

β -Tridymite (SiO_2 , $C10$) Structure: A2B_hP12_194_cg_f-001

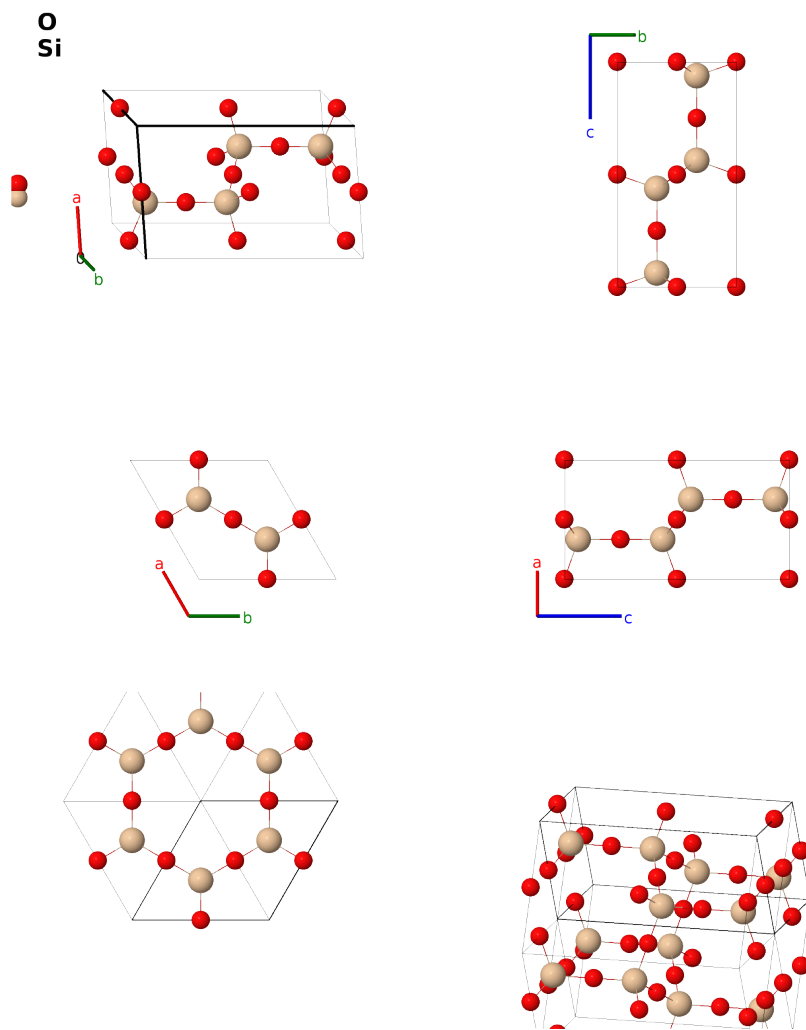
This structure previously used the label(s) **A2B_hP12_194_cg_f**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

<https://aflow.org/prototype-encyclopedia/3KTM>

https://aflow.org/prototype-encyclopedia/A2B_hP12_194_cg_f-001

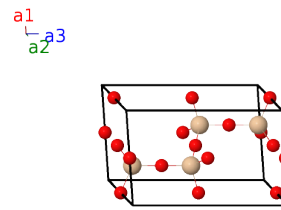


Prototype	O_2Si
AFLOW prototype label	A2B_hP12_194_cg_f-001
<i>Strukturbericht</i> designation	$C10$
Mineral name	tridymite
ICSD	200478

CCDC	1705387
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A2B_hP12_194_cg_f-001</code> <code>--params=a, c/a, z₂</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.

Hexagonal primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c \hat{\mathbf{z}}
 \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	O II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}}$	(6g)	O II
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(6g)	O II
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(6g)	O II

References

- [1] K. Kihara, *Thermal change in unit-cell dimensions, and a hexagonal structure of tridymite*, Z. Krystallogr. **148**, 237–253 (1978), doi:10.1524/zkri.1978.148.3-4.237.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017