α-Quartz (low Quartz) Structure: A2B_hP9_152_c_a-001

This structure originally had the label `A2B_hP9_152_c_a`. Calls to that address will be redirected here.

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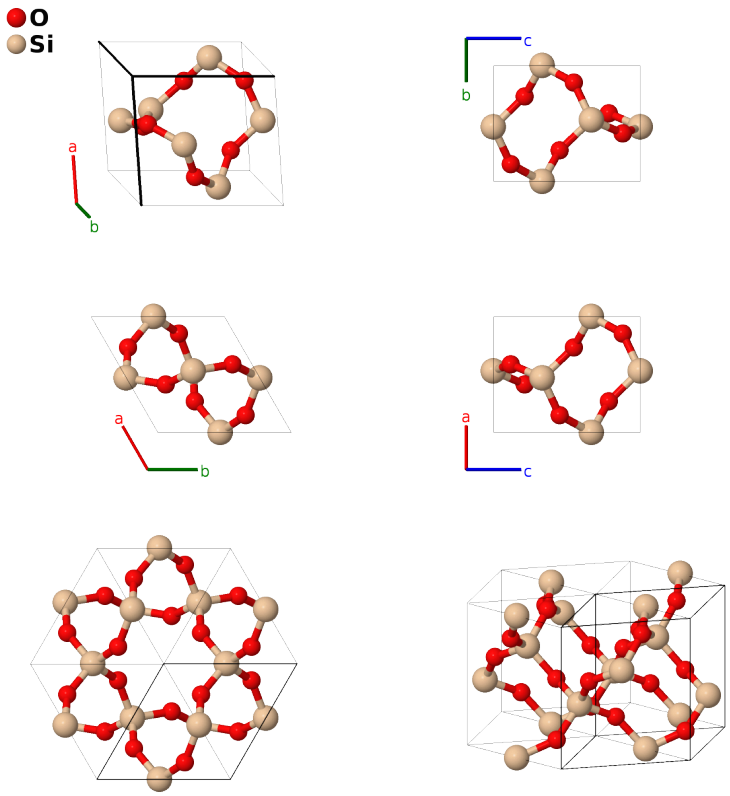
https://aflow.org/p/P53L

https://aflow.org/p/A2B_hP9_152_c_a-001

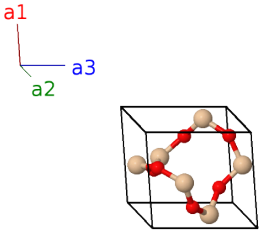


Prototype	O_2Si
AFLOW prototype label	A2B_hP9_152_c_a-001
Mineral name	quartz
ICSD	67121
Pearson symbol	hP9
Space group number	152
Space group symbol	$P3_121$
AFLOW prototype command	`aflow --proto=A2B_hP9_152_c_a-001 --params=`$a, c/a, x_1, x_2, y_2, z_2$

- When $x_1 = 1/2$, $y_2 = 2x_2$, and $z_2 = 1/2$ this tranforms into the high β-quartz ($C8$) structure. This structure can also be found in the enantiomorphic space group $P3_221$ #154.

Trigonal (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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3a)	Si I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(3a)	Si I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(3a)	Si I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_6}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2 + 2)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_7}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_8}$	=	$(x_2 - y_2)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - \left(z_2 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_2 - 2)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(6c)	O I

References

[1] R. M. Hazen, L. W. Finger, R. J. Hemley, and H. K. Mao, *High-pressure crystal chemistry and amorphization of α-quartz*, Solid State Commun. **72**, 507–511 (1989), doi:10.1016/0038-1098(89)90607-8.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).