigonal prism N ₄ Li ₅ Mn
Li3	12f	2..	0.2633	0	0		fourcapped trigonal prism N ₄ Li ₅ Mn
N4	8e	.3.	0.1093	0.1093	0.1093		square prism (cube) MnLi ₇
Li5	8e	.3.	0.2331	0.2331	0.2331		fourcapped trigonal prism N ₄ Li ₆
Mn6	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		fourcapped trigonal prism N ₄ Li ₆
Li7	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		fourcapped trigonal prism N ₄ Li ₆
Li8	6b	222..	0	$\frac{1}{2}$	$\frac{1}{2}$		fourcapped trigonal prism N ₄ Li ₄ Mn ₂
Mn9	2a	23.	0	0	0		fourcapped trigonal prism N ₄ Li ₆

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

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

Remarks: Idealized coordinates. Li₇VN₄ was later refined in space group (205) *Pa*-3 [6] (Li₇NbN₄ type), as recommended in [4].

References: [1] Niewa R., Wagner F.R., Schnelle W., Hochrein O., Kniep R. (2001), Inorg. Chem. 40, 5215-5222. [2] Juza R., Anschütz E., Puff H. (1959), Angew. Chem. 71, 161. [3] Schnick W., Luecke J. (1990), J. Solid State Chem. 87, 101-106. [4] Vennos D.A., Disalvo F.J. (1992), Acta Crystallogr. C 48, 610-612. [5] Juza R., Gieren W., Haug J. (1959), Z. Anorg. Allg. Chem. 300, 61-71. [6] Niewa R., Kniep R. (2001), Z. Kristallogr., New Cryst. Struct. 216, 5-6.

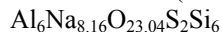
218
cP102

Na ₈ CaAl ₆ [SiO ₄] ₆ S _{0.86} [SO ₄] _{1.14}	cP102	(218) <i>P</i> -43 <i>n</i> – i ² e ⁵ dca
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(Na,Ca)₈Al₆Si₆O₂₄(SO₄,S,Cl)₂ [1], lazurite-1C, zeolite SOD-SO₄S

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO₄ tetrahedra (orientational disorder) or S²⁻ (substitutional disorder), Na at and above the centers of 6-rings (split site).

Hassan I. et al. (1985) [1]



$a = 0.9054 \text{ nm}, V = 0.7422 \text{ nm}^3, Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.026	0.339	0.347	0.4	
O2	24 <i>i</i>	1	0.133	0.144	0.449	0.37	
O3	8 <i>e</i>	.3.	0.098	0.098	0.098	0.21	
Na4	8 <i>e</i>	.3.	0.183	0.183	0.183	0.29	
Na5	8 <i>e</i>	.3.	0.255	0.255	0.255	0.3	
Na6	8 <i>e</i>	.3.	0.304	0.304	0.304	0.43	
O7	8 <i>e</i>	.3.	0.402	0.402	0.402	0.36	
Al8	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		
Si9	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		
Si10	2 <i>a</i>	23.	0	0	0		square prism (cube) O ₈

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

Experimental: single crystal, diffractometer, X-rays, R = 0.063

Remarks: Natural specimen from Baffin Island. Composition $\text{Ca}_{1.06}\text{Na}_{6.79}\text{K}_{0.01}\text{Si}_{6.20}\text{Al}_{5.80}\text{O}_x(\text{SO}_4)_{1.53}\text{S}_{0.60}\text{Cl}_{0.06}$ from chemical analysis. We adjusted the charge balance in the chemical formula given above by adding Ca, not located. Short interatomic distances for partly occupied site(s). Additional reflections indicate a possible superstructure with 6x6x6 cell volume, *a* = 5.42 nm.

References: [1] Hassan I., Peterson C., Grundy H.D. (1985), Acta Crystallogr. C 41, 827-832.

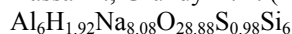
218
cP102

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6[\text{SO}_4][\text{H}_2\text{O}]$	<i>cP102</i>	(218) <i>P</i> -43 <i>n</i> – <i>i</i> ² <i>e</i> ⁵ <i>dca</i>
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Na₈Al₆Si₆O₂₄SO₄·H₂O [1], nosean, zeolite SOD-SO₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by SO₄ tetrahedra (orientational disorder) or H₂O (substitutional disorder, H₂O displaced into a split site); Na near and above the centers of 6-rings (split site).

Hassan I., Grundy H.D. (1989) [1]



$a = 0.9084 \text{ nm}, V = 0.7496 \text{ nm}^3, Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>i</i>	1	0.043	0.34	0.347	0.5	
O2	24 <i>i</i>	1	0.137	0.146	0.456	0.5	
(OH ₂)3	8 <i>e</i>	.3.	0.03	0.03	0.03	0.12	
O4	8 <i>e</i>	.3.	0.095	0.095	0.095	0.49	
Na5	8 <i>e</i>	.3.	0.197	0.197	0.197	0.21	
Na6	8 <i>e</i>	.3.	0.267	0.267	0.267	0.46	
Na7	8 <i>e</i>	.3.	0.326	0.326	0.326	0.34	
Al8	6 <i>d</i>	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		
Si9	6 <i>c</i>	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		
Si10	2 <i>a</i>	23.	0	0	0	0.49	

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

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

Remarks: Natural specimen from Laacher See, Germany. Composition $\text{Na}_{7.20}\text{Ca}_{0.24}\text{K}_{0.23}[\text{Al}_6\text{Si}_6\text{O}_{24}](\text{SO}_4)_{0.87}\cdot 0.51\text{H}_2\text{O}$ from chemical analysis, small amounts of Fe, Mg, Cl, and S^{2-} detected. Average structure; the authors state that the real structure is incommensurate. A model for local ordering was proposed in space group (195) $P23$. 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] Hassan I., Grundy H.D. (1989), Can. Mineral. 27, 165-172.

218
cP142

$\text{HNa}_8\text{Al}_6[\text{SiO}_4]_6[\text{CO}_3]_{1.5}[\text{H}_2\text{O}]_2$	cP142	(218) $P\text{-}43n - i^4e^4dca$
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$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{HCO}_3)(\text{CO}_3)_{0.5}\cdot 2\text{H}_2\text{O}$ [1], zeolite SOD- $\text{HCO}_3, \text{CO}_3$

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra) centered by CO_3 trigonal units (orientational disorder); Na distributed over several sites along $\langle 111 \rangle$ (disorder), H_2O opposite 4-rings.

Gesing T.M., Buhl J.C. (2000) [1]

$\text{Al}_6\text{C}_{1.50}\text{H}_{3.98}\text{Na}_{7.67}\text{O}_{30.53}\text{Si}_6$

$a = 0.9033 \text{ nm}$, $V = 0.7370 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	24i	1	0.026	0.036	0.1622	0.083	
O2	24i	1	0.034	0.1167	0.0684	0.138	
O3	24i	1	0.04749	0.34788	0.35767		non-colinear SiAl
O4	24i	1	0.0653	0.1023	0.0688	0.051	
Na5	8e	.3.	0.2009	0.2009	0.2009	0.131	
Na6	8e	.3.	0.2692	0.2692	0.2692	0.237	
Na7	8e	.3.	0.3064	0.3064	0.3064	0.214	
Na8	8e	.3.	0.3159	0.3159	0.3159	0.377	
Al9	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si10	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄
C11	2a	23.	0	0	0	0.75	

Experimental: single crystal, diffractometer, X-rays, $R = 0.013$

Remarks: H of HCO_3 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. In [1] the number of formula units per unit cell Z is misprinted as 2 instead of 1.

References: [1] Gesing T.M., Buhl J.C. (2000), Z. Kristallogr. 215, 413-418.

218
cP148

$\text{Na}_8\text{Al}_6[\text{SiO}_4]_6[\text{NO}_3]_2$	cP148	(218) $P\text{-}43n - i^5e^2dc$
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$\text{Na}_8\text{Al}_6\text{Si}_6\text{O}_{24}(\text{NO}_3)_2$ [1], zeolite SOD- NO_3

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); NO_3 trigonal units near the cage centers (orientational disorder), Na above the centers of 6-rings (split site).

Buhl J.C., Löns J. (1996) [1]

$\text{Al}_6\text{N}_{1.92}\text{Na}_{7.88}\text{O}_{29.76}\text{Si}_6$

$a = 0.8978 \text{ nm}$, $V = 0.7237 \text{ nm}^3$, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
N1	24i	1	0.006	0.009	0.013	0.08	
O2	24i	1	0.019	0.022	0.15	0.08	
O3	24i	1	0.041	0.051	0.123	0.08	
O4	24i	1	0.0516	0.3585	0.3486		single atom Si
O5	24i	1	0.052	0.072	0.109	0.08	
Na6	8e	.3.	0.296	0.296	0.296	0.209	
Na7	8e	.3.	0.3089	0.3089	0.3089	0.776	
Si8	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Al9	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

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

Experimental: single crystal, diffractometer, X-rays, $wR = 0.020$, $T = 295 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). In table 3 of [1] the x -coordinate of former O1 is misprinted as 0.115 instead of 0.1415 (checked on interatomic distances) and the occupancy of former O22 as 0.050 instead of 0.080 (agreement with other partial occupancies).

References: [1] Buhl J.C., Löns J. (1996), J. Alloys Compd. 235, 41-47.

218
cP160

SeCl_4	$cP160$	$(218) P-43n - i^6e^2$
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SeCl_4 α [1]

Structural features: Cubane-like $\text{Se}_4\text{Cl}_{16}$ units consisting of four edge-sharing SeCl_6 octahedra (Se_4Cl_4 cube with three additional Cl bonded to each Se). See Fig. II.4.

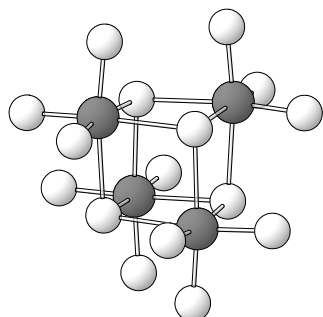


Fig. II.4. **SeCl_4 α**

$\text{Se}_4\text{Cl}_{16}$ unit (Se atoms dark, Cl atoms light).

Kniep R. et al. (1981) [1]

Cl_4Se

$a = 1.6433 \text{ nm}$, $V = 4.4376 \text{ nm}^3$, $Z = 32$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	24i	1	0.0371	0.1	0.5982		single atom Se
Cl2	24i	1	0.0747	0.4163	0.1646		non-coplanar triangle Se ₃
Cl3	24i	1	0.078	0.2709	0.3191		single atom Se
Cl4	24i	1	0.0794	0.0842	0.2211		single atom Se
Se5	24i	1	0.0924	0.4001	0.3312		octahedron Cl ₆

Cl6	24i	1	0.2225	0.4014	0.3162	single atom Se
Se7	8e	.3.	0.0893	0.0893	0.0893	octahedron Cl ₆
Cl8	8e	.3.	0.418	0.418	0.418	non-coplanar triangle Se ₃

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

Remarks: The only stable modification of SeCl₄.

References: [1] Kniep R., Korte L., Mootz D. (1981), Z. Naturforsch. B 36, 1660-1662.

218
cP160

CsI ₃ F ₁₆	cP160	(218) <i>P</i> -43 <i>n</i> – i ⁶ eba
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CsI₃F₁₆ [1]

Structural features: I₃F₁₆ units consisting of three IF₅ square pyramids loosely interconnected via an additional F.

Mahjoub A.R. et al. (1989) [1]

CsF₁₆I₃

a = 1.379 nm, *V* = 2.6224 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
I1	24i	1	0.0289	0.2548	0.2484		octahedron F ₆
F2	24i	1	0.041	0.317	0.371		non-colinear FI
F3	24i	1	0.042	0.136	0.317		single atom I
F4	24i	1	0.134	0.473	0.211		non-coplanar triangle F ₂ I
F5	24i	1	0.228	0.27	0.402		non-coplanar triangle IF ₂
F6	24i	1	0.316	0.446	0.36		4-vertex polyhedron F ₃ I
F7	8e	.3.	0.19	0.19	0.19		non-coplanar triangle I ₃
Cs8	6b	222..	0	¹ / ₂	¹ / ₂		12-vertex polyhedron F ₁₂
Cs9	2a	23.	0	0	0		icosahedron F ₁₂

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.028

References: [1] Mahjoub A.R., Hoser A., Fuchs J., Seppelt K. (1989), Angew. Chem. 101, 1528-1529.

218
cP200

Na ₂ Zn ₃ [CO ₃] ₄ [H ₂ O] ₃	cP200	(218) <i>P</i> -43 <i>n</i> – i ⁷ hfe
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Na₂Zn₃(CO₃)₄·3H₂O [1]

Structural features: ZnO₄ tetrahedra and CO₃ trigonal units share vertices to form a 3D-framework where the central atoms form a defect diamond-type sublattice; Na and H₂O in larger voids.

Gier T.E. et al. (1996) [1]

C₄H₆Na₂O₁₅Zn₃

a = 1.37549 nm, *V* = 2.6024 nm³, *Z* = 8

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH ₂)1	24i	1	0.07	0.088	0.429		non-colinear Na ₂
O2	24i	1	0.078	0.13	0.21		single atom C
O3	24i	1	0.094	0.354	0.277		single atom C
O4	24i	1	0.148	0.281	0.413		single atom C

C5	24i	1	0.148	0.349	0.342	non-coplanar triangle O ₃
O6	24i	1	0.218	0.4118	0.3589	single atom C
Zn7	24i	1	0.2514	0.4976	0.2583	tetrahedron O ₄
Na8	12h	2..	0.205	0	$\frac{1}{2}$	0.333
Na9	12f	2..	0.2929	0	0	octahedron O ₄ (OH ₂) ₂
C10	8e	.3.	0.134	0.134	0.134	non-coplanar triangle O ₃

Experimental: single crystal, diffractometer, X-rays, R = 0.069, 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] Gier T.E., Bu X., Wang S.L., Stucky G.D. (1996), J. Am. Chem. Soc. 118, 3039-3040.

218
cP212

Na _{7.5} Al ₆ [SiO ₄] ₆ B _{1.5} [OH] ₆ [H ₂ O] ₂	cP212	(218) <i>P</i> -43 <i>n</i> – i ⁷ e ⁴ dc
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Na_{7.5}Al₆Si₆O₂₄[B(OH)₄]_{1.5}·2H₂O [1], zeolite SOD-B(OH)₄

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); B(OH)₄ tetrahedra (orientational disorder) and H₂O near the cage centers (substitutional disorder), Na above the centers of 6-rings (split site).

Buhi J.C. et al. (1994) [1]

Al₆B_{1.68}H_{10.66}Na_{7.55}O_{32.69}Si₆

a = 0.9024 nm, *V* = 0.7348 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
B1	24i	1	0.0028	0.0755	0.0256	0.07	
(OH)2	24i	1	0.008	0.1708	0.0219	0.07	
(OH)3	24i	1	0.0503	0.1497	0.0868	0.07	
O4	24i	1	0.1422	0.1522	0.4523		non-collinear SiAl
(OH)5	24i	1	0.3408	0.4538	0.4637	0.07	
(OH)6	24i	1	0.3846	0.4459	0.447	0.07	
(OH ₂)7	24i	1	0.395	0.423	0.431	0.082	
Na8	8e	.3.	0.1827	0.1827	0.1827	0.499	
Na9	8e	.3.	0.1963	0.1963	0.1963	0.113	
Na10	8e	.3.	0.2038	0.2038	0.2038	0.152	
Na11	8e	.3.	0.2274	0.2274	0.2274	0.18	
Al12	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si13	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

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

Experimental: single crystal, diffractometer, X-rays, wR = 0.021, T = 295 K

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

References: [1] Buhi J.C., Mundus C., Löns J., Hoffmann W. (1994), Z. Naturforsch. A 49, 1171-1178.

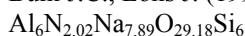
218
cP228

Na ₈ Al ₆ [SiO ₄] ₆ [NO ₂][NO ₃]	cP228	(218) <i>P</i> -43 <i>n</i> – i ⁸ e ³ dc
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Na₈Al₆Si₆O₂₄(NO₂)(NO₃) [1], zeolite SOD-NO₂,NO₃

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a SOD-type zeolite framework with condensed β cages (14-face truncated octahedra); NO_2 non-linear units and NO_3 trigonal units near the cage centers (substitutional and orientational disorder), Na near the centers of 6-rings (split site).

Buhl J.C., Löns J. (1994) [1]



$$a = 0.8958 \text{ nm}, V = 0.7188 \text{ nm}^3, Z = 1$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.0035	0.0243	0.1457	0.048	
N2	24i	1	0.0074	0.0174	0.009	0.048	
O3	24i	1	0.0268	0.1288	0.0542	0.036	
O4	24i	1	0.0388	0.1319	0.0419	0.036	
O5	24i	1	0.0518	0.0667	0.1243	0.048	
O6	24i	1	0.05426	0.3491	0.35899		non-colinear SiAl
O7	24i	1	0.0571	0.0713	0.1021	0.048	
N8	24i	1	0.4943	0.4956	0.4963	0.036	
Na9	8e	.3.	0.2974	0.2974	0.2974	0.148	
Na10	8e	.3.	0.3091	0.3091	0.3091	0.473	
Na11	8e	.3.	0.31771	0.31771	0.31771	0.365	
Al12	6d	-4..	$\frac{1}{4}$	0	$\frac{1}{2}$		tetrahedron O ₄
Si13	6c	-4..	$\frac{1}{4}$	$\frac{1}{2}$	0		tetrahedron O ₄

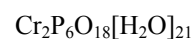
Transformation from published data: $-x, -y, -z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.016$, $T = 295 \text{ K}$

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

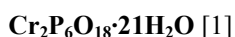
References: [1] Buhl J.C., Löns J. (1994), J. Solid State Chem. 112, 243-250.

218
cP424



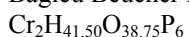
cP424

(218) $P\text{-}43n - i^{15}\text{hgf}^2\text{eba}$



Structural features: P_6O_{18} units (rings formed by six vertex-sharing PO_4 tetrahedra), $\text{Cr}(\text{OH}_2)_6$ octahedra and additional H_2O molecules.

Bagieu Beucher M. et al. (1991) [1]



$$a = 1.9052 \text{ nm}, V = 6.9155 \text{ nm}^3, Z = 8$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24i	1	0.0004	0.1106	0.1906		single atom P
O2	24i	1	0.0307	0.1124	0.3214		single atom P
(OH ₂)3	24i	1	0.032	0.088	0.054	0.157	non-coplanar square (OH ₂) ₄
P4	24i	1	0.05078	0.12682	0.24743		tetrahedron O ₄
P5	24i	1	0.06546	0.26868	0.18996		tetrahedron O ₄
O6	24i	1	0.0737	0.2075	0.2461		non-colinear P ₂
O7	24i	1	0.0877	0.4224	0.3232		tetrahedron O ₄
O8	24i	1	0.0895	0.2271	0.122		non-colinear P ₂
(OH ₂)9	24i	1	0.1108	0.1658	0.4521		non-colinear O ₂
O10	24i	1	0.1155	0.325	0.2084		single atom P
O11	24i	1	0.1255	0.3075	0.4185		tetrahedron O ₃ (OH ₂)
O12	24i	1	0.2116	0.4916	0.3185		single atom P

O13	24i	1	0.2276	0.2501	0.3404		single atom Cr
O14	24i	1	0.2732	0.383	0.3666		single atom Cr
(OH ₂)15	24i	1	0.416	0.472	0.451	0.166	
O16	12h	2..	0.1045	0	$\frac{1}{2}$		single atom Cr
O17	12g	2..	0.1024	$\frac{1}{2}$	0		single atom Cr
(OH ₂)18	12f	2..	0.1024	0	0	0.186	
O19	12f	2..	0.396	0	0		single atom Cr
Cr20	8e	.3.	0.30709	0.30709	0.30709		octahedron O ₆
Cr21	6b	222..	0	$\frac{1}{2}$	$\frac{1}{2}$		octahedron O ₆
Cr22	2a	23.	0	0	0		
H23	24i	1	0.015	0.043	0.371		
H24	24i	1	0.041	0.132	0.473		
H25	24i	1	0.051	0.518	0.125		
H26	24i	1	0.081	0.413	0.279		
H27	24i	1	0.105	0.337	0.392		
H28	24i	1	0.11	0.475	0.317		
H29	24i	1	0.141	0.336	0.457		
H30	24i	1	0.194	0.271	0.363		
H31	24i	1	0.216	0.346	0.224		
H32	24i	1	0.266	0.42	0.356		
H33	24i	1	0.286	0.387	0.41		

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

Experimental: single crystal, diffractometer, X-rays, R = 0.053

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] Bagieu Beucher M., Averbuch Pouchot M.T., Rzaigui M. (1991), Acta Crystallogr. C 47, 1364-1366.