

α (High) Tridymite (SiO_2) Structure: A2B_oC24_20_abc_c-001

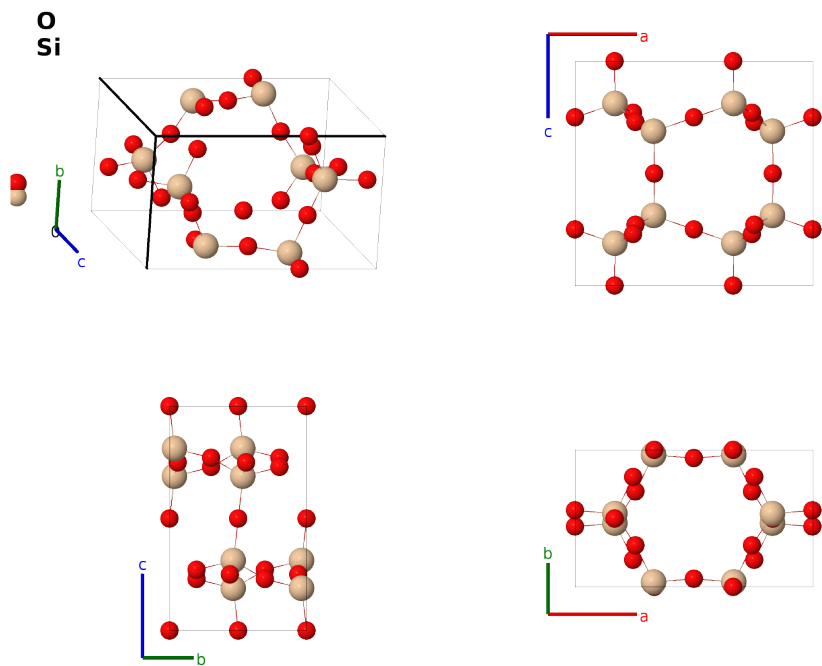
This structure previously used the label(s) **A2B_oC24_20_abc_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/NDBQ>

https://aflow.org/prototype-encyclopedia/A2B_oC24_20_abc_c-001

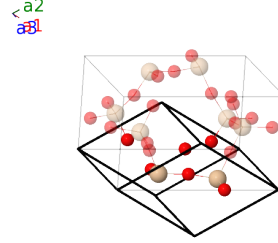


Prototype	O_2Si
AFLOW prototype label	A2B_oC24_20_abc_c-001
Mineral name	high tridymite
ICSD	15321
CCDC	1596085
Pearson symbol	oC24
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	<code>aflow --proto=A2B_oC24_20_abc_c-001</code> <code>--params=a, b/a, c/a, x₁, y₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

- Tridymite undergoes a series of temperature-driven phase transitions. We also have an extensive list of the many phases of SiO₂ and related compounds.
- (Dollase, 1967) used a non-standard origin for the atomic positions, so there has been a considerable rearrangement of the coordinates, even from the previous version of this file. We have chosen the ordering of the axes so that it is obvious that the primitive base-centered orthorhombic lattice is very close to a tetragonal primitive lattice.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}}$	(4a)	O I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_5$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_6$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_7$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_8$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{10}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{11}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Si I
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8c)	Si I

References

- [1] W. A. Dollase, *The crystal structure at 220° C of orthorhombic high tridymite from the Steinbach meteorite*, Acta Cryst. **23**, 617–623 (1967), doi:10.1107/S0365110X67003287.

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