

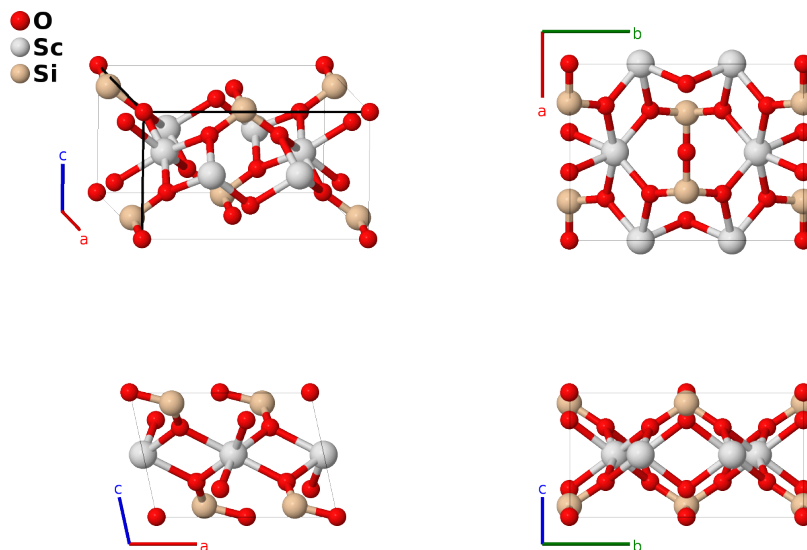
Thortveitite ($[\text{Sc}, \text{Y}]_2\text{Si}_2\text{O}_7$, $S2_1$) Structure: A7B2C2_mC22_12_aij_h_i-001

This structure originally had the label A7B2C2_mC22_12_aij_h_i. Calls to that address will be redirected here.

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<https://aflow.org/p/0J1F>

https://aflow.org/p/A7B2C2_mC22_12_aij_h_i-001



Prototype	$\text{O}_7\text{Sc}_2\text{Si}_2$
AFLOW prototype label	A7B2C2_mC22_12_aij_h_i-001
<i>Strukturbericht</i> designation	$S2_1$
Mineral name	thortveitite
ICSD	202633
Pearson symbol	mC22
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A7B2C2_mC22_12_aij_h_i-001 --params=a, b/a, c/a, β, y_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5</pre>

Other compounds with this structure

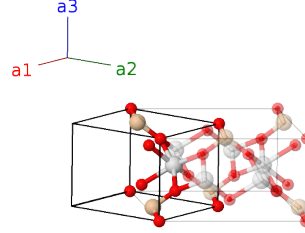
$\beta\text{Er}_2\text{Si}_2\text{O}_7$, $\beta\text{Ho}_2\text{Si}_2\text{O}_7$, $\beta\text{In}_2\text{Si}_2\text{O}_7$, $\beta\text{Lu}_2\text{Si}_2\text{O}_7$, $\beta\text{Sc}_2\text{Si}_2\text{O}_7$, $\beta\text{Tm}_2\text{Si}_2\text{O}_7$, $\beta\text{Y}_2\text{Si}_2\text{O}_7$, $\beta\text{Yb}_2\text{Si}_2\text{O}_7$, $\beta[\text{Y}, \text{Sc}]_2\text{Si}_2\text{O}_7$, $\beta[\text{Y}, \text{Yb}]_2\text{Si}_2\text{O}_7$

- Thortveitite is the primary source of scandium and is one of the simplest sorosilicates, minerals with isolated Si_2O_7 groups. (Bianchi, 1988)

- Although the (4h) Wyckoff position is randomly occupied by both Sc and Y atoms, we use Sc to represent the site.
- (Bianchi, 1988) gives structural information for several samples of thortveitite.
- In addition, the Si (4i) site contains 2% aluminum.
- We use the data from sample 1, collected in Iveland, Norway.

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	(2a)	O I
\mathbf{B}_2	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Sc I
\mathbf{B}_3	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Sc I
\mathbf{B}_4	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_5	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
\mathbf{B}_6	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Si I
\mathbf{B}_7	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Si I
\mathbf{B}_8	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_9	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{10}	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
\mathbf{B}_{11}	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O III

References

- [1] R. Bianchi, T. Pilati, V. Diella, C. M. Gramacciou, and G. Mannucci, *A re-examination of thortveitite*, *American Mineralogist* **73**, 601–607 (1988).

Found in

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