Staurolite ($H_2Al_5Fe_2Si_2O_{12}$) Structure: A5B2C2D10E2_mC84_12_acghj_bdi_2i_5j_j-001

This structure originally had the label `A5B2C10D2E2_mC84_12_acghj_bdi_5j_2i_j`. Calls to that address will be redirected here.

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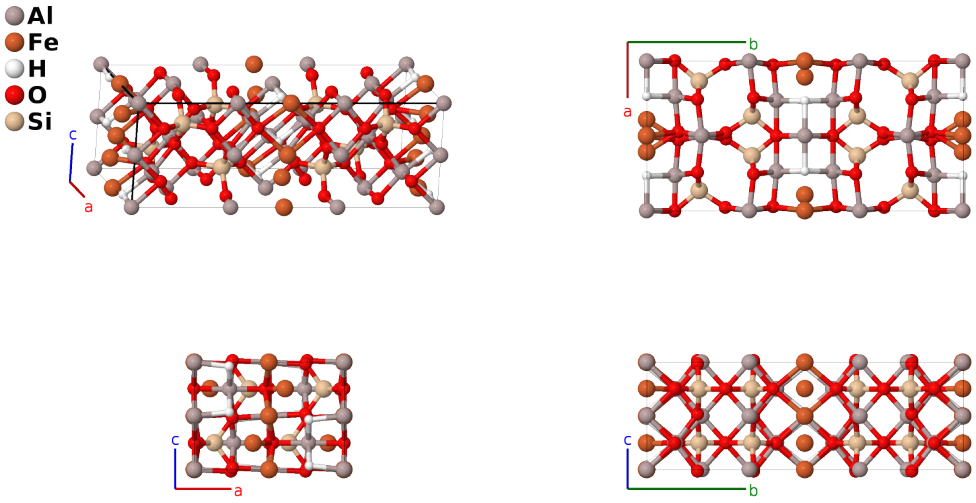
https://aflow.org/p/QHVX

https://aflow.org/p/A5B2C2D10E2_mC84_12_acghj_bdi_2i_5j_j-001



Prototype	$Al_5Fe_2H_2O_{12}Si_2$
AFLOW prototype label	A5B2C2D10E2_mC84_12_acghj_bdi_2i_5j_j-001
Mineral name	staurolite
ICSD	22051
Pearson symbol	mC84
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A5B2C2D10E2_mC84_12_acghj_bdi_2i_5j_j-001 --params=`$a, b/a, c/a, \beta, y_5, y_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}$

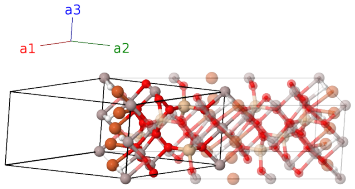
- The orthorhombic structure of staurolite determined by (Náray-Szabó, 1929) was given the *Strukturbericht* designation $S0_4$ by (Hermann, 1937). (Smith, 1968) showed that the structure is actually monoclinic with $\beta \approx 90°$. This paper also corrected the chemical composition of the mineral.
- The hydrogen positions are undetermined, but they part of a "complex distribution of OH ions," and are "probably" associated with the atoms on the (4i) sites (Smith, 1968). We therefore label the (4i) sites as OH.
- The metallic sites are actually somewhat disordered. (Smith, 1968) gives the composition of the various sites as:

- Al (2a) $Al_{0.67}$ $Fe_{0.33}$
- Fe (2b) $Fe_{0.68}$ $Mn_{0.32}$
- Al (2c) $Al_{0.67}$ $Fe_{0.33}$
- Fe (2d) $Fe_{0.68}$ $Mn_{0.32}$
- Al (4g) $Al_{0.95}$ $Mg_{0.05}$
- Al (4h) $Al_{0.95}$ $Mg_{0.05}$
- Fe (4i) $Fe_{0.64}$ $Al_{0.32}$ $Ti_{0.04}$
- Si (8j) $Si_{0.936}$ $Al_{0.064}$

More (see reference in Donnay, 1983) presents a history of the difficulties in determining the staurolite structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}\left(a + c\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2d)	Fe II
$\mathbf{B_5}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$by_5\,\hat{\mathbf{y}}$	(4g)	Al III
$\mathbf{B_6}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-by_5\,\hat{\mathbf{y}}$	(4g)	Al III
$\mathbf{B_7}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Al IV
$\mathbf{B_8}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Al IV
$\mathbf{B_9}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Fe III
$\mathbf{B_{10}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Fe III
$\mathbf{B_{11}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_{12}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	H I
$\mathbf{B_{13}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	H II
$\mathbf{B_{14}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-\left(ax_9 + cz_9\cos\beta\right)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	H II
$\mathbf{B_{15}}$	=	$\left(x_{10} - y_{10}\right)\,\mathbf{a}_1 + \left(x_{10} + y_{10}\right)\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al V
$\mathbf{B_{16}}$	=	$-\left(x_{10} + y_{10}\right)\,\mathbf{a}_1 - \left(x_{10} - y_{10}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al V
$\mathbf{B_{17}}$	=	$-\left(x_{10} - y_{10}\right)\,\mathbf{a}_1 - \left(x_{10} + y_{10}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al V
$\mathbf{B_{18}}$	=	$\left(x_{10} + y_{10}\right)\,\mathbf{a}_1 + \left(x_{10} - y_{10}\right)\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\left(ax_{10} + cz_{10}\cos\beta\right)\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(8j)	Al V
$\mathbf{B_{19}}$	=	$\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 + \left(x_{11} + y_{11}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\left(ax_{11} + cz_{11}\cos\beta\right)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(8j)	O I

$$\mathbf{B_{20}} = -(x_{11}+y_{11})\,\mathbf{a}_1 - (x_{11}-y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O I}$$

$$\mathbf{B_{21}} = -(x_{11}-y_{11})\,\mathbf{a}_1 - (x_{11}+y_{11})\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O I}$$

$$\mathbf{B_{22}} = (x_{11}+y_{11})\,\mathbf{a}_1 + (x_{11}-y_{11})\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = (ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O I}$$

$$\mathbf{B_{23}} = (x_{12}-y_{12})\,\mathbf{a}_1 + (x_{12}+y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = (ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O II}$$

$$\mathbf{B_{24}} = -(x_{12}+y_{12})\,\mathbf{a}_1 - (x_{12}-y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O II}$$

$$\mathbf{B_{25}} = -(x_{12}-y_{12})\,\mathbf{a}_1 - (x_{12}+y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O II}$$

$$\mathbf{B_{26}} = (x_{12}+y_{12})\,\mathbf{a}_1 + (x_{12}-y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = (ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O II}$$

$$\mathbf{B_{27}} = (x_{13}-y_{13})\,\mathbf{a}_1 + (x_{13}+y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = (ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O III}$$

$$\mathbf{B_{28}} = -(x_{13}+y_{13})\,\mathbf{a}_1 - (x_{13}-y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -(ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O III}$$

$$\mathbf{B_{29}} = -(x_{13}-y_{13})\,\mathbf{a}_1 - (x_{13}+y_{13})\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -(ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O III}$$

$$\mathbf{B_{30}} = (x_{13}+y_{13})\,\mathbf{a}_1 + (x_{13}-y_{13})\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = (ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O III}$$

$$\mathbf{B_{31}} = (x_{14}-y_{14})\,\mathbf{a}_1 + (x_{14}+y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = (ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O IV}$$

$$\mathbf{B_{32}} = -(x_{14}+y_{14})\,\mathbf{a}_1 - (x_{14}-y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -(ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O IV}$$

$$\mathbf{B_{33}} = -(x_{14}-y_{14})\,\mathbf{a}_1 - (x_{14}+y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -(ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O IV}$$

$$\mathbf{B_{34}} = (x_{14}+y_{14})\,\mathbf{a}_1 + (x_{14}-y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = (ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O IV}$$

$$\mathbf{B_{35}} = (x_{15}-y_{15})\,\mathbf{a}_1 + (x_{15}+y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O V}$$

$$\mathbf{B_{36}} = -(x_{15}+y_{15})\,\mathbf{a}_1 - (x_{15}-y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O V}$$

$$\mathbf{B_{37}} = -(x_{15}-y_{15})\,\mathbf{a}_1 - (x_{15}+y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O V}$$

$$\mathbf{B_{38}} = (x_{15}+y_{15})\,\mathbf{a}_1 + (x_{15}-y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{O V}$$

$$\mathbf{B_{39}} = (x_{16}-y_{16})\,\mathbf{a}_1 + (x_{16}+y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Si I}$$

$$\mathbf{B_{40}} = -(x_{16}+y_{16})\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Si I}$$

$$\mathbf{B_{41}} = -(x_{16}-y_{16})\,\mathbf{a}_1 - (x_{16}+y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Si I}$$

$$\mathbf{B_{42}} = (x_{16}+y_{16})\,\mathbf{a}_1 + (x_{16}-y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8j) \quad \text{Si I}$$

References

[1] J. V. Smith, *The crystal structure of staurolite*, Am. Mineral. **53**, 1139–1155 (1968).

[2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[3] S. Náray-Szabó, *The structure of staurolite*, Z. Krystallogr. **71**, 103–116 (1929), doi:10.1524/zkri.1929.71.1.103.

[4] J. D. H. Donnay and G. Donnay, *The staurolite story*, TMPM Tschermaks Min. Petr. Mitt. **31**, 1–15 (1983), doi:10.1007/BF01084757.