

Space group (192) *P6/mcc*192
hP58

$\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$	<i>hP58</i>	(192) <i>P6/mcc</i> – ml^2fc
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Be₃Al₂Si₆O₁₈ [2], beryl, Strukturbericht notation G3₁

Structural features: Si₆O₁₈ units (6-rings formed by six vertex-linked SiO₄ tetrahedra) share vertices with distorted BeO₄ tetrahedra and AlO₆ octahedra to form a 3D-framework with channels parallel to [001] delimited by the 6-rings.

Hazen R.M. et al. (1986) [1]

 $\text{Al}_2\text{Be}_3\text{O}_{18}\text{Si}_6$ $a = 0.9214$, $c = 0.9194$ nm, $c/a = 0.998$, $V = 0.6760$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>m</i>	1	0.1456	0.4985	0.1453		non-coplanar triangle SiBeAl
Si2	12 <i>l</i>	<i>m</i> ..	0.1159	0.3876	0		tetrahedron O ₄
O3	12 <i>l</i>	<i>m</i> ..	0.3103	0.0734	0		non-colinear Si ₂
Be4	6 <i>f</i>	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
Al5	4 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

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

Remarks: Small amounts of Cr on the Al site (1.3%) are ignored here. Natural beryl generally contains water molecules and/or alkaline metal atoms (charge compensation for partial substitution of Al and/or Si) on partly occupied sites. In [2] the origin is shifted by 0 0 $\frac{1}{4}$ from the description in the International Tables for Crystallography.

References: [1] Hazen R.M., Au A.Y., Finger L.W. (1986), Am. Mineral. 71, 977-984. [2] Bragg W.L., West J. (1926), Proc. R. Soc. London, Ser. A 111, 691-714.

192
hP58

$\text{Mg}_2(\text{Al}_{0.45}\text{Si}_{0.55})_9\text{O}_{18}$	<i>hP58</i>	(192) <i>P6/mcc</i> – ml^2fc
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(Mg,Fe)₂Al₄Si₅O₁₈ [2], indialite

Structural features: (Si,Al)₆O₁₈ units (6-rings formed by six vertex-linked (Si,Al)O₄ tetrahedra) share vertices with additional (Si,Al)O₄ tetrahedra and MgO₆ octahedra to form a 3D-framework with channels parallel to [001] delimited by the 6-rings.

Thomas P. et al. (1995) [1]

 $\text{Al}_{4.01}\text{Mg}_2\text{O}_{18}\text{Si}_{4.99}$ $a = 0.9769$, $c = 0.9337$ nm, $c/a = 0.956$, $V = 0.7717$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	24 <i>m</i>	1	0.1351	0.481	0.1433		non-colinear Si ₂
M2	12 <i>l</i>	<i>m</i> ..	0.1051	0.3692	0		tetrahedron O ₄
O3	12 <i>l</i>	<i>m</i> ..	0.299	0.0759	0		non-colinear Si ₂
M4	6 <i>f</i>	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
Mg5	4 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆

M2 = 0.555Si + 0.445Al; M4 = 0.555Si + 0.445Al

Experimental: powder, diffractometer, X-rays, $R_B = 0.090$

Remarks: This modification of Fe-free $Mg_2Al_4Si_5O_{18}$ is stable at $T > 1677$ K. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition.

References: [1] Thomas P., Gouby I., Mercurio D., Merle T., Frit B. (1995), Mater. Res. Bull. 30, 141-148. [2] Meagher E.P., Gibbs G.V. (1977), Can. Mineral. 15, 43-49.

192
hP60

$Be_3Al_2Si_6O_{18}[H_2O]_{0.1}$

hP60

(192) $P6/mcc - ml^2fca$

$Be_3Al_2Si_6O_{18} \cdot xH_2O$ [2], beryl; $Be_3(Sc,Al,Fe)_2Si_6O_{18} \cdot xH_2O$ [2], bazzite

Structural features: Si_6O_{18} units (6-rings formed by six vertex-linked SiO_4 tetrahedra) share vertices with distorted BeO_4 tetrahedra and AlO_6 octahedra to form a 3D-framework; H_2O in channels parallel to $[001]$ delimited by the 6-rings. See Fig. III.64.

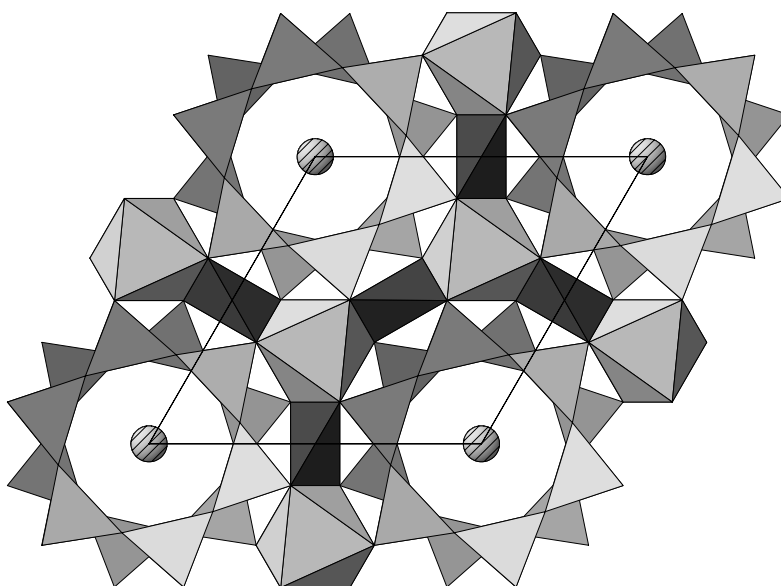


Fig. III.64. **$Be_3Al_2Si_6O_{18} \cdot xH_2O$**

Arrangement of BeO_4 (dark) and SiO_4 tetrahedra, AlO_6 octahedra and H_2O molecules (O atoms hatched) viewed along $[001]$.

Morosin B. (1972) [1]

$Al_2Be_3H_{0.20}O_{18.10}Si_6$

$a = 0.92088$, $c = 0.91896$ nm, $c/a = 0.998$, $V = 0.6749$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24m	1	0.14551	0.49884	0.14529		non-coplanar triangle SiBeAl
Si2	12l	$m..$	0.11584	0.38749	0		tetrahedron O_4
O3	12l	$m..$	0.31001	0.0734	0		non-colinear Si_2
Be4	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O_4
Al5	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O_6
$(OH_2)6$	2a	622	0	0	$\frac{1}{4}$	0.099	hexagonal prism O_{12}

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.020$

Remarks: 0.1 wt.% Fe, < 0.001 wt.% K and Ca detected by spectroscopy. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Morosin B. (1972), Acta Crystallogr. B 28, 1899-1903. [2] Bergerhoff G., Nowacki W. (1955), Schweiz. Mineral. Petrogr. Mitt. 35, 410-421.

192
hP62

$(\text{Cs}_{0.15}[\text{H}_2\text{O}]_{0.7})\text{Na}_{0.35}(\text{Li}_{0.1}\text{Be}_{0.9})_3\text{Si}_6\text{Al}_2\text{O}_{18}$	hP62	(192) $P6/mcc - \text{ml}^2\text{fcba}$
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$(\text{Cs}_{0.14}[\text{H}_2\text{O}]_{0.66})\text{Na}_{0.31}(\text{Li}_{0.1}\text{Be}_{0.9})_3\text{Al}_2\text{Si}_6\text{O}_{18}$ [1], beryl

Structural features: Si_6O_{18} units (6-rings formed by six vertex-linked SiO_4 tetrahedra) share vertices with distorted $(\text{Be},\text{Li})\text{O}_4$ tetrahedra and AlO_6 octahedra to form a 3D-framework; Na, Cs and H_2O in channels parallel to [001] delimited by the 6-rings.

Hawthorne F.C., Cerny P. (1977) [1]

$\text{Al}_2\text{Be}_{2.70}\text{Cs}_{0.14}\text{H}_{1.25}\text{Li}_{0.30}\text{Na}_{0.31}\text{O}_{18.62}\text{Si}_6$

$a = 0.9212$, $c = 0.9236$ nm, $c/a = 1.003$, $V = 0.6788$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24m	1	0.1473	0.4983	0.1445		non-coplanar triangle SiBeAl
Si2	12l	m..	0.1189	0.3892	0		tetrahedron O ₄
O3	12l	m..	0.3048	0.0696	0		non-colinear Si ₂
M4	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
Al5	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆
Na6	2b	6/m..	0	0	0	0.31	8-vertex polyhedron $(\text{OH}_2)_2\text{O}_6$
M7	2a	622	0	0	$\frac{1}{4}$	0.76	colinear Na ₂

$\text{M4} = 0.9\text{Be} + 0.1\text{Li}$; $\text{M7} = 0.82\text{OH}_2 + 0.18\text{Cs}$

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Remarks: Natural specimen from the Tanco deposit, Manitoba. Composition $\text{Fe}_{0.003}\text{Mg}_{0.005}\text{Mn}_{0.001}\text{Li}_{0.873}\text{Ca}_{0.006}\text{Na}_{0.626}\text{K}_{0.065}\text{Rb}_{0.013}\text{Cs}_{0.268}\text{Be}_{5.225}\text{Al}_{4.01}\text{Si}_{11.91}\text{O}_{36} \cdot 1.32\text{H}_2\text{O}$ from chemical analysis. Non-framework species could not be identified with certainty. 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] Hawthorne F.C., Cerny P. (1977), Can. Mineral. 15, 414-421.

192
hP62

$\text{KMg}_2(\text{Al}_{0.55}\text{Si}_{0.45})_9\text{O}_{18}$	hP62	(192) $P6/mcc - \text{ml}^2\text{fec}$
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$\text{KMg}_2\text{Al}_5\text{Si}_4\text{O}_{18}$ [2], indialite-(K)

Structural features: $(\text{Al},\text{Si})_6\text{O}_{18}$ units (6-rings formed by six vertex-linked $(\text{Al},\text{Si})\text{O}_4$ tetrahedra) share vertices with additional $(\text{Al},\text{Si})\text{O}_4$ tetrahedra and MgO_6 octahedra to form a 3D-framework; K in channels parallel to [001] delimited by the 6-rings (disorder).

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

$\text{Al}_{5.01}\text{KMg}_2\text{O}_{18}\text{Si}_{3.99}$

$a = 0.98001$, $c = 0.94105$ nm, $c/a = 0.960$, $V = 0.7827$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24m	1	0.1365	0.4862	0.1437		non-colinear Al ₂
M2	12l	m..	0.1076	0.3735	0		tetrahedron O ₄
O3	12l	m..	0.2995	0.0739	0		non-colinear Al ₂
M4	6f	222	1/2	0	1/4		tetrahedron O ₄
K5	4e	6..	0	0	0.1805	0.5	
Mg6	4c	3.2	1/3	2/3	1/4		octahedron O ₆

M2 = 0.54Al + 0.46Si; M4 = 0.59Al + 0.41Si

Experimental: powder, diffractometer, neutrons, time-of-flight, R_p = 0.050

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

References: [1] Thomas P., Mercurio D., Mercurio J.P., Frit B. (1991), Eur. J. Solid State Inorg. Chem. 28, 1011-1020. [2] Kim Y.H., Mercurio D., Mercurio J.P., Frit B. (1984), Mater. Res. Bull. 19, 209-217.

192
hP72

(Al _{0.5} P _{0.5})O ₂	hP72	(192) P6/mcc – mlk ² j
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AlPO₄ form 5 [1]; SiO₂ SSZ-24 [2], zeolite AFI

Structural features: (Al,P)O₄ tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001].

Richardson J.W. Jr. et al. (1987) [1]

Al_{0.50}O₂P_{0.50}

a = 1.37707, c = 0.83789 nm, c/a = 0.608, V = 1.3760 nm³, Z = 24

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24m	1	0.1207	0.4574	0.1905		tetrahedron O ₄
O2	12l	m..	0.1194	0.453	0		non-colinear Al ₂
O3	12k	..2	0.2098	0.4196	1/4		non-colinear Al ₂
O4	12k	..2	0.5778	0.1556	1/4		non-colinear Al ₂
O5	12j	.2.	0.3639	0	1/4		non-colinear Al ₂

M1 = 0.5Al + 0.5P

Experimental: powder, diffractometer, neutrons, time-of-flight, R_p = 0.019, T = 295 K

Remarks: A model in space group (184) P6cc with an ordered arrangement of Al and P could not be rejected. The structure was later again refined in this space group [3].

References: [1] Richardson J.W. Jr., Pluth J.J., Smith J.V. (1987), Acta Crystallogr. C 43, 1469-1472. [2] Bialek R., Meier W.M., Davis M., Annen M.J. (1991), Zeolites 11, 438-442. [3] Klap G.J., Van Koningsveld H., Graafsma H., Schreurs A.M.M. (2000), Microporous Mesoporous Mater. 38, 403-412.

192
hP84

SiO ₂	hP84	(192) P6/mcc – ml ² k ² j
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SiO₂ SSZ-24 [1], zeolite AFI

Structural features: SiO₄ tetrahedra share vertices to form an AFI-type zeolite framework (partial disorder) with channels delimited by 12-rings parallel to [001]. Variant of AlPO₄-5 with one split O site.

Bialek R. et al. (1991) [1]

O₂Si

$a = 1.3671$, $c = 0.8328$ nm, $c/a = 0.609$, $V = 1.3479$ nm³, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24 <i>m</i>	1	0.1210	0.4568	0.1898		
O2	12 <i>l</i>	<i>m</i> ..	0.1106	0.4389	0	0.5	
O3	12 <i>l</i>	<i>m</i> ..	0.1410	0.4863	0	0.5	
O4	12 <i>k</i>	..2	0.2106	0.4212	1/4		non-colinear Si ₂
O5	12 <i>k</i>	..2	0.5804	0.1608	1/4		non-colinear Si ₂
O6	12 <i>j</i>	..2	0.3583	0	1/4		non-colinear Si ₂

Experimental: powder, diffractometer, X-rays, $R = 0.093$

Remarks: Short interatomic distances for partly occupied site(s). Small amounts of template molecules (N,N,N-trimethyl-1-adamantammonium hydroxide) incorporated; refinement of the occupancy of a non-framework site in Wyckoff position 4e (0 0 0.125) considering $f(O)$ gave $occ = 1.6(1)$, $U = 0.052(3)$ nm².

References: [1] Bialek R., Meier W.M., Davis M., Annen M.J. (1991), Zeolites 11, 438-442.

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hP96

KCa ₂ (Be _{0.67} Al _{0.33}) ₃ Si ₁₂ O ₃₀	hP96	(192) <i>P6/mcc</i> – m ³ lfc
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KCa₂Be₂AlSi₁₂O₃₀ [2], milarite

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with distorted (Be,Al)O₄ tetrahedra to form a 3D-framework; K and Ca in channels parallel to [001] (K inside the columns formed by superposed double 6-rings). See Fig. III.65.

Pasheva Z.P., Tarkhova T.N. (1953) [1]

AlBe₂Ca₂KO₃₀Si₁₂

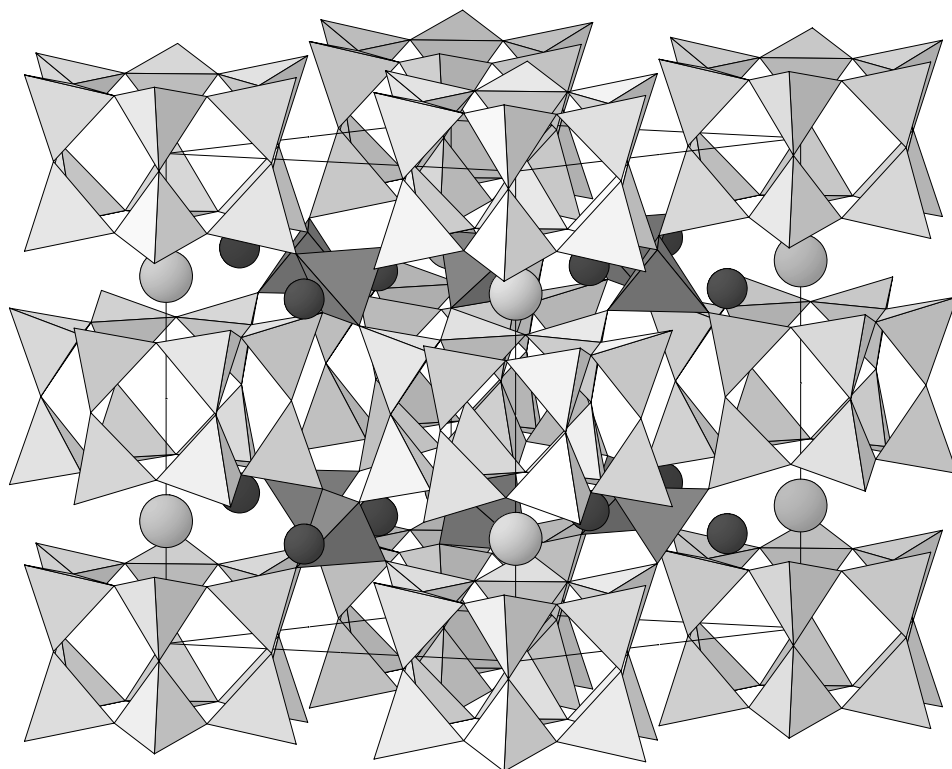
$a = 1.043$, $c = 1.385$ nm, $c/a = 1.328$, $V = 1.3048$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24 <i>m</i>	1	0.083	0.333	0.115		tetrahedron O ₄
O2	24 <i>m</i>	1	0.12	0.47	0.18		non-colinear SiBe
O3	24 <i>m</i>	1	0.28	0.08	0.14		non-colinear Si ₂
O4	12 <i>l</i>	<i>m</i> ..	0.09	0.375	0		non-colinear Si ₂
M5	6 <i>f</i>	222	1/2	0	1/4		tetrahedron O ₄
Ca6	4 <i>c</i>	3.2	1/3	2/3	1/4		octahedron O ₆
K7	2 <i>a</i>	622	0	0	1/4		hexagonal prism O ₁₂

M5 = 0.667Be + 0.333Al

Remarks: Natural specimen from the Alps, Switzerland. Adjustment of earlier published atom coordinates based on diffraction data from [2]. Cell parameters omitted, we took values from [2]. The data from [2] are also reported in [3].

References: [1] Pasheva Z.P., Tarkhova T.N. (1953), Dokl. Akad. Nauk SSSR 88, 807-810. [2] Belov N.V., Tarkhova T.N. (1949), Dokl. Akad. Nauk SSSR 69, 365-368. [3] Belov N.V., Tarkhova T.N. (1951), Tr. Inst. Kristallogr., Akad. Nauk SSSR 6, 83-140.

Fig. III.65. $\text{KCa}_2\text{Be}_2\text{AlSi}_{12}\text{O}_{30}$

Arrangement of $(\text{Be,Al})\text{O}_4$ (dark) and SiO_4 (light) tetrahedra, K (large) and Ca (small) atoms.

192
hP98

$\text{KCa}_2(\text{Be}_{0.13}\text{Al}_{0.07}\text{Si}_{0.80})_{15}\text{O}_{30}[\text{H}_2\text{O}]_{0.5}$

hP98

(192) $P6/mcc - m^3\text{fcba}$

$\text{KCa}_2\text{Be}_2\text{AlSi}_{12}\text{O}_{30} \cdot 0.5\text{H}_2\text{O}$ [1], milarite

Structural features: $(\text{Si,Be})_{12}\text{O}_{30}$ units (double 6-rings formed by twelve vertex-linked $(\text{Si,Be})\text{O}_4$ tetrahedra) share vertices with distorted $(\text{Si,Al,Be})\text{O}_4$ tetrahedra to form a 3D-framework; Ca, K and H_2O in channels parallel to $[001]$ (the latter two inside the columns formed by superposed double 6-rings).

Ito T. et al. (1952) [1]

$\text{Al}_{0.99}\text{Be}_{2.01}\text{Ca}_2\text{HKO}_{30.50}\text{Si}_{12}$

$a = 1.054$, $c = 1.396$ nm, $c/a = 1.324$, $V = 1.3431$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24m	1	0.076	0.331	0.111		tetrahedron O ₄
O2	24m	1	0.12	0.467	0.185		non-colinear Si ₂
O3	24m	1	0.283	0.084	0.128		non-colinear Si ₂
O4	12l	m..	0.091	0.388	0		non-colinear Si ₂
M5	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
Ca6	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆
(OH ₂)7	2b	6/m..	0	0	0	0.5	hexagonal prism O ₁₂

K8 2a 622 0 0 $\frac{1}{4}$ hexagonal prism O₁₂

M1 = 0.90Si + 0.10Be; M5 = 0.40Si + 0.33Al + 0.27Be

Experimental: single crystal, Weissenberg and oscillation photographs, X-rays, R = 0.300

Remarks: Natural specimen from Val Giuf, Graubünden, Switzerland. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Ito T., Morimoto M., Sadanaga R. (1952), Acta Crystallogr. 5, 209-213.

192
hP100

K₂Mg₅Si₁₂O₃₀ hP100 (192) P6/mcc – m³lfdca

K₂Mg₅Si₁₂O₃₀ [1], merrihueite

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with distorted MgO₄ tetrahedra and MgO₆ octahedra to form a 3D-framework; K inside the columns formed by superposed double 6-rings and between MgO₆ octahedra.

Khan A.A. et al. (1972) [1]

K₂Mg₅O₃₀Si₁₂

$a = 1.0222$, $c = 1.4152$ nm, $c/a = 1.384$, $V = 1.2806$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24m	1	0.1126	0.3484	0.1124		tetrahedron O ₄
O2	24m	1	0.1551	0.4968	0.1708		single atom Si
O3	24m	1	0.2763	0.058	0.1396		non-colinear Si ₂
O4	12l	m..	0.1239	0.3788	0		non-colinear Si ₂
Mg5	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
K6	4d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0	0.5	coplanar triangle O ₃
Mg7	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆
K8	2a	622	0	0	$\frac{1}{4}$		hexagonal prism O ₁₂

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

Remarks: Refinement on powder diffraction data in [2].

References: [1] Khan A.A., Baur W.H., Forbes W.C. (1972), Acta Crystallogr. B 28, 267-272. [2] Wohlfart A. (1998), Heidelb. Geowiss. Abh. 1998, 1-91.

192
hP102

K_{1.07}Ca_{2.15}(Be_{0.79}Al_{0.21})₃Si₁₂O₃₀ hP102 (192) P6/mcc – m³lfdca

K_{1.07}Ca_{2.15}Be_{2.37}Al_{0.63}Si₁₂O₃₀ [1], milarite dehydrated

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with distorted (Be,Al)O₄ tetrahedra to form a 3D-framework; K and Ca in channels parallel to [001] (main part of K inside the columns formed by superposed double 6-rings).

Armbruster T. et al. (1989) [1]

Al_{0.64}Be_{2.36}Ca₂K_{1.22}O₃₀Si₁₂

$a = 1.0363$, $c = 1.3827$ nm, $c/a = 1.334$, $V = 1.2860$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24m	1	0.08214	0.33739	0.11237		tetrahedron O ₄
O2	24m	1	0.1159	0.4742	0.18059		non-colinear SiBe

O3	24m	1	0.2771	0.0809	0.1345	non-colinear Si ₂
O4	12l	m..	0.0954	0.3854	0	non-colinear Si ₂
M5	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$	tetrahedron O ₄
K6	4d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0	0.1 coplanar triangle O ₃
Ca7	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	octahedron O ₆
K8	2b	6/m..	0	0	0	0.017 hexagonal prism O ₁₂
K9	2a	622	0	0	$\frac{1}{4}$	hexagonal prism O ₁₂

$$M5 = 0.787Be + 0.213Al$$

Experimental: single crystal, diffractometer, X-rays, R = 0.022, T = 100 K

Remarks: Natural specimen from Fuorcla da Crispalt, Val Giuf, Graubünden, Switzerland, dehydrated at 1100 K. Cation content $K_{0.111}Na_{0.039}Ca_{2.112}Be_{2.281}Al_{0.719}Si_{12}$ from electron microprobe analysis before heating. Partial substitution by Ca on sites K6 and K8 could not be excluded.

References: [1] Armbruster T., Bermanec V., Wenger M., Oberhansli R. (1989), Eur. J. Mineral. 1, 353-362.

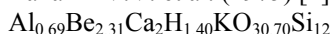
192
hP104

$KCa_2(Be_{0.77}Al_{0.23})_3Si_{12}O_{29.7}[OH]_{0.3}[H_2O]_{0.70}$	hP104	(192) <i>P6/mcc</i> – m ³ lhfca
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KCa₂Be_{2.3}Al_{0.7}Si₁₂O_{29.7}(OH)_{0.3}•0.7H₂O [1], milarite; BaCa₂Al₆Si₉O₃₀•2H₂O [1], armenite; KNa₂(Fe,Mn,Al)₂Li₃Si₁₂O₃₀ [2], sugilite

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with distorted (Be,Al)O₄ tetrahedra to form a 3D-framework; K, Ca and H₂O in channels parallel to [001] (K inside the columns formed by superposed double 6-rings).

Bakakin V.V. et al. (1975) [1]



$$a = 1.04, c = 1.38 \text{ nm}, c/a = 1.327, V = 1.2926 \text{ nm}^3, Z = 2$$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24m	1	0.082	0.3374	0.1119		tetrahedron O ₄
O2	24m	1	0.1154	0.4731	0.1811		non-colinear SiBe
O3	24m	1	0.272	0.0787	0.1347		non-colinear Si ₂
O4	12l	m..	0.0936	0.3834	0		non-colinear Si ₂
(OH ₂)5	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.06	0.175	single atom (OH ₂)
M6	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
Ca7	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		square prism (cube) O ₆ (OH ₂) ₂
K8	2a	622	0	0	$\frac{1}{4}$		hexagonal prism O ₁₂

$$M6 = 0.77Be + 0.23Al$$

Experimental: single crystal, diffractometer, X-rays, R = 0.120

Remarks: Natural specimen from the Kent deposit, central Kazakhstan. OH not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bakakin V.V., Balko V.P., Solov'eva L.P. (1975), Sov. Phys. Crystallogr. 19, 460-462 (Kristallografiya 19, 741-745). [2] Armbruster T., Oberhansli R. (1988), Am. Mineral. 73, 595-600.

192
hP108

$K_{0.7}Na_{0.3}Mg_{0.9}Fe_{0.9}(Fe_{0.12}Al_{0.88})_3(Al_{0.15}Si_{0.85})_{12}O_{30}[H_2O]$	hP108	(192) <i>P6/mcc</i> – m ³ l ² fca
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K_{0.7}Na_{0.3}Mg_{0.9}Fe_{1.3}Al_{4.4}Si_{10.2}O₃₀·H₂O [1], osumilite

Structural features: (Si,Al)₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked (Si,Al)O₄ tetrahedra) share vertices with distorted (Al,Fe)O₄ tetrahedra to form a 3D-framework; additional cations in channels parallel to [001] (partial disorder; alkaline metals and H₂O inside the columns formed by superposed double 6-rings).

Brown G.E., Gibbs G.V. (1969) [1]

Al_{4.44}Ca_{0.01}Fe_{1.28}H₂K_{0.71}Mg_{0.92}Mn_{0.16}Na_{0.28}O₃₁Si_{10.20}

$a = 1.0155$, $c = 1.4284$ nm, $c/a = 1.407$, $V = 1.2757$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24 <i>m</i>	1	0.1037	0.3513	0.1085		tetrahedron O ₄
O2	24 <i>m</i>	1	0.1372	0.4913	0.1789		non-coplanar triangle SiAlFe
O3	24 <i>m</i>	1	0.2837	0.0695	0.1316		non-coplanar Si ₂
(OH ₂)4	12 <i>l</i>	<i>m</i> ..	0.031	0.114	0	0.167	non-coplanar (OH ₂) ₂
O5	12 <i>l</i>	<i>m</i> ..	0.1267	0.4046	0		non-coplanar Si ₂
M6	6 <i>f</i>	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
M7	4 <i>c</i>	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆
M8	2 <i>a</i>	622	0	0	$\frac{1}{4}$		hexagonal prism O ₁₂

M1 = 0.85Si + 0.15Al; M6 = 0.88Al + 0.12Fe; M7 = 0.46Fe + 0.46Mg + 0.08Mn; M8 = 0.712K + 0.283Na + 0.005Ca

Experimental: single crystal, diffractometer, X-rays, R = 0.066

Remarks: Natural specimen. Composition (Ca_{0.005}Na_{0.31}K_{0.78})(Fe_{0.92}Mg_{0.92}Mn_{0.16})(Si_{10.22}Al_{4.41}Fe_{0.37})O₃₀·H₂O from electron microprobe analysis. We assigned an approximate value to the cation ratio of site M8 based on the chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Brown G.E., Gibbs G.V. (1969), Am. Mineral. 54, 101-116.

192
hP108

K _{1.1} Ca ₂ (Be _{0.7} Al _{0.3}) ₃ Si ₁₂ O ₃₀ [H ₂ O] _{0.75}	hP108	(192) <i>P6/mcc</i> – m ³ lh ² fa
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KCa₂Be₂AlSi₁₂O₃₀·H₂O [1], milarite

Structural features: Si₁₂O₃₀ units (double 6-rings formed by twelve vertex-linked SiO₄ tetrahedra) share vertices with distorted (Be,Al)O₄ tetrahedra to form a 3D-framework; K, Ca and H₂O in channels parallel to [001] (main part of K inside the columns formed by superposed double 6-rings).

Hawthorne F.C. et al. (1991) [1]

Al_{0.90}Be_{2.10}Ca₂H_{1.50}K_{1.10}O_{30.75}Si₁₂

$a = 1.0404$, $c = 1.3825$ nm, $c/a = 1.329$, $V = 1.2960$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24 <i>m</i>	1	0.08168	0.33625	0.11257		tetrahedron O ₄
O2	24 <i>m</i>	1	0.1154	0.4729	0.1804		non-coplanar SiBe
O3	24 <i>m</i>	1	0.2759	0.0808	0.134		non-coplanar Si ₂
O4	12 <i>l</i>	<i>m</i> ..	0.0946	0.383	0		non-coplanar Si ₂
M5	8 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0349	0.213	
Ca6	8 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.241	0.5	
M7	6 <i>f</i>	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
K8	2 <i>a</i>	622	0	0	$\frac{1}{4}$		hexagonal prism O ₁₂

M5 = 0.88OH₂ + 0.12K; M7 = 0.70Be + 0.30Al

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

Remarks: Natural specimen from Tittling, Bavaria, Germany. Composition $K_{1.07}Na_{0.01}Ca_{1.97}Be_{2.13}Al_{0.84}Si_{12.03}O_{30} \sim 0.75H_2O$ from electron microprobe analysis. We assigned approximate values to the occupancies of the cation sites based on the chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Hawthorne F.C., Kimata M., Cerny P., Ball N., Rossman G.R., Grice J.D. (1991), Am. Mineral. 76, 1836-1856.

192
hP110

$KCa_{2.15}(Be_{0.77}Al_{0.23})_3Si_{12}O_{30}[H_2O]_{0.6}$	hP110	(192) $P6/mcc - m^3lhfdcba$
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$KCa_{2.15}Be_{2.31}Al_{0.69}Si_{12}O_{30} \cdot 0.6H_2O$ [1], milarite

Structural features: $Si_{12}O_{30}$ units (double 6-rings formed by twelve vertex-linked SiO_4 tetrahedra) share vertices with distorted $(Be,Al)O_4$ tetrahedra to form a 3D-framework; K, Ca and H_2O in channels parallel to [001] (partial disorder, main part of K inside the columns formed by superposed double 6-rings).

Armbruster T. et al. (1989) [1]

$Al_{0.69}Be_{2.31}Ca_2H_{1.18}K_{1.15}O_{30.59}Si_{12}$

$a = 1.0398$, $c = 1.3771$ nm, $c/a = 1.324$, $V = 1.2894$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Si1	24m	1	0.08115	0.33622	0.11286		tetrahedron O ₄
O2	24m	1	0.1149	0.4731	0.181		non-colinear SiBe
O3	24m	1	0.276	0.0809	0.13492		non-colinear Si ₂
O4	12l	m..	0.0937	0.3831	0		non-colinear Si ₂
(OH ₂)5	8h	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0476	0.147	
M6	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$		tetrahedron O ₄
K7	4d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	0	0.07	
Ca8	4c	3.2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		octahedron O ₆
K9	2b	6/m..	0	0	0	0.013	hexagonal prism O ₁₂
K10	2a	622	0	0	$\frac{1}{4}$		hexagonal prism O ₁₂

$M6 = 0.770Be + 0.230Al$

Experimental: single crystal, diffractometer, X-rays, $R = 0.020$, $T = 100$ K

Remarks: Natural specimen from Fuorcla da Crispalt, Val Giuf, Graubünden, Switzerland. Cation content $K_{0.111}Na_{0.039}Ca_{2.112}Be_{2.281}Al_{0.719}Si_{12}$ from electron microprobe analysis. Partial substitution by Ca on sites K7 and K9 could not be excluded. 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] Armbruster T., Bermanec V., Wenger M., Oberhansli R. (1989), Eur. J. Mineral. 1, 353-362.

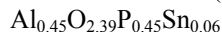
192
hP158

$Al_{0.48}Sn_{0.04}P_{0.48}O_2$	hP158	(192) $P6/mcc - m^3l^4k^2ja$
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$AlPO_4$ form 5:Sn [1], zeolite AFI-Sn

Structural features: $(Al,P)O_4$ tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001]; Sn substitutes for (Al,P) in the framework (displaced into a tetrahedron face, an additional O completes a surrounding trigonal bipyramid).

Flavell W.R. et al. (2001) [1]



$a = 1.36935$, $c = 0.84689$ nm, $c/a = 0.618$, $V = 1.3753$ nm³, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24 <i>m</i>	1	0.054	0.1279	0.117	0.04	non-coplanar triangle O ₃
Sn2	24 <i>m</i>	1	0.1196	0.4569	0.23	0.064	
M3	24 <i>m</i>	1	0.4568	0.1216	0.1809	0.906	
O4	12 <i>l</i>	<i>m</i> ..	0.0665	0.2579	0	0.136	single atom O
O5	12 <i>l</i>	<i>m</i> ..	0.1147	0.452	0	0.29	non-collinear Sn ₂
O6	12 <i>l</i>	<i>m</i> ..	0.1878	0.0414	0	0.194	non-coplanar triangle O ₃
O7	12 <i>l</i>	<i>m</i> ..	0.4465	0.1317	0		non-collinear Al ₂
O8	12 <i>k</i>	..2	0.2081	0.4163	$\frac{1}{4}$		
O9	12 <i>k</i>	..2	0.5769	0.1538	$\frac{1}{4}$		
O10	12 <i>j</i>	..2	0.3578	0	$\frac{1}{4}$		
O11	2 <i>a</i>	622	0	0	$\frac{1}{4}$	0.444	hexagonal prism O ₁₂

$\text{M3} = 0.5\text{Al} + 0.5\text{P}$

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: powder, diffractometer, X-rays, synchrotron, $R_B = 0.012$

Remarks: Short interatomic distances for partly occupied site(s). Ambiguous data: ideal composition not clear, large amount of non-framework species refined as O. We assume that in table 2 of [1] the occupancy of former O(A) is misprinted as 0.400 instead of 0.040 (better agreement with the description of the structure).

References: [1] Flavell W.R., Nicholson D.G., Nilsen M.H., Stahl K. (2001), J. Mater. Chem. 11, 620-627.

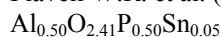
192
hP160

$\text{Al}_{0.48}\text{Sn}_{0.04}\text{P}_{0.48}\text{O}_2$	<i>hP160</i>	(192) <i>P6/mcc</i> – $m^4l^2k^2jd$
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AlPO₄ form 5:Sn [1], zeolite AFI-Sn

Structural features: (Al,P)O₄ tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001]; Sn substitutes for (Al,P) in the framework (displaced into a tetrahedron face).

Flavell W.R. et al. (2001) [1]



$a = 1.36965$, $c = 0.84231$ nm, $c/a = 0.615$, $V = 1.3684$ nm³, $Z = 24$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
M1	24 <i>m</i>	1	0.1236	0.4542	0.1855		
Sn2	24 <i>m</i>	1	0.1245	0.3523	0.0881	0.021	
O3	24 <i>m</i>	1	0.185	0.0468	0.1415	0.188	single atom O
Sn4	24 <i>m</i>	1	0.4986	0.1598	0.1301	0.033	
O5	12 <i>l</i>	<i>m</i> ..	0.0301	0.1864	0	0.372	non-collinear O ₂
O6	12 <i>l</i>	<i>m</i> ..	0.1089	0.4732	0		non-collinear Al ₂
O7	12 <i>k</i>	..2	0.2084	0.4169	$\frac{1}{4}$		non-collinear Al ₂
O8	12 <i>k</i>	..2	0.5817	0.1635	$\frac{1}{4}$		non-collinear Sn ₂
O9	12 <i>j</i>	..2	0.356	0	$\frac{1}{4}$		non-collinear Al ₂

O10 4d -6.. $\frac{1}{3}$ $\frac{2}{3}$ 0 0.216 trigonal prism Sn₆

M1 = 0.5Al + 0.5P

Experimental: powder, diffractometer, X-rays, synchrotron, $R_B = 0.010$

Remarks: Refinement of the occupancy of site M1 assuming 0.5Al + 0.5P gave occ = 1.016(8). Short interatomic distances for partly occupied site(s). Ambiguous data: ideal composition not clear, large amount of non-framework species refined as O.

References: [1] Flavell W.R., Nicholson D.G., Nilsen M.H., Stahl K. (2001), J. Mater. Chem. 11, 620-627.

192
hP166

Ag₁₆[P₂O₇]I₁₂

hP166

(192) *P6/mcc* – m⁵l³fe

Ag₁₆P₂O₇I₁₂ [1]

Structural features: Close-packed (I₆□) layers in approximate h stacking; disordered arrangement of units of two vertex-linked PO₄ tetrahedra in the channels formed by the vacant positions.

Garrett J.D. et al. (1982) [1]

Ag_{16.08}I₁₂O_{6.97}P₂

$a = 1.2054$, $c = 0.7504$ nm, $c/a = 0.623$, $V = 0.9442$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	24m	1	0.04	0.14	0.2	0.083	
O2	24m	1	0.05	0.1	0.15	0.083	
Ag3	24m	1	0.053	0.3018	0.1754	0.29	
Ag4	24m	1	0.0947	0.4747	0.1605	0.12	
O5	24m	1	0.15	0.07	0.2	0.083	
Ag6	12l	m..	0.0489	0.2467	0	0.26	
O7	12l	m..	0.05	0.02	0	0.083	
I8	12l	m..	0.45	0.1479	0		
Ag9	6f	222	$\frac{1}{2}$	0	$\frac{1}{4}$	0.52	
P10	4e	6..	0	0	0.2018	0.5	

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

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

References: [1] Garrett J.D., Greedan J.E., Faggiani R., Carbotte S., Brown I.D. (1982), J. Solid State Chem. 42, 183-190.

192
hP184

Cu_{0.023}Al_{0.48}Sn_{0.04}P_{0.48}O_{2.023}

hP184

(192) *P6/mcc* – m⁵l²k²j_d

AlPO₄ form 5:Sn,Cu [1], zeolite AFI-Sn,Cu

Structural features: (Al,P)O₄ tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001]; Sn substitutes for (Al,P) in the framework (displaced into a tetrahedron face), Cu at interstitial positions (disorder).

Flavell W.R. et al. (2001) [1]

Al_{0.46}Cu_{0.01}O_{2.20}P_{0.46}Sn_{0.04}

$a = 1.37579$, $c = 0.83604$ nm, $c/a = 0.608$, $V = 1.3704$ nm³, $Z = 24$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Sn1	24 <i>m</i>	1	0.1245	0.3523	0.0881	0.017	
M2	24 <i>m</i>	1	0.1306	0.4621	0.1845	0.924	
O3	24 <i>m</i>	1	0.1688	0.0358	0.2392	0.099	
Cu4	24 <i>m</i>	1	0.185	0.0468	0.1415	0.014	
Sn5	24 <i>m</i>	1	0.4986	0.1598	0.1301	0.022	
O6	12 <i>l</i>	<i>m</i> ..	0.0231	0.1465	0	0.132	non-colinear Cu ₂
O7	12 <i>l</i>	<i>m</i> ..	0.1118	0.4783	0		non-colinear Al ₂
O8	12 <i>k</i>	..2	0.2053	0.4107	¹ / ₄		tetrahedron Al ₂ Sn ₂
O9	12 <i>k</i>	..2	0.5775	0.155	¹ / ₄		
O10	12 <i>j</i>	..2	0.3502	0	¹ / ₄		non-colinear Al ₂
O11	4 <i>d</i>	-6..	¹ / ₃	² / ₃	0	0.234	trigonal prism Sn ₆

M2 = 0.5Al + 0.5P

Experimental: powder, diffractometer, X-rays, synchrotron, R_B = 0.006

Remarks: The authors state that former site O(C) (occ = 0.178 for f(O)), is occupied by Cu; we assigned an approximate value to the site occupancy assuming Cu. Short interatomic distances for partly occupied site(s). Ambiguous data: ideal composition not clear, large amount of non-framework species refined as O. Tetragonally distorted octahedral environment for Cu from EXAFS spectroscopy; the square coordination formed by interstitial O stated in the text is not confirmed by the published coordinates.

References: [1] Flavell W.R., Nicholson D.G., Nilsen M.H., Stahl K. (2001), J. Mater. Chem. 11, 620-627.