Coesite (SiO_2) Structure: A2B_mC48_15_ae3f_2f-001

This structure originally had the label `A2B_mC48_15_ae3f_2f`. Calls to that address will be redirected here.

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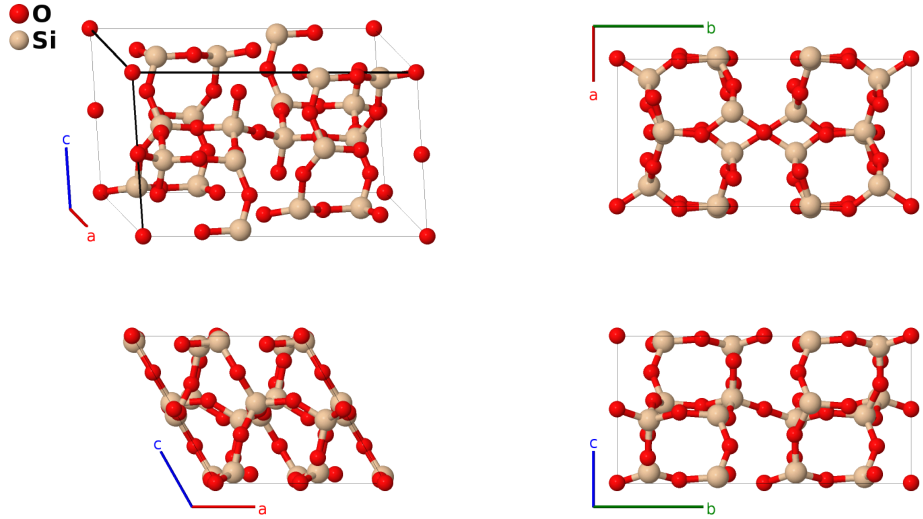
https://aflow.org/p/QHEE

https://aflow.org/p/A2B_mC48_15_ae3f_2f-001

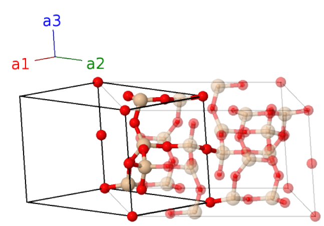


Prototype	O_2Si
AFLOW prototype label	A2B_mC48_15_ae3f_2f-001
Mineral name	coesite
ICSD	100749
Pearson symbol	mC48
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B_mC48_15_ae3f_2f-001` `--params=`$a, b/a, c/a, \beta, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- Our original work (Mehl, 2017) misplaced the O II Wycoff position. This is corrected here.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\mathbf{\hat{x}}+\frac{1}{2}c\sin\beta\,\mathbf{\hat{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\mathbf{\hat{x}}+by_2\,\mathbf{\hat{y}}+\frac{1}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	O II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\mathbf{\hat{x}}-by_2\,\mathbf{\hat{y}}+\frac{3}{4}c\sin\beta\,\mathbf{\hat{z}}$	(4e)	O II
$\mathbf{B_5}$	=	$\left(x_3-y_3\right)\,\mathbf{a}_1+\left(x_3+y_3\right)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\left(ax_3+cz_3\cos\beta\right)\,\mathbf{\hat{x}}+by_3\,\mathbf{\hat{y}}+cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_6}$	=	$-\left(x_3+y_3\right)\,\mathbf{a}_1-\left(x_3-y_3\right)\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3+c\left(z_3-\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}+by_3\,\mathbf{\hat{y}}-c\left(z_3-\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_7}$	=	$-\left(x_3-y_3\right)\,\mathbf{a}_1-\left(x_3+y_3\right)\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-\left(ax_3+cz_3\cos\beta\right)\,\mathbf{\hat{x}}-by_3\,\mathbf{\hat{y}}-cz_3\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_8}$	=	$\left(x_3+y_3\right)\,\mathbf{a}_1+\left(x_3-y_3\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3+c\left(z_3+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}-by_3\,\mathbf{\hat{y}}+c\left(z_3+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O III
$\mathbf{B_9}$	=	$\left(x_4-y_4\right)\,\mathbf{a}_1+\left(x_4+y_4\right)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$\left(ax_4+cz_4\cos\beta\right)\,\mathbf{\hat{x}}+by_4\,\mathbf{\hat{y}}+cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O IV
$\mathbf{B_{10}}$	=	$-\left(x_4+y_4\right)\,\mathbf{a}_1-\left(x_4-y_4\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4+c\left(z_4-\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}+by_4\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O IV
$\mathbf{B_{11}}$	=	$-\left(x_4-y_4\right)\,\mathbf{a}_1-\left(x_4+y_4\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-\left(ax_4+cz_4\cos\beta\right)\,\mathbf{\hat{x}}-by_4\,\mathbf{\hat{y}}-cz_4\sin\beta\,\mathbf{\hat{z}}$	(8f)	O IV
$\mathbf{B_{12}}$	=	$\left(x_4+y_4\right)\,\mathbf{a}_1+\left(x_4-y_4\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4+c\left(z_4+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}-by_4\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O IV
$\mathbf{B_{13}}$	=	$\left(x_5-y_5\right)\,\mathbf{a}_1+\left(x_5+y_5\right)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$\left(ax_5+cz_5\cos\beta\right)\,\mathbf{\hat{x}}+by_5\,\mathbf{\hat{y}}+cz_5\sin\beta\,\mathbf{\hat{z}}$	(8f)	O V
$\mathbf{B_{14}}$	=	$-\left(x_5+y_5\right)\,\mathbf{a}_1-\left(x_5-y_5\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5+c\left(z_5-\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}+by_5\,\mathbf{\hat{y}}-c\left(z_5-\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O V
$\mathbf{B_{15}}$	=	$-\left(x_5-y_5\right)\,\mathbf{a}_1-\left(x_5+y_5\right)\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-\left(ax_5+cz_5\cos\beta\right)\,\mathbf{\hat{x}}-by_5\,\mathbf{\hat{y}}-cz_5\sin\beta\,\mathbf{\hat{z}}$	(8f)	O V
$\mathbf{B_{16}}$	=	$\left(x_5+y_5\right)\,\mathbf{a}_1+\left(x_5-y_5\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5+c\left(z_5+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}-by_5\,\mathbf{\hat{y}}+c\left(z_5+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	O V
$\mathbf{B_{17}}$	=	$\left(x_6-y_6\right)\,\mathbf{a}_1+\left(x_6+y_6\right)\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$\left(ax_6+cz_6\cos\beta\right)\,\mathbf{\hat{x}}+by_6\,\mathbf{\hat{y}}+cz_6\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si I
$\mathbf{B_{18}}$	=	$-\left(x_6+y_6\right)\,\mathbf{a}_1-\left(x_6-y_6\right)\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6+c\left(z_6-\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}+by_6\,\mathbf{\hat{y}}-c\left(z_6-\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si I
$\mathbf{B_{19}}$	=	$-\left(x_6-y_6\right)\,\mathbf{a}_1-\left(x_6+y_6\right)\,\mathbf{a}_2-z_6\,\mathbf{a}_3$	=	$-\left(ax_6+cz_6\cos\beta\right)\,\mathbf{\hat{x}}-by_6\,\mathbf{\hat{y}}-cz_6\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si I
$\mathbf{B_{20}}$	=	$\left(x_6+y_6\right)\,\mathbf{a}_1+\left(x_6-y_6\right)\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6+c\left(z_6+\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}-by_6\,\mathbf{\hat{y}}+c\left(z_6+\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si I
$\mathbf{B_{21}}$	=	$\left(x_7-y_7\right)\,\mathbf{a}_1+\left(x_7+y_7\right)\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\left(ax_7+cz_7\cos\beta\right)\,\mathbf{\hat{x}}+by_7\,\mathbf{\hat{y}}+cz_7\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si II
$\mathbf{B_{22}}$	=	$-\left(x_7+y_7\right)\,\mathbf{a}_1-\left(x_7-y_7\right)\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7+c\left(z_7-\frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}}+by_7\,\mathbf{\hat{y}}-c\left(z_7-\frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si II
$\mathbf{B_{23}}$	=	$-\left(x_7-y_7\right)\,\mathbf{a}_1-\left(x_7+y_7\right)\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-\left(ax_7+cz_7\cos\beta\right)\,\mathbf{\hat{x}}-by_7\,\mathbf{\hat{y}}-cz_7\sin\beta\,\mathbf{\hat{z}}$	(8f)	Si II

$$\mathbf{B_{24}} = \left(x_7+y_7\right)\mathbf{a}_1+\left(x_7-y_7\right)\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3 = \left(ax_7+c\left(z_7+\frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(8f)} \quad \text{Si II}$$

References

[1] L. Levien and C. T. Prewitt, *High-pressure crystal structure and compressibility of coesite*, Am. Mineral. **66**, 324–333 (1981).

[2] 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–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.