Fresnoite ($Ba_2TiSi_2O_8$) Structure: A2B8C2D_tP26_100_c_abcd_c_a-001

This structure originally had the label `A2B8C2D_tP26_100_c_abcd_c_a`. Calls to that address will be redirected here.

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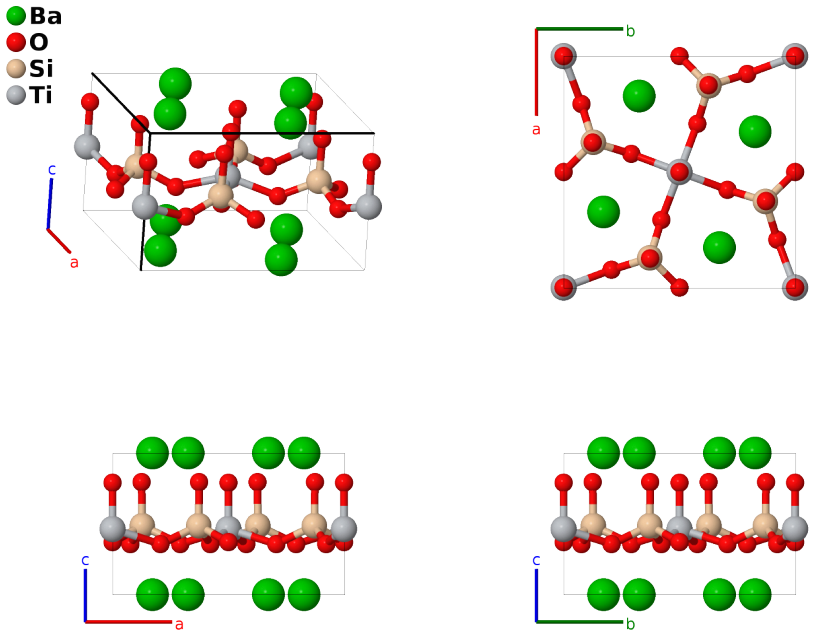
https://aflow.org/p/QC0E

https://aflow.org/p/A2B8C2D_tP26_100_c_abcd_c_a-001

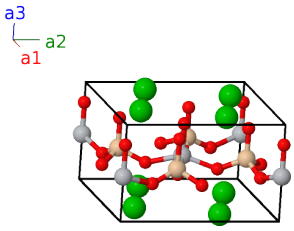


Prototype	$Ba_2O_8Si_2Ti$
AFLOW prototype label	A2B8C2D_tP26_100_c_abcd_c_a-001
Mineral name	fresnoite
ICSD	201844
Pearson symbol	tP26
Space group number	100
Space group symbol	*P4bm*
AFLOW prototype command	`aflow --proto=A2B8C2D_tP26_100_c_abcd_c_a-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, y_7, z_7$

- Found in the Big Creek – Rush Creek sanbornite deposit, 8 km (5 miles) NE of Trimmer, Fresno Co. California.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2a)	Ti I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_9}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_{10}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{13}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{14}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{17}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{18}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Si I
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{21}}$	=	$-y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{22}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{23}}$	=	$\left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{24}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{25}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B_{26}}$	=	$\left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$a\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	O IV

References

[1] S. A. Markgraf, A. Halliya, A. S. Bhalla, R. E. Newnham, and C. T. Prewitt, *X-ray structure refinement and pyroelectric investigation of fresnoite, Ba2TiSi2O8*, Ferroelectrics **62**, 17–26 (1985), doi:10.1080/00150198508017914.