

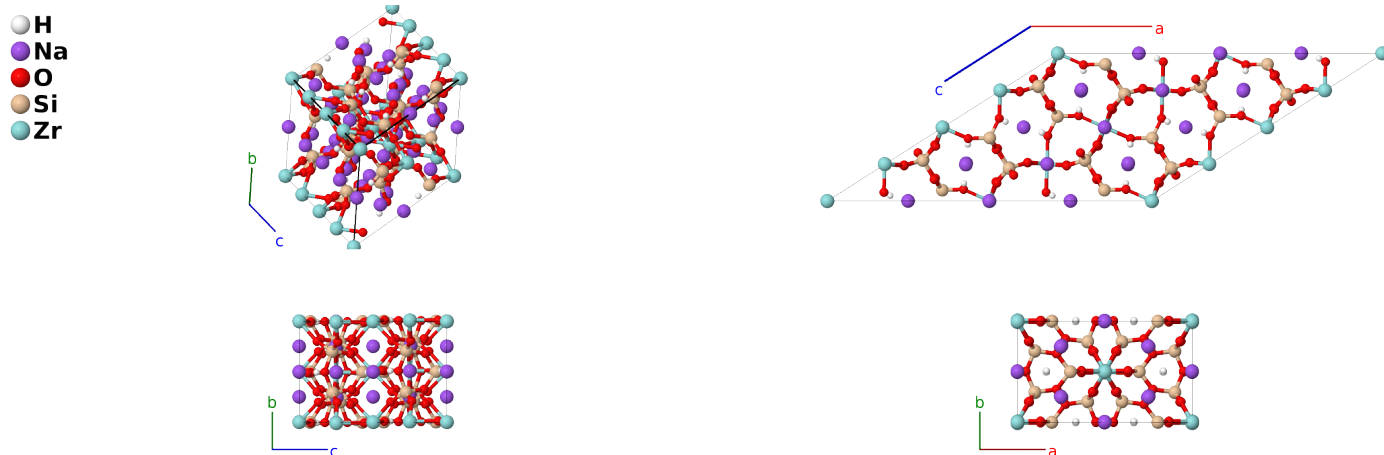
Catapleiite ($\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$) Structure: A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001

This structure originally had the label A2B3C9D3E_mC144_15_2f_bcdef_9f_3f_ae. Calls to that address will be redirected here.

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<https://afLOW.org/p/L4VZ>

https://afLOW.org/p/A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001

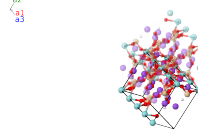


Prototype	$(\text{H}_2\text{O})_2\text{Na}_2\text{O}_9\text{Si}_3\text{Zr}$
AFLOW prototype label	A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001
Mineral name	catapleiite
ICSD	20267
Pearson symbol	mC144
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	<pre>afLOW --proto=A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001 --params=a, b/a, c/a, β, $y_5, y_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}$</pre>

- This is a refinement of the crystal structure of catapleiite. The original hexagonal structure was given the *Strukturbericht* designation $S3_4$ by (Gottfried, 1937).
- Only 66.7% of the sodium atom sites are occupied.
- (Ilyushin, 1981) gave the lattice parameters and Wyckoff positions in terms of the $B2/b$ setting of space group #15. We used findsym to transform this to the standard $C2/c$ setting. This required the y - and z -axes to be swapped.
- The hydrogen positions are unknown, so the water molecules are designated H_2O .

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	0	$=$	0	(4a)	Na I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4a)	Na I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(4b)	Na II
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}(a + c \cos \beta) \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4b)	Na II
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4c)	Na III
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{a}{4} + \frac{c \cos \beta}{2}\right) \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4c)	Na III
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\left(\frac{a}{4} + \frac{c \cos \beta}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4d)	Zr I
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}}$	(4d)	Zr I
\mathbf{B}_9	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Na IV
\mathbf{B}_{10}	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Na IV
\mathbf{B}_{11}	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Zr II
\mathbf{B}_{12}	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	Zr II
\mathbf{B}_{13}	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{14}	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{15}	$-(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{16}	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H I
\mathbf{B}_{17}	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(8f)	H II
\mathbf{B}_{18}	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_8 + c(z_8 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H II
\mathbf{B}_{19}	$-(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(8f)	H II
\mathbf{B}_{20}	$(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	H II
\mathbf{B}_{21}	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(8f)	Na V
\mathbf{B}_{22}	$-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_9 + c(z_9 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Na V
\mathbf{B}_{23}	$-(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(8f)	Na V
\mathbf{B}_{24}	$(x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Na V

$$\begin{aligned}
\mathbf{B}_{48} &= (x_{15} + y_{15}) \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{15} + c(z_{15} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VI} \\
\mathbf{B}_{49} &= (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}} &(8f) & \text{O VII} \\
\mathbf{B}_{50} &= -(x_{16} + y_{16}) \mathbf{a}_1 - (x_{16} - y_{16}) \mathbf{a}_2 - (z_{16} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{16} + c(z_{16} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VII} \\
\mathbf{B}_{51} &= -(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}} &(8f) & \text{O VII} \\
\mathbf{B}_{52} &= (x_{16} + y_{16}) \mathbf{a}_1 + (x_{16} - y_{16}) \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{16} + c(z_{16} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VII} \\
\mathbf{B}_{53} &= (x_{17} - y_{17}) \mathbf{a}_1 + (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= (ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VIII} \\
\mathbf{B}_{54} &= -(x_{17} + y_{17}) \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{17} + c(z_{17} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VIII} \\
\mathbf{B}_{55} &= -(x_{17} - y_{17}) \mathbf{a}_1 - (x_{17} + y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3 &= -(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VIII} \\
\mathbf{B}_{56} &= (x_{17} + y_{17}) \mathbf{a}_1 + (x_{17} - y_{17}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{17} + c(z_{17} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O VIII} \\
\mathbf{B}_{57} &= (x_{18} - y_{18}) \mathbf{a}_1 + (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= (ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}} &(8f) & \text{O IX} \\
\mathbf{B}_{58} &= -(x_{18} + y_{18}) \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 - (z_{18} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{18} + c(z_{18} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O IX} \\
\mathbf{B}_{59} &= -(x_{18} - y_{18}) \mathbf{a}_1 - (x_{18} + y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= -(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}} &(8f) & \text{O IX} \\
\mathbf{B}_{60} &= (x_{18} + y_{18}) \mathbf{a}_1 + (x_{18} - y_{18}) \mathbf{a}_2 + (z_{18} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{18} + c(z_{18} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{O IX} \\
\mathbf{B}_{61} &= (x_{19} - y_{19}) \mathbf{a}_1 + (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= (ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si I} \\
\mathbf{B}_{62} &= -(x_{19} + y_{19}) \mathbf{a}_1 - (x_{19} - y_{19}) \mathbf{a}_2 - (z_{19} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{19} + c(z_{19} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c(z_{19} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si I} \\
\mathbf{B}_{63} &= -(x_{19} - y_{19}) \mathbf{a}_1 - (x_{19} + y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= -(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si I} \\
\mathbf{B}_{64} &= (x_{19} + y_{19}) \mathbf{a}_1 + (x_{19} - y_{19}) \mathbf{a}_2 + (z_{19} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{19} + c(z_{19} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si I} \\
\mathbf{B}_{65} &= (x_{20} - y_{20}) \mathbf{a}_1 + (x_{20} + y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= (ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si II} \\
\mathbf{B}_{66} &= -(x_{20} + y_{20}) \mathbf{a}_1 - (x_{20} - y_{20}) \mathbf{a}_2 - (z_{20} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{20} + c(z_{20} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si II} \\
\mathbf{B}_{67} &= -(x_{20} - y_{20}) \mathbf{a}_1 - (x_{20} + y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= -(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si II} \\
\mathbf{B}_{68} &= (x_{20} + y_{20}) \mathbf{a}_1 + (x_{20} - y_{20}) \mathbf{a}_2 + (z_{20} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{20} + c(z_{20} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si II} \\
\mathbf{B}_{69} &= (x_{21} - y_{21}) \mathbf{a}_1 + (x_{21} + y_{21}) \mathbf{a}_2 + z_{21} \mathbf{a}_3 &= (ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si III} \\
\mathbf{B}_{70} &= -(x_{21} + y_{21}) \mathbf{a}_1 - (x_{21} - y_{21}) \mathbf{a}_2 - (z_{21} - \frac{1}{2}) \mathbf{a}_3 &= -(ax_{21} + c(z_{21} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} - c(z_{21} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(8f) & \text{Si III}
\end{aligned}$$

$$\mathbf{B}_{71} = \begin{matrix} -(x_{21} - y_{21}) \mathbf{a}_1 - \\ (x_{21} + y_{21}) \mathbf{a}_2 - z_{21} \mathbf{a}_3 \end{matrix} = \begin{matrix} -(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} - \\ cz_{21} \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Si III}$$

$$\mathbf{B}_{72} = \begin{matrix} (x_{21} + y_{21}) \mathbf{a}_1 + \\ (x_{21} - y_{21}) \mathbf{a}_2 + (z_{21} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_{21} + c(z_{21} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + \\ c(z_{21} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Si III}$$

References

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