β-SiO_2 ($C8$) Structure: A2B_hP9_181_i_d-001

This structure originally had the label `A2B_hP9_181_j_c`. Calls to that address will be redirected here.

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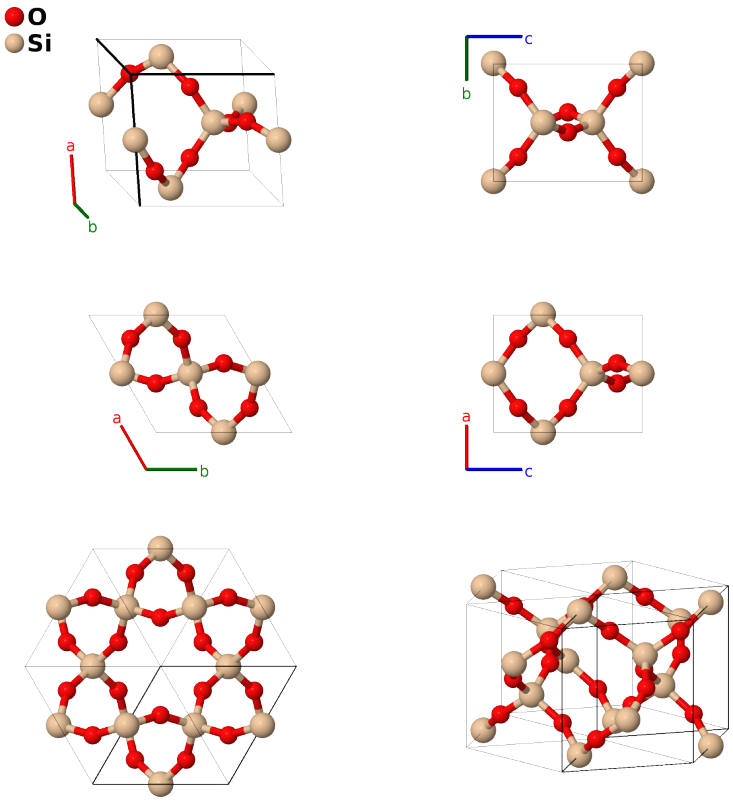
https://aflow.org/p/VH37

https://aflow.org/p/A2B_hP9_181_i_d-001



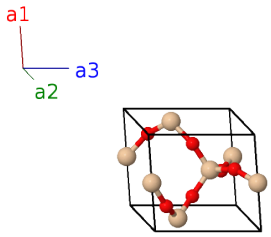
Prototype	O_2Si
AFLOW prototype label	A2B_hP9_181_i_d-001
***Strukturbericht* designation**	$C8$
ICSD	26430
Pearson symbol	hP9
Space group number	181
Space group symbol	$P6_422$
AFLOW prototype command	`aflow --proto=A2B_hP9_181_i_d-001 --params=`$a, c/a, x_2$

- This is the high-temperature structure of α-quartz. It can also be found in the enantiomorphic space group $P6_222$ #180.

- (Wright, 1981) put the oxygen atoms on half-filled (12k) sites, with pairs of oxygen sites separated by only 0.4Å. We approximate the structure here by moving the oxygen atoms to fully-filled (6i) sites.
- The ICSD entry is for the $P6_222$ representation of the structure.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3d)	Si I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(3d)	Si I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	Si I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6i)	O I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6i)	O I
$\mathbf{B_8}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6i)	O I

References

[1] A. F. Wright and M. S. Lehmann, *The Structure of Quartz at 25 and 590° C Determined by Neutron Diffraction*, J. Solid State Chem. **36**, 371–380 (1981), doi:10.1016/0022-4596(81)90449-7.

Found in

[1] *Mineral Web β-quartz structure.*