

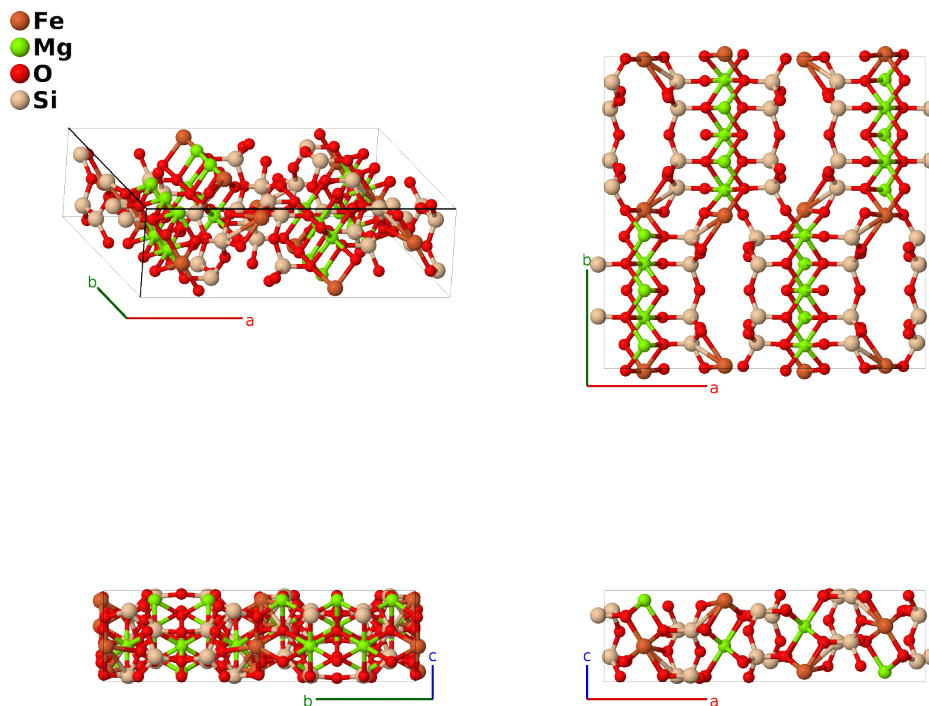
Anthophyllite ($\text{Mg}_5\text{Fe}_2\text{Si}_8\text{O}_{22}(\text{OH})_2$, $S4_4$) Structure: A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d-001

This structure originally had the label A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d. Calls to that address will be redirected here.

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<https://aflow.org/p/P9BG>

https://aflow.org/p/A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d-001



Prototype	$\text{Fe}_2\text{Mg}_5\text{O}_{22}(\text{OH})_2\text{Si}_8$
AFLOW prototype label	A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d-001
<i>Strukturbericht</i> designation	$S4_4$
Mineral name	anthophyllite
ICSD	40294
Pearson symbol	oP156
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=A2B5C22D2E8_oP156_62_d_c2d_2c10d_2c_4d-001 --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22</pre>

Other compounds with this structure

$\text{Mg}_7\text{Si}_8\text{O}_{22}(\text{OH})_2$

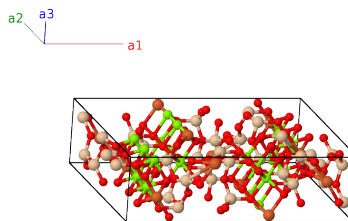
- (Warren, 1930) analyzed their sample of anthophyllite under the assumption that it was free of iron, and this structure was given the $S4_4$ designation by (Hermann, 1937).
- (Walitzi, 1989) found a more accurate determination of the structure, but their sample included substantial amounts of iron. The Mg-I (4c) site is actually $(\text{Mg}_{0.99}\text{Fe}_{0.01})$, Mg-II (8d) is $(\text{Mg}_{0.98}\text{Fe}_{0.02})$, and Fe (8d) is $(\text{Mg}_{0.38}\text{Fe}_{0.62})$. Trace amounts of calcium, manganese and sodium were found on the magnesium/iron sites, and trace amounts of aluminum were found on the silicon sites. Neither paper was able to determine the positions of the hydrogen atoms, which are included in the OH radicals.
- The ICSD entry for (Walitzi, 1989) does give positions for the hydrogens, but we can not find any evidence of this in the publication.
- Anthophyllite can be thought of as an approximation to a doubled unit cell of protoanthophyllite, where the hydrogen atoms have been located.

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_2	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_3	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_4	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mg I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_6	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_7	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_8	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_9	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{10}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{11}	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{12}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	OH I

$$\begin{aligned}
\mathbf{B}_{136} &= \begin{pmatrix} x_{20} + \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{20} - \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 = \begin{pmatrix} a(x_{20} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{20} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (8d) & \text{Si II} \\
\mathbf{B}_{137} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3 = -ax_{20} \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{138} &= \begin{pmatrix} x_{20} + \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{20} \mathbf{a}_2 - \mathbf{a}_3 = a(x_{20} + \frac{1}{2}) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{139} &= x_{20} \mathbf{a}_1 - \begin{pmatrix} y_{20} - \frac{1}{2} \\ z_{20} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_{20} \mathbf{a}_3 = ax_{20} \hat{\mathbf{x}} - b(y_{20} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{140} &= -\begin{pmatrix} x_{20} - \frac{1}{2} \\ z_{20} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{20} + \frac{1}{2} \\ z_{20} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = -a(x_{20} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{20} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si II} \\
\mathbf{B}_{141} &= x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3 = ax_{21} \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{142} &= -\begin{pmatrix} x_{21} - \frac{1}{2} \\ z_{21} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + \mathbf{a}_3 = -a(x_{21} - \frac{1}{2}) \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + c(z_{21} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{143} &= -x_{21} \mathbf{a}_1 + \begin{pmatrix} y_{21} + \frac{1}{2} \\ z_{21} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_{21} \mathbf{a}_3 = -ax_{21} \hat{\mathbf{x}} + b(y_{21} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{21} \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{144} &= \begin{pmatrix} x_{21} + \frac{1}{2} \\ z_{21} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{21} - \frac{1}{2} \\ z_{21} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 = a(x_{21} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{21} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{21} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{145} &= -x_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 - z_{21} \mathbf{a}_3 = -ax_{21} \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} - cz_{21} \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{146} &= \begin{pmatrix} x_{21} + \frac{1}{2} \\ z_{21} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{21} \mathbf{a}_2 - \mathbf{a}_3 = a(x_{21} + \frac{1}{2}) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} - c(z_{21} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{147} &= x_{21} \mathbf{a}_1 - \begin{pmatrix} y_{21} - \frac{1}{2} \\ z_{21} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_{21} \mathbf{a}_3 = ax_{21} \hat{\mathbf{x}} - b(y_{21} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{148} &= -\begin{pmatrix} x_{21} - \frac{1}{2} \\ z_{21} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{21} + \frac{1}{2} \\ z_{21} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = -a(x_{21} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{21} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{21} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si III} \\
\mathbf{B}_{149} &= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 = ax_{22} \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{150} &= -\begin{pmatrix} x_{22} - \frac{1}{2} \\ z_{22} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + \mathbf{a}_3 = -a(x_{22} - \frac{1}{2}) \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} + c(z_{22} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{151} &= -x_{22} \mathbf{a}_1 + \begin{pmatrix} y_{22} + \frac{1}{2} \\ z_{22} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - z_{22} \mathbf{a}_3 = -ax_{22} \hat{\mathbf{x}} + b(y_{22} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{22} \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{152} &= \begin{pmatrix} x_{22} + \frac{1}{2} \\ z_{22} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{22} - \frac{1}{2} \\ z_{22} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 = a(x_{22} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{22} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{22} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{153} &= -x_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 - z_{22} \mathbf{a}_3 = -ax_{22} \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} - cz_{22} \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{154} &= \begin{pmatrix} x_{22} + \frac{1}{2} \\ z_{22} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + y_{22} \mathbf{a}_2 - \mathbf{a}_3 = a(x_{22} + \frac{1}{2}) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} - c(z_{22} - \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{155} &= x_{22} \mathbf{a}_1 - \begin{pmatrix} y_{22} - \frac{1}{2} \\ z_{22} - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + z_{22} \mathbf{a}_3 = ax_{22} \hat{\mathbf{x}} - b(y_{22} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}} & (8d) & \text{Si IV} \\
\mathbf{B}_{156} &= -\begin{pmatrix} x_{22} - \frac{1}{2} \\ z_{22} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{22} + \frac{1}{2} \\ z_{22} + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 = -a(x_{22} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{22} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{22} + \frac{1}{2}) \hat{\mathbf{z}} & (8d) & \text{Si IV}
\end{aligned}$$

References

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