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

This structure originally had the label `A2B_hP12_194_cg_f`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. 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

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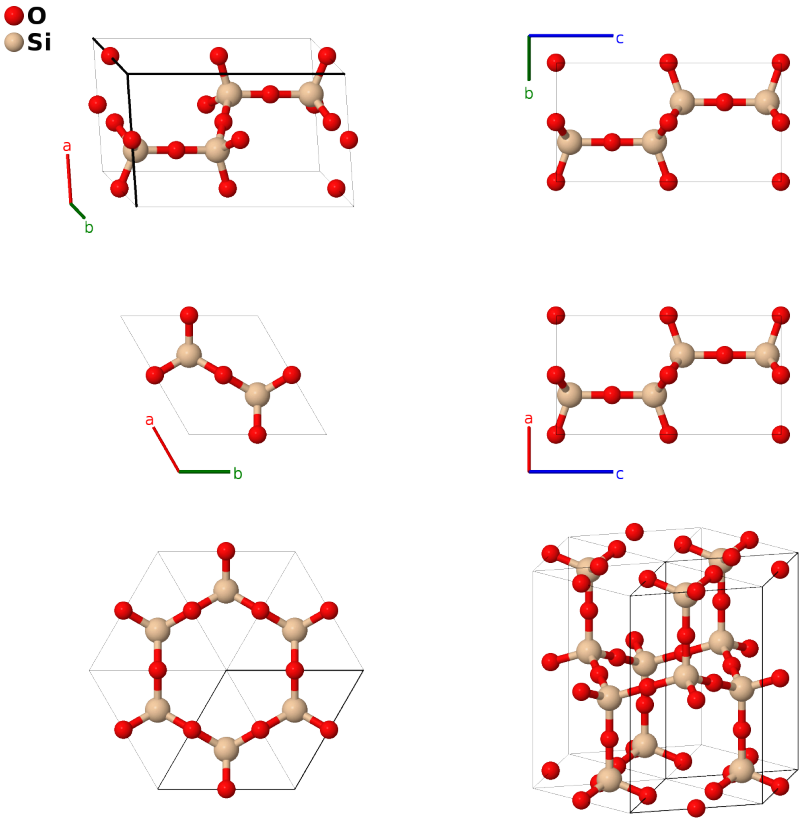
https://aflow.org/p/3KTM

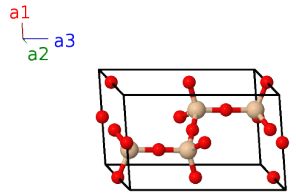
https://aflow.org/p/A2B_hP12_194_cg_f-001



Prototype	O_2Si
AFLOW prototype label	A2B_hP12_194_cg_f-001
***Strukturbericht* designation**	$C10$
Mineral name	tridymite
ICSD	200478
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A2B_hP12_194_cg_f-001 --params=`$a, c/a, z_2$

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_2}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_3}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_4}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_5}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_6}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Si I
$\mathbf{B_7}$	=	$\tfrac{1}{2}\,\mathbf{a}_1$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	O II
$\mathbf{B_8}$	=	$\tfrac{1}{2}\,\mathbf{a}_2$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	O II
$\mathbf{B_9}$	=	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	O II
$\mathbf{B_{10}}$	=	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{11}}$	=	$\tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{12}}$	=	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(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.