Ideal β-Cristobalite (SiO_2, $C9$) Structure: A2B_cF24_227_c_a-001

This structure originally had the label `A2B_cF24_227_c_a`. Calls to that address will be redirected here.

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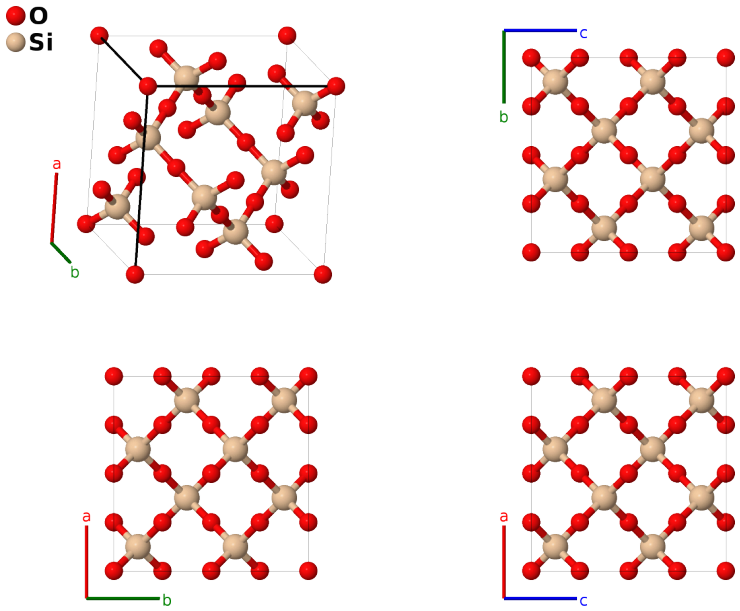
https://aflow.org/p/QDSV

https://aflow.org/p/A2B_cF24_227_c_a-001



Prototype	O_2Si
AFLOW prototype label	A2B_cF24_227_c_a-001
***Strukturbericht* designation**	$C9$
Mineral name	cristobalite
ICSD	35536
Pearson symbol	cF24
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B_cF24_227_c_a-001 --params=`a

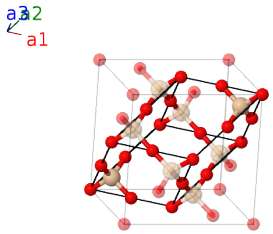
Other compounds with this structure
BeF_2, $AlPO_4$

- This is an idealized version of the high-temperature phase of α-cristobalite originally proposed by (Wyckoff, 1925).

- (Peacor, 1973) concludes that the oxygen atoms partially occupy the (96g) positions in the space group $Fd\bar{3}m$ #227. We average those positions to put the oxygen on the (16c) sites and return to the original structure.
- β-cristobalite is also known as "high" cristobalite.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Si I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Si I
$\mathbf{B_3}$	=	0	=	0	(16c)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	O I

References

[1] R. W. G. Wyckoff, *The crystal structure of the high temperature form of cristobalite (SiO_2*, Am. J. Science **9**, 448–459 (1925).

[2] D. R. Peacor, *High-temperature single-crystal study of the cristobalite inversion*, Z. Krystallogr. **138**, 274–298 (1973), doi:10.1524/zkri.1973.138.1-4.274.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).