

β (high) quartz (SiO_2 , $C8$) Structure: A2B_hP9_180_i_d-001

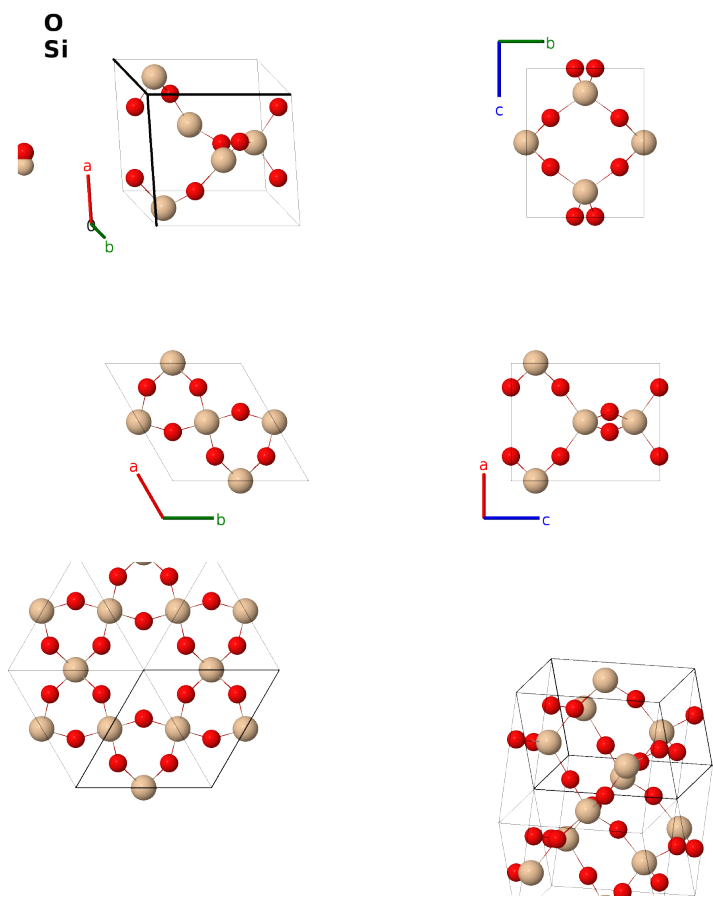
This structure previously used the label(s) **A2B_hP9_180_j_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/MK1H>

https://aflow.org/prototype-encyclopedia/A2B_hP9_180_i_d-001



Prototype	O_2Si
AFLOW prototype label	A2B_hP9_180_i_d-001
<i>Strukturbericht</i> designation	$C8$
ICSD	26430
CCDC	1601837
Pearson symbol	hP9
Space group number	180

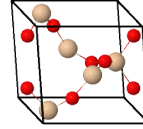
Space group symbol $P6_222$

AFLOW prototype command `aflow --proto=A2B_hP9_180_i_d-001`
`--params=a,c/a,x2`

- This is the high-temperature structure of α -quartz, stable above 573°C (Wright, 1981). It can also be found in the enantiomorphic space group $P6_422$ #181.
- (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.
- More information about SiO₂ structures can be found in our article on SiO₂ and AlPO₄.

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
$\mathbf{B}_1$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3d)	Si I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{6}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\hat{\mathbf{y}} + \frac{1}{6}c\hat{\mathbf{z}}$	(3d)	Si I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{5}{6}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{5}{6}c\hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$= -2x_2\mathbf{a}_1 - x_2\mathbf{a}_2 + \frac{2}{3}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}} + \frac{2}{3}c\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B}_6$	$= x_2\mathbf{a}_1 - x_2\mathbf{a}_2 + \frac{1}{3}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_2\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$= 2x_2\mathbf{a}_1 + x_2\mathbf{a}_2 + \frac{2}{3}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_2\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}} + \frac{2}{3}c\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B}_9$	$= -x_2\mathbf{a}_1 + x_2\mathbf{a}_2 + \frac{1}{3}\mathbf{a}_3$	$=$	$\sqrt{3}ax_2\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$	(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*.

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