Catapleiite ($Na_2ZrSi_3O_9{\cdot}2H_2O$) Structure: A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001

This structure previously used the label(s) `A2B3C9D3E_mC144_15_2f_bcdef_9f_3f_ae`. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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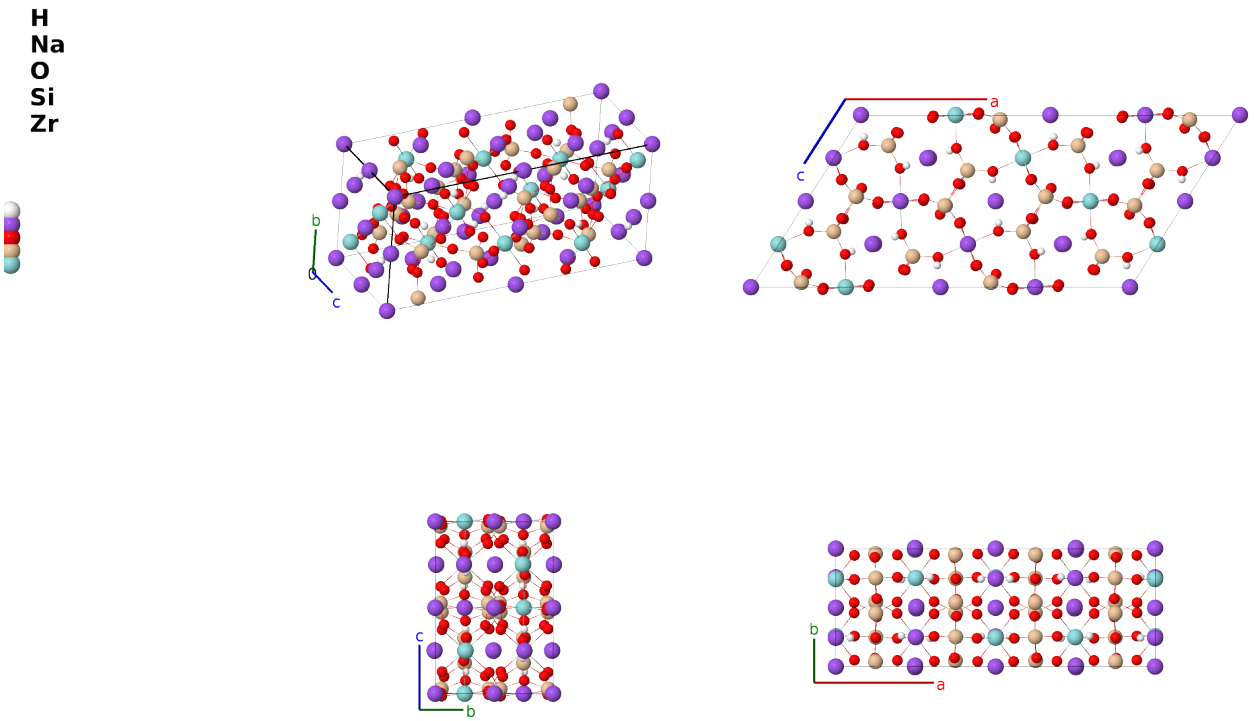
https://aflow.org/prototype-encyclopedia/L4VZ

https://aflow.org/prototype-encyclopedia/A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001



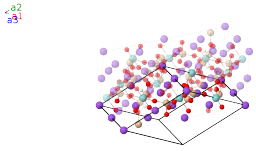
Prototype	$(H_2O)_2Na_2O_9Si_3Zr$
AFLOW prototype label	A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001
Mineral name	catapleiite
ICSD	20267
CCDC	1598089
Pearson symbol	mC144
Space group number	15
Space group symbol	$C2/c$

AFLOW prototype command `aflow --proto=A2B3C9D3E_mC144_15_2f_abcef_9f_3f_de-001 --params=`$a, b/a, c/a, \beta, y_5, y_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}$

- 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}\left(a + c\cos\beta\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{16}}$	=	$(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(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

$$\mathbf{B_{18}} = -(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_8+c\left(z_8-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{H II}$$

$$\mathbf{B_{19}} = -(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3 = -(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{H II}$$

$$\mathbf{B_{20}} = (x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_8+c\left(z_8+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{H II}$$

$$\mathbf{B_{21}} = (x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 = (ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Na V}$$

$$\mathbf{B_{22}} = -(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_9+c\left(z_9-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Na V}$$

$$\mathbf{B_{23}} = -(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3 = -(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Na V}$$

$$\mathbf{B_{24}} = (x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_9+c\left(z_9+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Na V}$$

$$\mathbf{B_{25}} = (x_{10}-y_{10})\,\mathbf{a}_1+(x_{10}+y_{10})\,\mathbf{a}_2+z_{10}\,\mathbf{a}_3 = (ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{26}} = -(x_{10}+y_{10})\,\mathbf{a}_1-(x_{10}-y_{10})\,\mathbf{a}_2-\left(z_{10}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{10}+c\left(z_{10}-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}-c\left(z_{10}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{27}} = -(x_{10}-y_{10})\,\mathbf{a}_1-(x_{10}+y_{10})\,\mathbf{a}_2-z_{10}\,\mathbf{a}_3 = -(ax_{10}+cz_{10}\cos\beta)\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}-cz_{10}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{28}} = (x_{10}+y_{10})\,\mathbf{a}_1+(x_{10}-y_{10})\,\mathbf{a}_2+\left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{10}+c\left(z_{10}+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+c\left(z_{10}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{29}} = (x_{11}-y_{11})\,\mathbf{a}_1+(x_{11}+y_{11})\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3 = (ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{30}} = -(x_{11}+y_{11})\,\mathbf{a}_1-(x_{11}-y_{11})\,\mathbf{a}_2-\left(z_{11}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{11}+c\left(z_{11}-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}-c\left(z_{11}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{31}} = -(x_{11}-y_{11})\,\mathbf{a}_1-(x_{11}+y_{11})\,\mathbf{a}_2-z_{11}\,\mathbf{a}_3 = -(ax_{11}+cz_{11}\cos\beta)\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}-cz_{11}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{32}} = (x_{11}+y_{11})\,\mathbf{a}_1+(x_{11}-y_{11})\,\mathbf{a}_2+\left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{11}+c\left(z_{11}+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+c\left(z_{11}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B_{33}} = (x_{12}-y_{12})\,\mathbf{a}_1+(x_{12}+y_{12})\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3 = (ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{34}} = -(x_{12}+y_{12})\,\mathbf{a}_1-(x_{12}-y_{12})\,\mathbf{a}_2-\left(z_{12}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{12}+c\left(z_{12}-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}-c\left(z_{12}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{35}} = -(x_{12}-y_{12})\,\mathbf{a}_1-(x_{12}+y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3 = -(ax_{12}+cz_{12}\cos\beta)\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-cz_{12}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{36}} = (x_{12}+y_{12})\,\mathbf{a}_1+(x_{12}-y_{12})\,\mathbf{a}_2+\left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{12}+c\left(z_{12}+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+c\left(z_{12}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O III}$$

$$\mathbf{B_{37}} = (x_{13}-y_{13})\,\mathbf{a}_1+(x_{13}+y_{13})\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3 = (ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{38}} = -(x_{13}+y_{13})\,\mathbf{a}_1-(x_{13}-y_{13})\,\mathbf{a}_2-\left(z_{13}-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_{13}+c\left(z_{13}-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}-c\left(z_{13}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{39}} = -(x_{13}-y_{13})\,\mathbf{a}_1-(x_{13}+y_{13})\,\mathbf{a}_2-z_{13}\,\mathbf{a}_3 = -(ax_{13}+cz_{13}\cos\beta)\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}-cz_{13}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{40}} = (x_{13}+y_{13})\,\mathbf{a}_1+(x_{13}-y_{13})\,\mathbf{a}_2+\left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_{13}+c\left(z_{13}+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+c\left(z_{13}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IV}$$

$$\mathbf{B_{41}} = (x_{14}-y_{14})\,\mathbf{a}_1 + (x_{14}+y_{14})\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = (ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{42}} = -(x_{14}+y_{14})\,\mathbf{a}_1 - (x_{14}-y_{14})\,\mathbf{a}_2 - \left(z_{14}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{14}+c\left(z_{14}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - c\left(z_{14}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{43}} = -(x_{14}-y_{14})\,\mathbf{a}_1 - (x_{14}+y_{14})\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -(ax_{14}+cz_{14}\cos\beta)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{44}} = (x_{14}+y_{14})\,\mathbf{a}_1 + (x_{14}-y_{14})\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{14}+c\left(z_{14}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O V}$$

$$\mathbf{B_{45}} = (x_{15}-y_{15})\,\mathbf{a}_1 + (x_{15}+y_{15})\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = (ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VI}$$

$$\mathbf{B_{46}} = -(x_{15}+y_{15})\,\mathbf{a}_1 - (x_{15}-y_{15})\,\mathbf{a}_2 - \left(z_{15}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{15}+c\left(z_{15}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} - c\left(z_{15}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VI}$$

$$\mathbf{B_{47}} = -(x_{15}-y_{15})\,\mathbf{a}_1 - (x_{15}+y_{15})\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -(ax_{15}+cz_{15}\cos\beta)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} - cz_{15}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VI}$$

$$\mathbf{B_{48}} = (x_{15}+y_{15})\,\mathbf{a}_1 + (x_{15}-y_{15})\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{15}+c\left(z_{15}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VI}$$

$$\mathbf{B_{49}} = (x_{16}-y_{16})\,\mathbf{a}_1 + (x_{16}+y_{16})\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = (ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VII}$$

$$\mathbf{B_{50}} = -(x_{16}+y_{16})\,\mathbf{a}_1 - (x_{16}-y_{16})\,\mathbf{a}_2 - \left(z_{16}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{16}+c\left(z_{16}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} - c\left(z_{16}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VII}$$

$$\mathbf{B_{51}} = -(x_{16}-y_{16})\,\mathbf{a}_1 - (x_{16}+y_{16})\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -(ax_{16}+cz_{16}\cos\beta)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} - cz_{16}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VII}$$

$$\mathbf{B_{52}} = (x_{16}+y_{16})\,\mathbf{a}_1 + (x_{16}-y_{16})\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{16}+c\left(z_{16}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VII}$$

$$\mathbf{B_{53}} = (x_{17}-y_{17})\,\mathbf{a}_1 + (x_{17}+y_{17})\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = (ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} + cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VIII}$$

$$\mathbf{B_{54}} = -(x_{17}+y_{17})\,\mathbf{a}_1 - (x_{17}-y_{17})\,\mathbf{a}_2 - \left(z_{17}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{17}+c\left(z_{17}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} - c\left(z_{17}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VIII}$$

$$\mathbf{B_{55}} = -(x_{17}-y_{17})\,\mathbf{a}_1 - (x_{17}+y_{17})\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -(ax_{17}+cz_{17}\cos\beta)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} - cz_{17}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VIII}$$

$$\mathbf{B_{56}} = (x_{17}+y_{17})\,\mathbf{a}_1 + (x_{17}-y_{17})\,\mathbf{a}_2 + \left(z_{17}+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{17}+c\left(z_{17}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O VIII}$$

$$\mathbf{B_{57}} = (x_{18}-y_{18})\,\mathbf{a}_1 + (x_{18}+y_{18})\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = (ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} + cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IX}$$

$$\mathbf{B_{58}} = -(x_{18}+y_{18})\,\mathbf{a}_1 - (x_{18}-y_{18})\,\mathbf{a}_2 - \left(z_{18}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{18}+c\left(z_{18}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} - c\left(z_{18}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IX}$$

$$\mathbf{B_{59}} = -(x_{18}-y_{18})\,\mathbf{a}_1 - (x_{18}+y_{18})\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -(ax_{18}+cz_{18}\cos\beta)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} - cz_{18}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IX}$$

$$\mathbf{B_{60}} = (x_{18}+y_{18})\,\mathbf{a}_1 + (x_{18}-y_{18})\,\mathbf{a}_2 + \left(z_{18}+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_{18}+c\left(z_{18}+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} + c\left(z_{18}+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O IX}$$

$$\mathbf{B_{61}} = (x_{19}-y_{19})\,\mathbf{a}_1 + (x_{19}+y_{19})\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = (ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} + cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{62}} = -(x_{19}+y_{19})\,\mathbf{a}_1 - (x_{19}-y_{19})\,\mathbf{a}_2 - \left(z_{19}-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_{19}+c\left(z_{19}-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} - c\left(z_{19}-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$$\mathbf{B_{63}} = -(x_{19}-y_{19})\,\mathbf{a}_1 - (x_{19}+y_{19})\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -(ax_{19}+cz_{19}\cos\beta)\,\hat{\mathbf{x}} - by_{19}\,\hat{\mathbf{y}} - cz_{19}\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{Si I}$$

$\mathbf{B_{64}}$	=	$(x_{19}+y_{19})\,\mathbf{a}_1+(x_{19}-y_{19})\,\mathbf{a}_2+\left(z_{19}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{19}+c\left(z_{19}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_{19}\,\hat{\mathbf{y}}+c\left(z_{19}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	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)	Si II
$\mathbf{B_{66}}$	=	$-(x_{20}+y_{20})\,\mathbf{a}_1-(x_{20}-y_{20})\,\mathbf{a}_2-\left(z_{20}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{20}+c\left(z_{20}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_{20}\,\hat{\mathbf{y}}-c\left(z_{20}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	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)	Si II
$\mathbf{B_{68}}$	=	$(x_{20}+y_{20})\,\mathbf{a}_1+(x_{20}-y_{20})\,\mathbf{a}_2+\left(z_{20}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{20}+c\left(z_{20}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_{20}\,\hat{\mathbf{y}}+c\left(z_{20}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	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)	Si III
$\mathbf{B_{70}}$	=	$-(x_{21}+y_{21})\,\mathbf{a}_1-(x_{21}-y_{21})\,\mathbf{a}_2-\left(z_{21}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_{21}+c\left(z_{21}-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_{21}\,\hat{\mathbf{y}}-c\left(z_{21}-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si III
$\mathbf{B_{71}}$	=	$-(x_{21}-y_{21})\,\mathbf{a}_1-(x_{21}+y_{21})\,\mathbf{a}_2-z_{21}\,\mathbf{a}_3$	=	$-(ax_{21}+cz_{21}\cos\beta)\,\hat{\mathbf{x}}-by_{21}\,\hat{\mathbf{y}}-cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si III
$\mathbf{B_{72}}$	=	$(x_{21}+y_{21})\,\mathbf{a}_1+(x_{21}-y_{21})\,\mathbf{a}_2+\left(z_{21}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_{21}+c\left(z_{21}+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_{21}\,\hat{\mathbf{y}}+c\left(z_{21}+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Si III

References

[1] G. D. Ilyushin, A. A. Voronkov, V. V. Ilyukhin, N. N. Nevskii, and N. V. Belov, *Crystal structure of natural monoclinic catapleiite, $Na_2ZrSi_3O_9\cdot 2H_2O$*, Dokl. Akad. Nauk SSSR **260**, 623–627 (1981).

[2] C. Gottfried, ed., *Strukturbericht Band V 1937* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1940).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.