

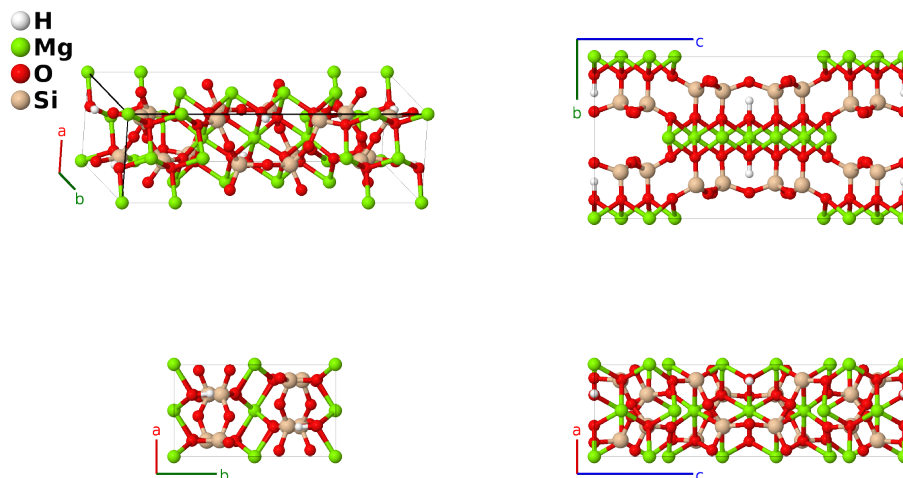
Protoanthophyllite ($\text{H}_2\text{Mg}_7\text{Si}_8\text{O}_{24}$) Structure: A2B7C24D8_oP82_58_g_ae2f_2g5h_2h-001

This structure originally had the label A2B7C24D8_oP82_58_g_ae2f_2g5h_2h. Calls to that address will be redirected here.

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

https://aflow.org/p/A2B7C24D8_oP82_58_g_ae2f_2g5h_2h-001

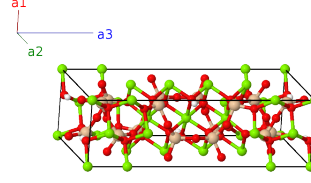


| | |
|--------------------------------|--|
| Prototype | $\text{H}_2\text{Mg}_7\text{O}_{24}\text{Si}_8$ |
| AFLOW prototype label | A2B7C24D8_oP82_58_g_ae2f_2g5h_2h-001 |
| Mineral name | protoanthophyllite |
| ICSD | 98791 |
| Pearson symbol | oP82 |
| Space group number | 58 |
| Space group symbol | $Pn\bar{m}$ |
| AFLOW prototype command | <pre>aflow --proto=A2B7C24D8_oP82_58_g_ae2f_2g5h_2h-001 --params=a,b/a,c/a,z2,z3,z4,x5,y5,x6,y6,x7,y7,x8,y8,z8,x9,y9,z9,x10,y10,z10,x11, y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14</pre> |

- This structure is approximately one-half of the unit cell of anthophyllite ($S4_4$).
- Like anthophyllite, iron is sometimes mixed with magnesium. For this sample, (Konishi, 2003) found that the Mg-I (2a) site contains 2.5% iron, Mg-III (4f) contains 2.1%, and Mg-IV (4f) contains 27.7% iron.
- Similarly, the silicon sites are have very small amounts of aluminum ($< 1\%$), and the (2b) site ($1/2\ 1/2\ 1/2$) is occupied by a sodium atom about 5% of the time. We ignore this later site.
- (Konishi, 2003) give the crystal structure in the $Pn\bar{m}n$ setting of space group #58. We used findsym to transform this to the standard $Pn\bar{m}$ orientation.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|---|-----|---|------------------|-----------|
| \mathbf{B}_1 | 0 | $=$ | 0 | (2a) | Mg I |
| \mathbf{B}_2 | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (2a) | Mg I |
| \mathbf{B}_3 | $z_2 \mathbf{a}_3$ | $=$ | $cz_2 \hat{\mathbf{z}}$ | (4e) | Mg II |
| \mathbf{B}_4 | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4e) | Mg II |
| \mathbf{B}_5 | $-z_2 \mathbf{a}_3$ | $=$ | $-cz_2 \hat{\mathbf{z}}$ | (4e) | Mg II |
| \mathbf{B}_6 | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4e) | Mg II |
| \mathbf{B}_7 | $\frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (4f) | Mg III |
| \mathbf{B}_8 | $\frac{1}{2} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4f) | Mg III |
| \mathbf{B}_9 | $\frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $\frac{1}{2} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (4f) | Mg III |
| \mathbf{B}_{10} | $\frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4f) | Mg III |
| \mathbf{B}_{11} | $\frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $\frac{1}{2} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (4f) | Mg IV |
| \mathbf{B}_{12} | $\frac{1}{2} \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (4f) | Mg IV |
| \mathbf{B}_{13} | $\frac{1}{2} \mathbf{a}_2 - z_4 \mathbf{a}_3$ | $=$ | $\frac{1}{2} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$ | (4f) | Mg IV |
| \mathbf{B}_{14} | $\frac{1}{2} \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $\frac{1}{2} a \hat{\mathbf{x}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (4f) | Mg IV |
| \mathbf{B}_{15} | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$ | $=$ | $ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$ | (4g) | H I |
| \mathbf{B}_{16} | $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$ | $=$ | $-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$ | (4g) | H I |
| \mathbf{B}_{17} | $-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | H I |
| \mathbf{B}_{18} | $(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | H I |
| \mathbf{B}_{19} | $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$ | $=$ | $ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$ | (4g) | O I |
| \mathbf{B}_{20} | $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$ | $=$ | $-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$ | (4g) | O I |
| \mathbf{B}_{21} | $-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | O I |
| \mathbf{B}_{22} | $(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | O I |
| \mathbf{B}_{23} | $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$ | $=$ | $ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$ | (4g) | O II |
| \mathbf{B}_{24} | $-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2$ | $=$ | $-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$ | (4g) | O II |
| \mathbf{B}_{25} | $-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | O II |
| \mathbf{B}_{26} | $(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$ | $=$ | $a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$ | (4g) | O II |
| \mathbf{B}_{27} | $x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$ | $=$ | $ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$ | (8h) | O III |
| \mathbf{B}_{28} | $-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$ | $=$ | $-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$ | (8h) | O III |

$$\begin{aligned}
\mathbf{B}_{58} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O VI} \\
\mathbf{B}_{59} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= & ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{60} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= & -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{61} &= -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{62} &= \left(x_{12} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{12} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{63} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= & -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{64} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= & ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{65} &= \left(x_{12} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{12} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{66} &= -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{O VII} \\
\mathbf{B}_{67} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= & ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{68} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= & -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{69} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{70} &= \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{71} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= & -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{72} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= & ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{73} &= \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{74} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si I} \\
\mathbf{B}_{75} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= & ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{76} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= & -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{77} &= -\left(x_{14} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{14} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{78} &= \left(x_{14} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{14} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{79} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= & -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{80} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= & ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{81} &= \left(x_{14} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{14} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{14} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si II} \\
\mathbf{B}_{82} &= -\left(x_{14} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{14} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{14} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8h) & \text{Si II}
\end{aligned}$$

References

- [1] H. Konishi, T. L. Groy, I. Dódony, R. Miyawaki, S. Matsubara, and P. R. Buseck, *Crystal structure of protoanthophyllite: A new mineral from the Takase ultramafic complex, Japan*, Am. Mineral. **88**, 1718–1723 (2003), doi:10.2138/am-2003-11-1212.