

Space group (196) *F*23196  
*cF*60

$\text{Cu}_2\text{Fe}[\text{CN}]_6$	<i>cF</i> 60	(196) <i>F</i> 23 – hcba
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 **$\text{Cu}_2\text{Fe}(\text{CN})_6$**  [1]

Structural features:  $\text{Fe}(\text{CN})_6$  and  $\text{Cu}(\text{CN})_6$  octahedra (CN units perpendicular to the Fe-Cu segments) share vertices to form a 3D-framework; additional Cu in cubic voids.

Rigamonti R. (1937) [1]

$\text{C}_6\text{Cu}_2\text{FeN}_6$

$a = 0.998 \text{ nm}$ ,  $V = 0.9940 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	48 <i>h</i>	1	0.0	0.0625	0.25		single atom C
Cu2	4 <i>c</i>	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		icosahedron $\text{C}_{12}$
Cu3	4 <i>b</i>	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		icosahedron $\text{C}_{12}$
Fe4	4 <i>a</i>	23.	0	0	0		icosahedron $\text{C}_{12}$

$\text{M1} = 0.5\text{C} + 0.5\text{N}$

Experimental: powder, film, X-rays

Remarks: We derived the space group from the coordinates of all atoms in the unit cell. A similar model with linear Fe-C-N segments could not be rejected.

References: [1] Rigamonti R. (1937), Gazz. Chim. Ital. 67, 137-146.

196  
*cF*136

$\text{Na}_{0.01}\text{Ca}_{1.04}\text{Mn}_{0.07}(\text{Ti}_{0.38}\text{Fe}_{0.09}\text{Al}_{0.03}\text{Sb}_{0.50})_2\text{Sb}_{0.65}\text{O}_6[\text{OH}]_{0.91}$	<i>cF</i> 136
(196) <i>F</i> 23 – hgfe <sup>2</sup> ca	

 **$(\text{Ca}_{1.04}\text{Mn}_{0.07}\text{Na}_{0.01})\text{Sb}_{0.65}(\text{Sb}_{0.99}\text{Ti}_{0.76}\text{Fe}_{0.19}\text{Al}_{0.06})\text{O}_6(\text{OH})_{0.91}$**  [1], lewisite, pyrochlore family

Structural features:  $(\text{Sb}^{5+}, \text{Ti}, \text{Fe}^{3+}, \text{Al})\text{O}_6$  octahedra share vertices to form a pyrochlore-type framework;  $(\text{Ca}, \text{Mn}, \text{Na})$ ,  $\text{Sb}^{3+}$  and OH in voids.

Rouse R.C. et al. (1998) [1]

$\text{Al}_{0.06}\text{Ca}_{1.04}\text{Fe}_{0.19}\text{H}_{0.91}\text{Mn}_{0.07}\text{Na}_{0.01}\text{O}_{6.91}\text{Sb}_{1.64}\text{Ti}_{0.76}$

$a = 1.0277 \text{ nm}$ ,  $V = 1.0854 \text{ nm}^3$ ,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
M1	48 <i>h</i>	1	0.0914	0.142	0.1431	0.147	
M2	24 <i>g</i>	2..	0.554	$\frac{1}{4}$	$\frac{1}{4}$	0.987	tetrahedron $\text{Sb}_2\text{Ca}_2$
M3	24 <i>f</i>	2..	0.2991	0	0	0.987	non-colinear $\text{Sb}_2$
M4	16 <i>e</i>	.3.	0.1223	0.1223	0.1223	0.442	
M5	16 <i>e</i>	.3.	0.62519	0.62519	0.62519		octahedron $\text{O}_6$
M6	4 <i>c</i>	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0.987	
M7	4 <i>a</i>	23.	0	0	0	0.987	

$\text{M1} = 0.5868\text{Ca} + 0.3672\text{Sb} + 0.0388\text{Mn} + 0.0072\text{Na}$ ;  $\text{M2} = 0.8684\text{O} + 0.1316\text{OH}$ ;  $\text{M3} = 0.8684\text{O} + 0.1316\text{OH}$ ;  $\text{M4} = 0.5868\text{Ca} + 0.3672\text{Sb} + 0.0388\text{Mn} + 0.0072\text{Na}$ ;  $\text{M5} = 0.495\text{Sb} + 0.3800\text{Ti} + 0.095\text{Fe} + 0.0300\text{Al}$ ;  $\text{M6} = 0.8684\text{O} + 0.1316\text{OH}$ ;  $\text{M7} = 0.8684\text{O} + 0.1316\text{OH}$

Transformation from published data:  $-y, -x, z$ ; origin shift  $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.014$ ,  $T = 297$  K

Remarks:  $[(\text{Ca}_{1.04}\text{Mn}^{2+}_{0.07}\text{Na}_{0.01})(\text{Sb}^{3+}_{0.65})](\text{Sb}^{5+}_{0.99}\text{Ti}^{4+}_{0.76}\text{Fe}^{3+}_{0.19}\text{Al}_{0.06})\text{O}_6(\text{OH})_{0.91}$ . Natural specimen from Tripuí, Ouro Preto, Minas Gerais. Composition  $\text{Ca}_{8.31}\text{Na}_{0.10}\text{Fe}_{1.53}\text{Mn}_{0.55}\text{Ti}_{6.07}\text{Al}_{0.44}\text{Sb}_{13.16}\text{O}_x$  from electron microprobe analysis, no F detected. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (227)  $Fd\text{-}3m$  was tested and rejected, space group (216)  $F\text{-}43m$  was retained as most probable.

References: [1] Rouse R.C., Dunn P.J., Peacor D.R., Wang L. (1998), J. Solid State Chem. 141, 562-569.

196  
cF204

$\text{Li}_{10}\text{B}_{14}\text{Cl}_2\text{O}_{25}$	cF204	(196) $F23 - h^2gfe^3cba$
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**$\text{Li}_5\text{B}_7\text{O}_{12.5}\text{Cl}$**  [1], boracite family

Structural features:  $\text{BO}_4$  tetrahedra and  $\text{BO}_3$  trigonal units (in the ratio 5:2) share vertices to form a 3D-framework; Li in tetrahedral ( $\text{O}_3\text{Cl}$ ) and square pyramidal ( $\text{O}_4\text{Cl}$ ) voids.

Vlasse M. et al. (1981) [1]

$\text{B}_{14}\text{Cl}_2\text{Li}_{10}\text{O}_{25}$

$a = 1.2136$  nm,  $V = 1.7874$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	48h	1	0.0695	0.2305	0.1527		non-collinear B <sub>2</sub>
O2	48h	1	0.1508	0.2273	0.5673		non-collinear B <sub>2</sub>
B3	24g	2..	0.5015	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
Li4	24f	2..	0.2084	0	0		square pyramid O <sub>4</sub> Cl
B5	16e	.3.	0.1692	0.1692	0.1692		tetrahedron O <sub>4</sub>
Li6	16e	.3.	0.385	0.385	0.385		non-coplanar triangle O <sub>3</sub>
B7	16e	.3.	0.6489	0.6489	0.6489		coplanar triangle O <sub>3</sub>
O8	4c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron B <sub>4</sub>
Cl9	4b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		tetrahedron Li <sub>4</sub>
Cl10	4a	23.	0	0	0		octahedron Li <sub>6</sub>

Transformation from published data:  $-x, -y, -z$ ; origin shift  $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays,  $R = 0.064$ ,  $T = 296$  K

References: [1] Vlasse M., Levasseur A., Hagenmuller P. (1981), Solid State Ionics 2, 33-37.

196  
cF240

$\text{Li}_4\text{B}_7\text{ClO}_{12}$	cF240	(196) $F23 - h^2gf^2e^4ba$
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**$\text{Li}_4\text{B}_7\text{O}_{12}\text{Cl}$**  [1], boracite family

Structural features:  $\text{BO}_4$  tetrahedra and  $\text{BO}_3$  trigonal units (in the ratio 3:4) share vertices to form a 3D-framework.

Levasseur A. et al. (1973) [1]

$\text{B}_7\text{ClLi}_4\text{O}_{12}$

$a = 1.2154$  nm,  $V = 1.7954$  nm<sup>3</sup>,  $Z = 8$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	48h	1	0.0689	0.2718	0.1522		non-collinear B <sub>2</sub>
O2	48h	1	0.1515	0.2732	0.5677		non-collinear B <sub>2</sub>

B3	24g	2..	0.0	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
Li4	24f	2..	0.208	0	0	0.5	
Li5	24f	2..	0.263	0	0	0.5	
Li6	16e	.3.	0.111	0.111	0.111	0.25	
Li7	16e	.3.	0.121	0.121	0.121	0.25	
B8	16e	.3.	0.3505	0.3505	0.3505		coplanar triangle O <sub>3</sub>
B9	16e	.3.	0.8494	0.8494	0.8494		non-coplanar triangle O <sub>3</sub>
Cl10	4b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Li <sub>6</sub>
Cl11	4a	23.	0	0	0		tetrahedron Li <sub>4</sub>

Transformation from published data:  $-y, -x, z$ ; origin shift  $\frac{1}{4} \frac{1}{4} \frac{1}{4}$

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

Remarks: Short interatomic distances for partly occupied site(s). In table 1 of [1] the y-coordinate of former Li(II)1 is misprinted as 0.316 instead of 0.361 (agreement with Wyckoff position 16e).

References: [1] Levasseur A., Lloyd D.J., Fouassier C., Hagenmuller P. (1973), J. Solid State Chem. 8, 318-324.

196  
cF260

Ca <sub>14</sub> Zn <sub>6</sub> Al <sub>10</sub> O <sub>35</sub>	cF260	(196) F23 – h <sup>2</sup> g <sup>2</sup> fe <sup>5</sup> dca
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### Ca<sub>14</sub>Zn<sub>6</sub>Al<sub>10</sub>O<sub>35</sub> [1]

Structural features: AlO<sub>4</sub> and ZnO<sub>4</sub> tetrahedra (partial disorder) share vertices to form a 3D-framework; additional Al and Ca in octahedral voids.

Barbanyagre V.D. et al. (1997) [1]

Al<sub>10</sub>Ca<sub>14</sub>O<sub>35</sub>Zn<sub>6</sub>

$a = 1.4868 \text{ nm}$ ,  $V = 3.2867 \text{ nm}^3$ ,  $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	48h	1	0.0054	0.0996	0.3196		non-colinear Al <sub>2</sub>
O2	48h	1	0.0061	0.1841	0.0997		non-colinear AlZn
Ca3	24g	2..	0.0358	$\frac{1}{4}$	$\frac{1}{4}$		7-vertex polyhedron O <sub>7</sub>
O4	24g	2..	0.6198	$\frac{1}{4}$	$\frac{1}{4}$		single atom Al
Al5	24f	2..	0.2523	0	0		tetrahedron O <sub>4</sub>
Zn6	16e	.3.	0.0776	0.0776	0.0776		tetrahedron O <sub>4</sub>
O7	16e	.3.	0.3167	0.3167	0.3167		colinear Al <sub>2</sub>
M8	16e	.3.	0.3929	0.3929	0.3929		tetrahedron O <sub>4</sub>
Ca9	16e	.3.	0.6369	0.6369	0.6369		octahedron O <sub>6</sub>
Ca10	16e	.3.	0.8624	0.8624	0.8624		octahedron O <sub>6</sub>
Al11	4d	23.	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		octahedron O <sub>6</sub>
Al12	4c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O13	4a	23.	0	0	0		tetrahedron Zn <sub>4</sub>

M8 = 0.50Al + 0.50Zn

Transformation from published data:  $y, x, -z$ ; origin shift  $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: single crystal, diffractometer, X-rays

References: [1] Barbanyagre V.D., Timoshenko T.I., Ilynets A.M., Shamshurov V.M. (1997), Powder Diffr. 12, 22-26.

196  
*cF432*

$\text{Li}_{22}\text{Si}_5$	<i>cF432</i>	(196) <i>F23</i> – $\text{h}^4\text{g}^2\text{f}^2\text{e}^8\text{dcba}$
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 **$\text{Li}_{22}\text{Si}_5$**  (see remark)

Structural features: Slightly distorted ordering variant of the W type (prototype for a b.c.c. arrangement).

Axel H. et al. (1966) [1]

 $\text{Li}_{22}\text{Si}_5$  $a = 1.875 \text{ nm}$ ,  $V = 6.5918 \text{ nm}^3$ ,  $Z = 16$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	48 <i>h</i>	1	0.003	0.158	0.333		rhombic dodecahedron $\text{Li}_{10}\text{Si}_4$
Li2	48 <i>h</i>	1	0.005	0.161	0.167		rhombic dodecahedron $\text{Li}_{12}\text{Si}_2$
Li3	48 <i>h</i>	1	0.083	0.25	0.583		rhombic dodecahedron $\text{Si}_3\text{Li}_{11}$
Li4	48 <i>h</i>	1	0.087	0.087	0.25		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Si5	24 <i>g</i>	2..	0.072	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron $\text{Li}_{14}$
Li6	24 <i>g</i>	2..	0.583	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Li7	24 <i>f</i>	2..	0.167	0	0		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Si8	24 <i>f</i>	2..	0.322	0	0		rhombic dodecahedron $\text{Li}_{14}$
Li9	16 <i>e</i>	.3.	0.08	0.08	0.08		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Li10	16 <i>e</i>	.3.	0.167	0.167	0.167		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Li11	16 <i>e</i>	.3.	0.33	0.33	0.33		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Li12	16 <i>e</i>	.3.	0.42	0.42	0.42		rhombic dodecahedron $\text{Li}_{11}\text{Si}_3$
Li13	16 <i>e</i>	.3.	0.583	0.583	0.583		rhombic dodecahedron $\text{Li}_{10}\text{Si}_4$
Si14	16 <i>e</i>	.3.	0.665	0.665	0.665		rhombic dodecahedron $\text{Li}_{14}$
Li15	16 <i>e</i>	.3.	0.833	0.833	0.833		rhombic dodecahedron $\text{Si}_4\text{Li}_{10}$
Si16	16 <i>e</i>	.3.	0.911	0.911	0.911		rhombic dodecahedron $\text{Li}_{14}$
Li17	4 <i>d</i>	23.	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		rhombic dodecahedron $\text{Li}_{10}\text{Si}_4$
Li18	4 <i>c</i>	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		rhombic dodecahedron $\text{Li}_8\text{Si}_6$
Li19	4 <i>b</i>	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		rhombic dodecahedron $\text{Li}_8\text{Si}_6$
Li20	4 <i>a</i>	23.	0	0	0		rhombic dodecahedron $\text{Li}_{10}\text{Si}_4$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.097$ 

Remarks: The structure was later refined in space group (216) *F-43m* and the composition corrected to  $\text{Li}_{21}\text{Si}_5$  [2] (Zintl compound). The description of  $\text{Li}_{22}\text{Si}_5$  in space group (196) *F23* in [3] does not take into consideration all symmetry elements of the proposed model; the data can be directly transformed to space group (216) *F-43m*. The same is true for  $\text{Li}_{22}\text{Pb}_5$  reported in [4].

References: [1] Axel H., Schäfer H., Weiss A. (1966), Z. Naturforsch. B 21, 115-117. [2] Nesper R., Von Schnering H.G. (1987), J. Solid State Chem. 70, 48-57. [3] Gladyshevskii E.I., Oleksiv G.I., Kripyakevich P.I. (1964), Sov. Phys. Crystallogr. (Engl. Transl.) 9, 269-271. [4] Zalkin A., Ramsey W.J. (1958), J. Phys. Chem. 62, 689-693.

196  
*cF536*

$\text{Ca}_2\text{Hg}_{11}\text{Cl}_{26}[\text{H}_2\text{O}]_{16}$	<i>cF536</i>	(196) <i>F23</i> – $\text{h}^{10}\text{fedcba}$
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 **$\text{Ca}_2\text{Hg}_{11}\text{Cl}_{26}\cdot 16\text{H}_2\text{O}$**  [1]

Structural features:  $\text{Hg}_6\text{Cl}_{13}$  icosahedral units (a central Cl surrounded by six linear Cl-Hg-Cl units arranged so that the Hg atoms form an octahedron and the Cl atoms an icosahedron),  $\text{Hg}_5\text{Cl}_{13}$  icosahedral units (distorted  $\text{ClCl}_{12}$  icosahedron, part of Hg in trigonal coordination) and  $\text{Ca}(\text{H}_2\text{O})_8$  units (all in orientational disorder).

Putzas D. et al. (1991) [1]

 $\text{Ca}_2\text{Cl}_{26}\text{H}_{31.97}\text{Hg}_{11}\text{O}_{15.98}$  $a = 1.817 \text{ nm}$ ,  $V = 5.9988 \text{ nm}^3$ ,  $Z = 4$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cl1	48h	1	0.0101	0.192	0.0995	0.5	
Hg2	48h	1	0.0126	0.0624	0.1394	0.066	
Hg3	48h	1	0.0585	0.0826	0.1303	0.12	
Hg4	48h	1	0.0837	0.3644	0.5446	0.132	
Cl5	48h	1	0.1139	0.5183	0.3192	0.5	
(OH <sub>2</sub> )6	48h	1	0.122	0.254	0.23	0.333	
Cl7	48h	1	0.1256	0.1728	0.5024		single atom Hg
(OH <sub>2</sub> )8	48h	1	0.136	0.191	0.269	0.333	
(OH <sub>2</sub> )9	48h	1	0.167	0.639	0.242	0.333	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )10	48h	1	0.203	0.285	0.627	0.333	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
Hg11	24f	2..	0.3308	0	0		non-colinear Cl <sub>2</sub>
Hg12	16e	.3.	0.0877	0.0877	0.0877	0.295	
Ca13	4d	23.	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3}{4}$		pseudo Frank-Kasper (OH <sub>2</sub> ) <sub>24</sub>
Ca14	4c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$		
Cl15	4b	23.	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		octahedron Hg <sub>6</sub>
Cl16	4a	23.	0	0	0		

Transformation from published data:  $-y, -x, z$ ; origin shift  $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays,  $wR = 0.051$ ,  $T = 293 \text{ K}$ 

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] Putzas D., Rotter H.W., Thiele G., Brodersen K., Pezzeti G. (1991), Z. Anorg. Allg. Chem. 595, 193-202.

196  
cF856

$\text{K}_{31.75}\text{Al}_{23.75}\text{Si}_{25.25}\text{O}_{96}$	cF856	(196) F23 – h <sup>15</sup> fe <sup>7</sup>
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**K<sub>128.4</sub>Al<sub>95</sub>Si<sub>97</sub>O<sub>384</sub>** [1], zeolite LTA-K<sub>12</sub>/K<sub>4</sub>Structural features: AlO<sub>4</sub> and SiO<sub>4</sub> tetrahedra share vertices to form a LTA-type zeolite framework with  $\beta$  cages (14-face truncated octahedra) interconnected via tetragonal prisms, and  $\alpha$  cages (26-face truncated cuboctahedra); different K<sup>+</sup> clusters in two different kinds of  $\alpha$  cage, additional K<sup>+</sup> distributed over several partly occupied sites.

Ikeda T. et al. (2000) [1]

 $\text{Al}_{23.76}\text{K}_{32.02}\text{O}_{96}\text{Si}_{24.24}$  $a = 2.46341 \text{ nm}$ ,  $V = 14.9489 \text{ nm}^3$ ,  $Z = 4$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
K1	48h	1	0.001	0.3671	0.1307	0.487	non-coplanar square O <sub>4</sub>
O2	48h	1	0.0035	0.2507	0.1266		non-colinear SiAl
K3	48h	1	0.016	0.232	0.017	0.16	
M4	48h	1	0.0585	0.1578	0.2541		tetrahedron O <sub>4</sub>
Si5	48h	1	0.0622	0.2528	0.1567		tetrahedron O <sub>4</sub>
O6	48h	1	0.0671	0.1964	0.195		non-colinear SiAl
O7	48h	1	0.0722	0.3065	0.191		non-colinear SiAl
O8	48h	1	0.1084	0.11	0.249		non-colinear SiAl

O9	48h	1	0.1102	0.2527	0.6074		non-colinear SiAl
K10	48h	1	0.119	0.503	0.374	0.283	single atom O
O11	48h	1	0.1268	0.2435	0.502		non-colinear SiAl
Si12	48h	1	0.1558	0.2511	0.5603		tetrahedron O <sub>4</sub>
M13	48h	1	0.1573	0.5623	0.2435		tetrahedron O <sub>4</sub>
O14	48h	1	0.1904	0.1954	0.5733		non-colinear AlSi
O15	48h	1	0.1911	0.3063	0.5658		non-colinear SiAl
K16	24f	2..	0.25	0	0	0.71	
K17	16e	.3.	0.0106	0.0106	0.0106	0.15	
K18	16e	.3.	0.123	0.123	0.123	0.582	
K19	16e	.3.	0.1488	0.1488	0.1488	0.418	
K20	16e	.3.	0.318	0.318	0.318	0.582	
K21	16e	.3.	0.3646	0.3646	0.3646	0.418	
K22	16e	.3.	0.6812	0.6812	0.6812		
K23	16e	.3.	0.8648	0.8648	0.8648		non-coplanar triangle O <sub>3</sub>

M4 = 0.990Al + 0.010Si; M13 = 0.990Al + 0.010Si

Transformation from published data: origin shift  $\frac{3}{4} \frac{3}{4} \frac{3}{4}$

Experimental: powder, diffractometer, neutrons, time-of-flight,  $R_p = 0.022$ ,  $T = 39.5$  K

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

References: [1] Ikeda T., Kodaira T., Izumi F., Kamiyama T., Ohshima K. (2000), Chem. Phys. Lett. 318, 93-101.