

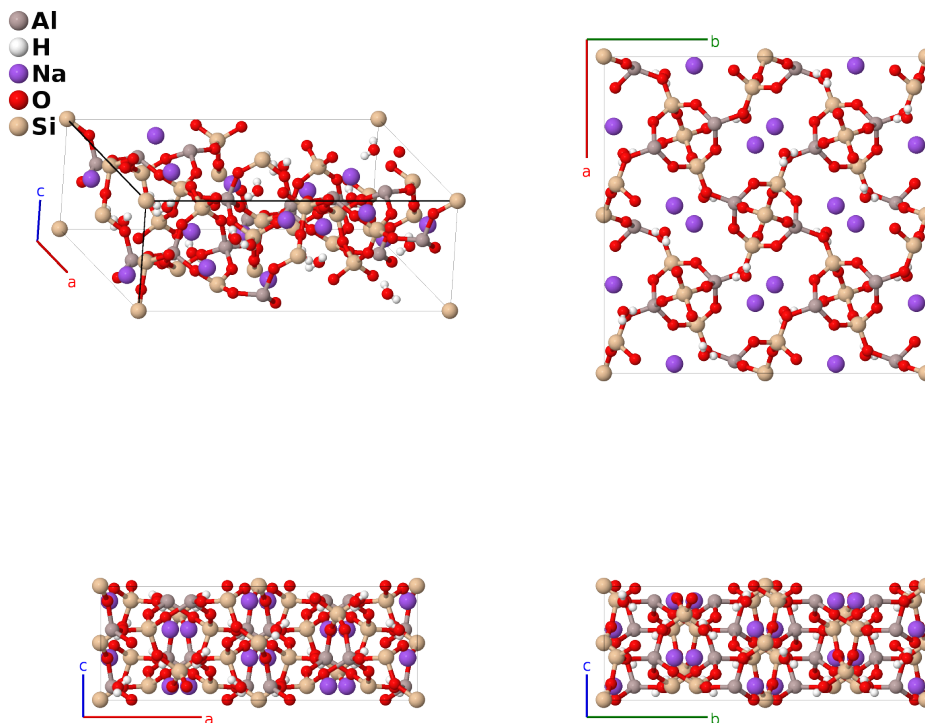
Natrolite ($\text{Na}_2\text{Al}_2\text{Si}_3\text{O}_{10}\cdot 2\text{H}_2\text{O}$, $S6_{10}$) Structure: A2B4C2D12E3_oF184_43_b_2b_b_6b_ab-001

This structure originally had the label A2B4C2D12E3_oF184_43_b_2b_b_6b_ab. Calls to that address will be redirected here.

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<https://aflow.org/p/FT02>

https://aflow.org/p/A2B4C2D12E3_oF184_43_b_2b_b_6b_ab-001

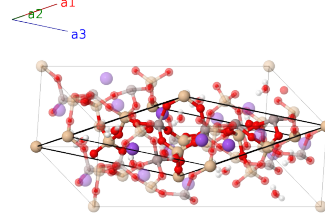


Prototype	$\text{Al}_2\text{H}_4\text{O}_{12}\text{Si}_3$
AFLOW prototype label	A2B4C2D12E3_oF184_43_b_2b_b_6b_ab-001
<i>Strukturbericht</i> designation	$S6_{10}$
Mineral name	natrolite
ICSD	201651
Pearson symbol	oF184
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	aflow --proto=A2B4C2D12E3_oF184_43_b_2b_b_6b_ab-001 --params= $a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- We use the data from the sample that (Kirfel, 1984) call Crystal II. The origin has been arbitrarily set so that $z_1 = 0$.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(8a)	Si I
\mathbf{B}_2	$= (z_1 + \frac{1}{4}) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 - (z_1 - \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + c(z_1 + \frac{1}{4})\hat{\mathbf{z}}$	(8a)	Si I
\mathbf{B}_3	$= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16b)	Al I
\mathbf{B}_4	$= (x_2 - y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16b)	Al I
\mathbf{B}_5	$= -(x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_1 + (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 + (x_2 - y_2 - z_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4})\hat{\mathbf{x}} - b(y_2 - \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$	(16b)	Al I
\mathbf{B}_6	$= (x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_1 - (x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - y_2 + z_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + b(y_2 + \frac{1}{4})\hat{\mathbf{y}} + c(z_2 + \frac{1}{4})\hat{\mathbf{z}}$	(16b)	Al I
\mathbf{B}_7	$= (-x_3 + y_3 + z_3) \mathbf{a}_1 + (x_3 - y_3 + z_3) \mathbf{a}_2 + (x_3 + y_3 - z_3) \mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(16b)	H I
\mathbf{B}_8	$= (x_3 - y_3 + z_3) \mathbf{a}_1 + (-x_3 + y_3 + z_3) \mathbf{a}_2 - (x_3 + y_3 + z_3) \mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} - by_3\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(16b)	H I
\mathbf{B}_9	$= -(x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_1 + (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + (x_3 - y_3 - z_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{4})\hat{\mathbf{x}} - b(y_3 - \frac{1}{4})\hat{\mathbf{y}} + c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$	(16b)	H I
\mathbf{B}_{10}	$= (x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_1 - (x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_2 - (x_3 - y_3 + z_3 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{4})\hat{\mathbf{x}} + b(y_3 + \frac{1}{4})\hat{\mathbf{y}} + c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$	(16b)	H I
\mathbf{B}_{11}	$= (-x_4 + y_4 + z_4) \mathbf{a}_1 + (x_4 - y_4 + z_4) \mathbf{a}_2 + (x_4 + y_4 - z_4) \mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(16b)	H II

$$\begin{aligned}
\mathbf{B}_{12} &= \begin{pmatrix} (x_4 - y_4 + z_4) \mathbf{a}_1 + \\ (-x_4 + y_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4 + z_4) \mathbf{a}_3 \end{pmatrix} &= -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16b) & \text{H II} \\
\mathbf{B}_{13} &= \begin{pmatrix} -(x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_4 - y_4 - z_4 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{H II} \\
\mathbf{B}_{14} &= \begin{pmatrix} (x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_4 - y_4 + z_4 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{H II} \\
\mathbf{B}_{15} &= \begin{pmatrix} (-x_5 + y_5 + z_5) \mathbf{a}_1 + \\ (x_5 - y_5 + z_5) \mathbf{a}_2 + \\ (x_5 + y_5 - z_5) \mathbf{a}_3 \end{pmatrix} &= ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{Na I} \\
\mathbf{B}_{16} &= \begin{pmatrix} (x_5 - y_5 + z_5) \mathbf{a}_1 + \\ (-x_5 + y_5 + z_5) \mathbf{a}_2 - \\ (x_5 + y_5 + z_5) \mathbf{a}_3 \end{pmatrix} &= -ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16b) & \text{Na I} \\
\mathbf{B}_{17} &= \begin{pmatrix} -(x_5 + y_5 - z_5 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_5 + y_5 + z_5 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_5 - y_5 - z_5 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= a(x_5 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{Na I} \\
\mathbf{B}_{18} &= \begin{pmatrix} (x_5 + y_5 + z_5 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_5 + y_5 - z_5 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_5 - y_5 + z_5 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= -a(x_5 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{Na I} \\
\mathbf{B}_{19} &= \begin{pmatrix} (-x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (x_6 - y_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6 - z_6) \mathbf{a}_3 \end{pmatrix} &= ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16b) & \text{O I} \\
\mathbf{B}_{20} &= \begin{pmatrix} (x_6 - y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_2 - \\ (x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} &= -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16b) & \text{O I} \\
\mathbf{B}_{21} &= \begin{pmatrix} -(x_6 + y_6 - z_6 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_6 + y_6 + z_6 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_6 - y_6 - z_6 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= a(x_6 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O I} \\
\mathbf{B}_{22} &= \begin{pmatrix} (x_6 + y_6 + z_6 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_6 + y_6 - z_6 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_6 - y_6 + z_6 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= -a(x_6 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O I} \\
\mathbf{B}_{23} &= \begin{pmatrix} (-x_7 + y_7 + z_7) \mathbf{a}_1 + \\ (x_7 - y_7 + z_7) \mathbf{a}_2 + \\ (x_7 + y_7 - z_7) \mathbf{a}_3 \end{pmatrix} &= ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16b) & \text{O II} \\
\mathbf{B}_{24} &= \begin{pmatrix} (x_7 - y_7 + z_7) \mathbf{a}_1 + \\ (-x_7 + y_7 + z_7) \mathbf{a}_2 - \\ (x_7 + y_7 + z_7) \mathbf{a}_3 \end{pmatrix} &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16b) & \text{O II} \\
\mathbf{B}_{25} &= \begin{pmatrix} -(x_7 + y_7 - z_7 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_7 + y_7 + z_7 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_7 - y_7 - z_7 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= a(x_7 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O II} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_7 + y_7 + z_7 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_7 + y_7 - z_7 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_7 - y_7 + z_7 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} &= -a(x_7 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O II} \\
\mathbf{B}_{27} &= \begin{pmatrix} (-x_8 + y_8 + z_8) \mathbf{a}_1 + \\ (x_8 - y_8 + z_8) \mathbf{a}_2 + \\ (x_8 + y_8 - z_8) \mathbf{a}_3 \end{pmatrix} &= ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16b) & \text{O III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{28} &= \begin{pmatrix} (x_8 - y_8 + z_8) \mathbf{a}_1 + \\ (-x_8 + y_8 + z_8) \mathbf{a}_2 - \\ (x_8 + y_8 + z_8) \mathbf{a}_3 \end{pmatrix} = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16b) & \text{O III} \\
\mathbf{B}_{29} &= \begin{pmatrix} -(x_8 + y_8 - z_8 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_8 + y_8 + z_8 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_8 - y_8 - z_8 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = a(x_8 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O III} \\
\mathbf{B}_{30} &= \begin{pmatrix} (x_8 + y_8 + z_8 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_8 + y_8 - z_8 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_8 - y_8 + z_8 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a(x_8 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O III} \\
\mathbf{B}_{31} &= \begin{pmatrix} (-x_9 + y_9 + z_9) \mathbf{a}_1 + \\ (x_9 - y_9 + z_9) \mathbf{a}_2 + \\ (x_9 + y_9 - z_9) \mathbf{a}_3 \end{pmatrix} = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{32} &= \begin{pmatrix} (x_9 - y_9 + z_9) \mathbf{a}_1 + \\ (-x_9 + y_9 + z_9) \mathbf{a}_2 - \\ (x_9 + y_9 + z_9) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{33} &= \begin{pmatrix} -(x_9 + y_9 - z_9 - \frac{1}{4}) \mathbf{a}_1 + \\ (x_9 + y_9 + z_9 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_9 - y_9 - z_9 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = a(x_9 + \frac{1}{4}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{34} &= \begin{pmatrix} (x_9 + y_9 + z_9 + \frac{1}{4}) \mathbf{a}_1 - \\ (x_9 + y_9 - z_9 - \frac{1}{4}) \mathbf{a}_2 - \\ (x_9 - y_9 + z_9 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a(x_9 - \frac{1}{4}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O IV} \\
\mathbf{B}_{35} &= \begin{pmatrix} (-x_{10} + y_{10} + z_{10}) \mathbf{a}_1 + \\ (x_{10} - y_{10} + z_{10}) \mathbf{a}_2 + \\ (x_{10} + y_{10} - z_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16b) & \text{O V} \\
\mathbf{B}_{36} &= \begin{pmatrix} (x_{10} - y_{10} + z_{10}) \mathbf{a}_1 + \\ (-x_{10} + y_{10} + z_{10}) \mathbf{a}_2 - \\ (x_{10} + y_{10} + z_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16b) & \text{O V} \\
\mathbf{B}_{37} &= \begin{pmatrix} -(x_{10} + y_{10} - z_{10} - \frac{1}{4}) \mathbf{a}_1 + \\ (x_{10} + y_{10} + z_{10} + \frac{1}{4}) \mathbf{a}_2 + \\ (x_{10} - y_{10} - z_{10} + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = a(x_{10} + \frac{1}{4}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{4}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O V} \\
\mathbf{B}_{38} &= \begin{pmatrix} (x_{10} + y_{10} + z_{10} + \frac{1}{4}) \mathbf{a}_1 - \\ (x_{10} + y_{10} - z_{10} - \frac{1}{4}) \mathbf{a}_2 - \\ (x_{10} - y_{10} + z_{10} - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a(x_{10} - \frac{1}{4}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{4}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O V} \\
\mathbf{B}_{39} &= \begin{pmatrix} (-x_{11} + y_{11} + z_{11}) \mathbf{a}_1 + \\ (x_{11} - y_{11} + z_{11}) \mathbf{a}_2 + \\ (x_{11} + y_{11} - z_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16b) & \text{O VI} \\
\mathbf{B}_{40} &= \begin{pmatrix} (x_{11} - y_{11} + z_{11}) \mathbf{a}_1 + \\ (-x_{11} + y_{11} + z_{11}) \mathbf{a}_2 - \\ (x_{11} + y_{11} + z_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16b) & \text{O VI} \\
\mathbf{B}_{41} &= \begin{pmatrix} -(x_{11} + y_{11} - z_{11} - \frac{1}{4}) \mathbf{a}_1 + \\ (x_{11} + y_{11} + z_{11} + \frac{1}{4}) \mathbf{a}_2 + \\ (x_{11} - y_{11} - z_{11} + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = a(x_{11} + \frac{1}{4}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{4}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O VI} \\
\mathbf{B}_{42} &= \begin{pmatrix} (x_{11} + y_{11} + z_{11} + \frac{1}{4}) \mathbf{a}_1 - \\ (x_{11} + y_{11} - z_{11} - \frac{1}{4}) \mathbf{a}_2 - \\ (x_{11} - y_{11} + z_{11} - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -a(x_{11} - \frac{1}{4}) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{4}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{4}) \hat{\mathbf{z}} & (16b) & \text{O VI} \\
\mathbf{B}_{43} &= \begin{pmatrix} (-x_{12} + y_{12} + z_{12}) \mathbf{a}_1 + \\ (x_{12} - y_{12} + z_{12}) \mathbf{a}_2 + \\ (x_{12} + y_{12} - z_{12}) \mathbf{a}_3 \end{pmatrix} = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (16b) & \text{Si II}
\end{aligned}$$

$$\mathbf{B}_{44} = \begin{pmatrix} (x_{12} - y_{12} + z_{12}) \mathbf{a}_1 + \\ (-x_{12} + y_{12} + z_{12}) \mathbf{a}_2 - \\ (x_{12} + y_{12} + z_{12}) \mathbf{a}_3 \end{pmatrix} = -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (16b) \quad \text{Si II}$$

$$\mathbf{B}_{45} = \begin{pmatrix} -(x_{12} + y_{12} - z_{12} - \frac{1}{4}) \mathbf{a}_1 + \\ (x_{12} + y_{12} + z_{12} + \frac{1}{4}) \mathbf{a}_2 + \\ (x_{12} - y_{12} - z_{12} + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(x_{12} + \frac{1}{4}) \hat{\mathbf{x}} - b(y_{12} - \frac{1}{4}) \hat{\mathbf{y}} + \\ c(z_{12} + \frac{1}{4}) \hat{\mathbf{z}} \end{pmatrix} \quad (16b) \quad \text{Si II}$$

$$\mathbf{B}_{46} = \begin{pmatrix} (x_{12} + y_{12} + z_{12} + \frac{1}{4}) \mathbf{a}_1 - \\ (x_{12} + y_{12} - z_{12} - \frac{1}{4}) \mathbf{a}_2 - \\ (x_{12} - y_{12} + z_{12} - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a(x_{12} - \frac{1}{4}) \hat{\mathbf{x}} + b(y_{12} + \frac{1}{4}) \hat{\mathbf{y}} + \\ c(z_{12} + \frac{1}{4}) \hat{\mathbf{z}} \end{pmatrix} \quad (16b) \quad \text{Si II}$$

References

- [1] A. Kirfel, M. Orthen, and G. Will, *Natrolite: refinement of the crystal structure of two samples from Marienberg (Usti nad Labem, CSSR)*, *Zeolites* **4**, 140–146 (1984), doi:10.1016/0144-2449(84)90052-6.