Thortveitite ($[Sc,Y]_2Si_2O_7$, $S2_1$) Structure: A7B2C2_mC22_12_aij_h_i-001

This structure previously used the label(s) `A7B2C2_mC22_12_aij_h_i`. Calls to these addresses will be redirected here.

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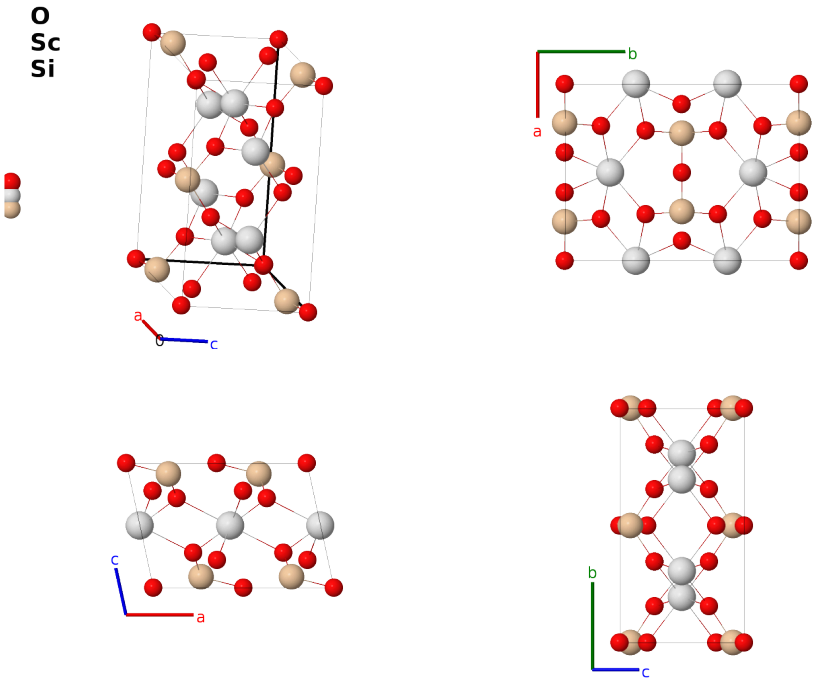
https://aflow.org/prototype-encyclopedia/0J1F

https://aflow.org/prototype-encyclopedia/A7B2C2_mC22_12_aij_h_i-001



Prototype	$O_7Sc_2Si_2$
AFLOW prototype label	A7B2C2_mC22_12_aij_h_i-001
***Strukturbericht* designation**	$S2_1$
Mineral name	thortveitite
ICSD	202633
CCDC	1707199
Pearson symbol	mC22
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A7B2C2_mC22_12_aij_h_i-001 --params=`$a, b/a, c/a, \beta, y_2, x_3, z_3, x_4, z_4, x_5, y_5, z_5$

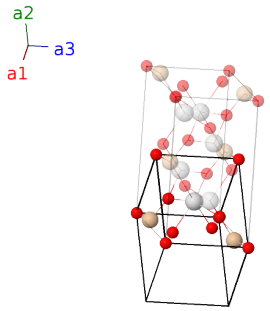
Other compounds with this structure

β-$Er_2Si_2O_7$, β-$Ho_2Si_2O_7$, β-$In_2Si_2O_7$, β-$Lu_2Si_2O_7$, β-$Sc_2Si_2O_7$, β-$Tm_2Si_2O_7$, β-$Y_2Si_2O_7$, β-$Yb_2Si_2O_7$ (keiviite), β-$[Y, Yb]_2Si_2O_7$

- 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).

First cited in

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