Marialite Scapolite [$Na_4Cl(AlSi_3)_3O_{24}$, $S6_4$] Structure: AB4C24D12_tI82_87_a_h_2h2i_hi-001

This structure originally had the label `AB4C24D12_tI82_87_a_h_2h2i_hi`. Calls to that address will be redirected here.

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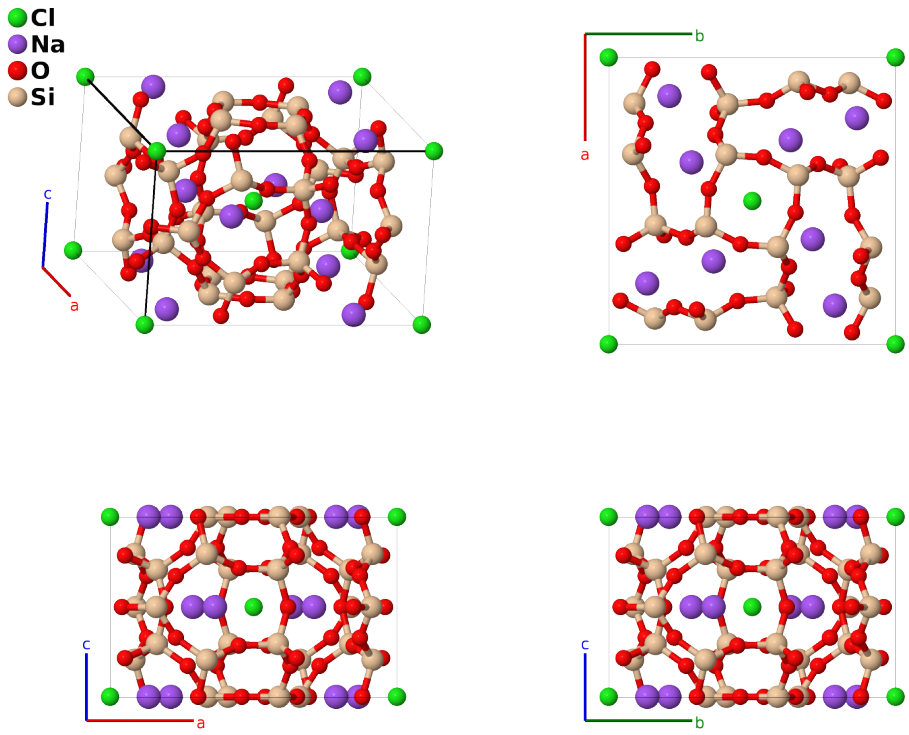
https://aflow.org/p/8NAD

https://aflow.org/p/AB4C24D12_tI82_87_a_h_2h2i_hi-001

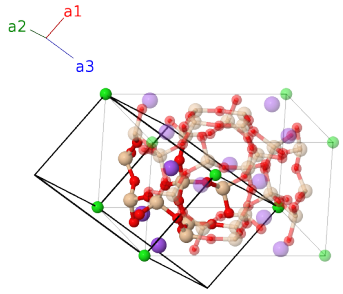


Prototype	$Al_3ClNa_4O_{24}Si_9$
AFLOW prototype label	AB4C24D12_tI82_87_a_h_2h2i_hi-001
***Strukturbericht* designation**	$S6_4$
Mineral name	marialite scapolite
ICSD	9502
Pearson symbol	tI82
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=AB4C24D12_tI82_87_a_h_2h2i_hi-001 --params=`$a, c/a, x_2, y_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- (Papike, 1965) found that the composition of the Si-II (16h) site was actually $Al_{0.458}Si_{0.542}$, and which we list as silicon. This is richer in aluminum than assumed by Pauli, who gave the total aluminum/silicon composition as $AlSi_3$. If we assume that the Si-I (8h) site is only filled by silicon atoms, then Pauli's composition for the Si-II site is $Al_{0.375}Si_{0.625}$. The name "marialite" scapolite distinguishes this from meionite scapolite, which replaces the sodium atoms by calcium but also includes SiO_4 and CO_3, which replace the chlorine atoms. According to Pauli, "The minerals of the scapolite group can be considered as solid solution of two end-members, marialite, $Na_4Al_3Si_9O_{24}Cl$, and meionite, $Ca_4Al_6Si_6O_{24}(SO_4,CO_3)$, in various proportions."

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cl I
$\mathbf{B_2}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(8h)	Na I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	O I
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{13}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{14}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(8h)	Si I
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(8h)	Si I
$\mathbf{B_{16}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + (x_5-y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8h)	Si I
$\mathbf{B_{17}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - (x_5-y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8h)	Si I
$\mathbf{B_{18}}$	=	$(y_6+z_6)\,\mathbf{a}_1 + (x_6+z_6)\,\mathbf{a}_2 + (x_6+y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{19}}$	=	$-(y_6-z_6)\,\mathbf{a}_1 - (x_6-z_6)\,\mathbf{a}_2 - (x_6+y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{20}}$	=	$(x_6+z_6)\,\mathbf{a}_1 - (y_6-z_6)\,\mathbf{a}_2 + (x_6-y_6)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16i)	O III

$$\mathbf{B_{21}} = -(x_6 - z_6)\,\mathbf{a}_1 + (y_6 + z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = a y_6\,\hat{\mathbf{x}} - a x_6\,\hat{\mathbf{y}} + c z_6\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{22}} = -(y_6 + z_6)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -a x_6\,\hat{\mathbf{x}} - a y_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{23}} = (y_6 - z_6)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3 = a x_6\,\hat{\mathbf{x}} + a y_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{24}} = -(x_6 + z_6)\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = a y_6\,\hat{\mathbf{x}} - a x_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{25}} = (x_6 - z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3 = -a y_6\,\hat{\mathbf{x}} + a x_6\,\hat{\mathbf{y}} - c z_6\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{26}} = (y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3 = a x_7\,\hat{\mathbf{x}} + a y_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{27}} = -(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -a x_7\,\hat{\mathbf{x}} - a y_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{28}} = (x_7 + z_7)\,\mathbf{a}_1 - (y_7 - z_7)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3 = -a y_7\,\hat{\mathbf{x}} + a x_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{29}} = -(x_7 - z_7)\,\mathbf{a}_1 + (y_7 + z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = a y_7\,\hat{\mathbf{x}} - a x_7\,\hat{\mathbf{y}} + c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{30}} = -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -a x_7\,\hat{\mathbf{x}} - a y_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{31}} = (y_7 - z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3 = a x_7\,\hat{\mathbf{x}} + a y_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{32}} = -(x_7 + z_7)\,\mathbf{a}_1 + (y_7 - z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = a y_7\,\hat{\mathbf{x}} - a x_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{33}} = (x_7 - z_7)\,\mathbf{a}_1 - (y_7 + z_7)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3 = -a y_7\,\hat{\mathbf{x}} + a x_7\,\hat{\mathbf{y}} - c z_7\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{34}} = (y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3 = a x_8\,\hat{\mathbf{x}} + a y_8\,\hat{\mathbf{y}} + c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{35}} = -(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3 = -a x_8\,\hat{\mathbf{x}} - a y_8\,\hat{\mathbf{y}} + c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{36}} = (x_8 + z_8)\,\mathbf{a}_1 - (y_8 - z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3 = -a y_8\,\hat{\mathbf{x}} + a x_8\,\hat{\mathbf{y}} + c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{37}} = -(x_8 - z_8)\,\mathbf{a}_1 + (y_8 + z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3 = a y_8\,\hat{\mathbf{x}} - a x_8\,\hat{\mathbf{y}} + c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{38}} = -(y_8 + z_8)\,\mathbf{a}_1 - (x_8 + z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3 = -a x_8\,\hat{\mathbf{x}} - a y_8\,\hat{\mathbf{y}} - c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{39}} = (y_8 - z_8)\,\mathbf{a}_1 + (x_8 - z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3 = a x_8\,\hat{\mathbf{x}} + a y_8\,\hat{\mathbf{y}} - c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{40}} = -(x_8 + z_8)\,\mathbf{a}_1 + (y_8 - z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3 = a y_8\,\hat{\mathbf{x}} - a x_8\,\hat{\mathbf{y}} - c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

$$\mathbf{B_{41}} = (x_8 - z_8)\,\mathbf{a}_1 - (y_8 + z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3 = -a y_8\,\hat{\mathbf{x}} + a x_8\,\hat{\mathbf{y}} - c z_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{Si II}$$

References

[1] J. J. Papike and T. Zoltai, *The crystal structure of a marialite scapolite*, Am. Mineral. **50**, 641–655 (1965).

[2] L. Pauling, *The Structure of Some Sodium nd Calcium Aluminosilicates*, Proc. Natl. Acad. Sci. **16**, 453–459 (1930), doi:10.1073/pnas.16.7.453.