

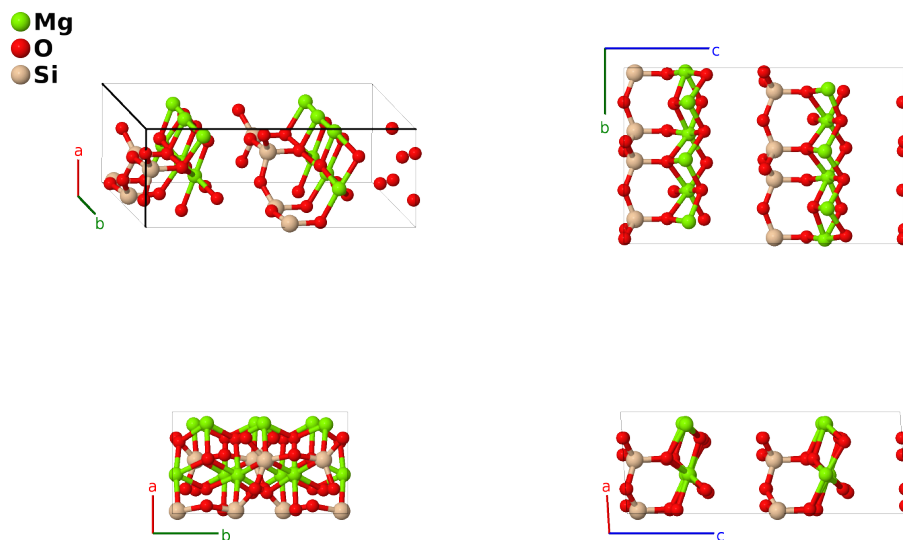
Chrysotile $[\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4]$ Structure: A3B5C4D2_mC56_9_3a_5a_4a_2a-001

This structure originally had the label A3B5C4D2_mC56_9_3a_5a_4a_2a. Calls to that address will be redirected here.

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<https://aflow.org/p/BT10>

https://aflow.org/p/A3B5C4D2_mC56_9_3a_5a_4a_2a-001

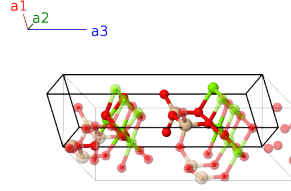


Prototype	$\text{Mg}_3\text{O}_5(\text{OH})_4\text{Si}_2$
AFLOW prototype label	A3B5C4D2_mC56_9_3a_5a_4a_2a-001
Mineral name	chrysotile
ICSD	413633
Pearson symbol	mC56
Space group number	9
Space group symbol	Cc
AFLOW prototype command	<pre>aflow --proto=A3B5C4D2_mC56_9_3a_5a_4a_2a-001 --params=a,b/a,c/a,beta,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14</pre>

- Chrysotile is more commonly known as “white asbestos.” Chrysotile sheets typically curl into tubular fibers and the crystal structure is difficult to determine. (Yada, 1967) has a partial list of the experiments performed to determine this structure.
- This structure differs from (Warren, 1931), $S4_5$, halving the size of the unit cell and removing the inversion site.
- For this prototype the OH molecules are centered on (4a) Wyckoff positions.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4a)	Mg I
\mathbf{B}_2	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Mg I
\mathbf{B}_3	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4a)	Mg II
\mathbf{B}_4	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Mg II
\mathbf{B}_5	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4a)	Mg III
\mathbf{B}_6	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Mg III
\mathbf{B}_7	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_8	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_9	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{10}	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{11}	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{12}	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	O III
\mathbf{B}_{13}	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{14}	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	O IV
\mathbf{B}_{15}	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4a)	O V
\mathbf{B}_{16}	$(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	O V
\mathbf{B}_{17}	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4a)	OH I

$$\begin{aligned}
\mathbf{B}_{18} &= (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= (ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{OH I} \\
\mathbf{B}_{19} &= (x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} &(4a) &\text{OH II} \\
\mathbf{B}_{20} &= (x_{10} + y_{10}) \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{OH II} \\
\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}} &(4a) &\text{OH III} \\
\mathbf{B}_{22} &= (x_{11} + y_{11}) \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{11} + c(z_{11} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{OH III} \\
\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}} &(4a) &\text{OH IV} \\
\mathbf{B}_{24} &= (x_{12} + y_{12}) \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{12} + c(z_{12} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{OH IV} \\
\mathbf{B}_{25} &= (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}} &(4a) &\text{Si I} \\
\mathbf{B}_{26} &= (x_{13} + y_{13}) \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{13} + c(z_{13} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{Si I} \\
\mathbf{B}_{27} &= (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}} &(4a) &\text{Si II} \\
\mathbf{B}_{28} &= (x_{14} + y_{14}) \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{14} + c(z_{14} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4a) &\text{Si II}
\end{aligned}$$

References

- [1] G. Falini, E. Foresti, M. Gazzano, A. F. Gualtieri, M. Leoni, I. G. Lesci, and N. Roveri, *Tubular-Shaped Stoichiometric Chrysotile Nanocrystals*, Chem. Eur. J. **10**, 3043–3049 (2004), doi:10.1002/chem.200305685.
- [2] K. Yada, *Study of Chrysotile Asbestos by a High Resolution Electron Microscope*, Acta Cryst. **23**, 704–707 (1967), doi:10.1107/S0365110X67003524.
- [3] B. E. Warren and W. L. Bragg, *The Structure of Chrysotile $H_4Mg_3Si_2O_9$* , Z. Krystallogr. **76**, 201–210 (1931), doi:10.1524/zkri.1931.76.1.201.