

Coesite (SiO₂) Structure: A2B_mC48_15_ae3f_2f-001

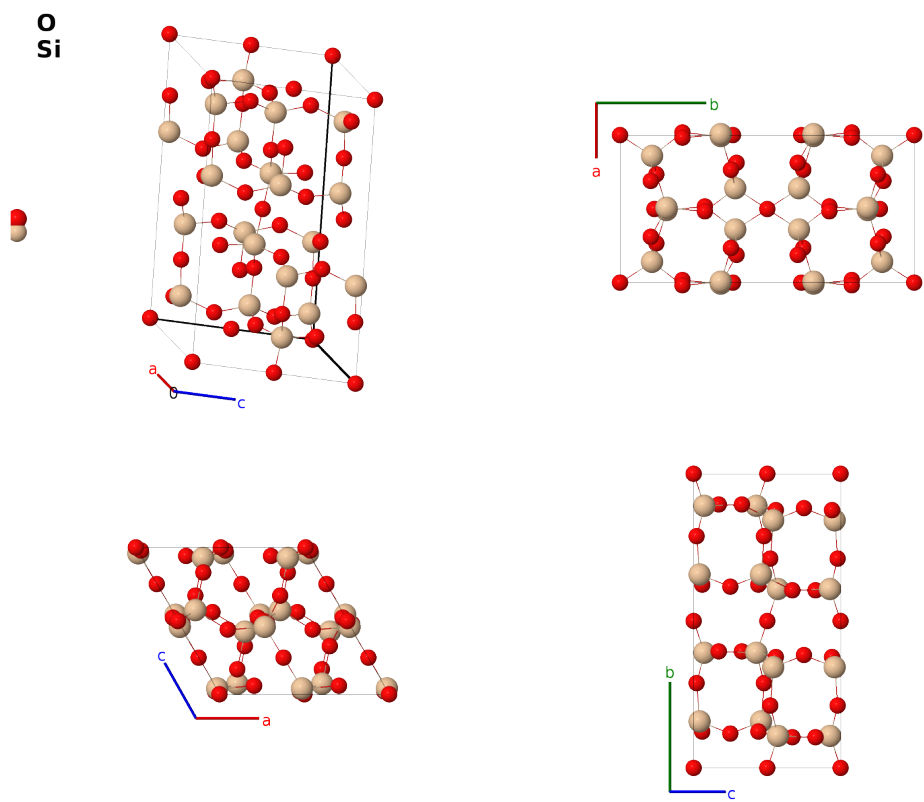
This structure previously used the label(s) **A2B_mC48_15_ae3f_2f**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/A2B_mC48_15_ae3f_2f-001



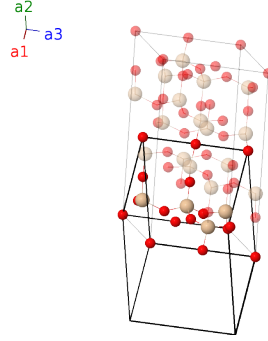
Prototype	O ₂ Si
AFLOW prototype label	A2B_mC48_15_ae3f_2f-001
Mineral name	coesite
ICSD	100749
CCDC	1659854
Pearson symbol	mC48
Space group number	15
Space group symbol	C2/c

AFLOW prototype command `aflow --proto=A2B_mC48_15_ae3f_2f-001`
 `--params=a,b/a,c/a, $\beta$ , $y_2$ , $x_3$ , $y_3$ , $z_3$ , $x_4$ , $y_4$ , $z_4$ , $x_5$ , $y_5$ , $z_5$ , $x_6$ , $y_6$ , $z_6$ , $x_7$ , $y_7$ , $z_7$`

- This was named for its original discoverer, Loring Coes, Jr. (Coes, 1953; Hazen, 1999).
 - At 2.92 gm/cm³ this is the densest form of silica we have found.
 - More information about SiO₂ structures can be found in our article on SiO₂ and AlPO₄.
 - Our original work (Mehl, 2017) misplaced the O II Wyckoff position. This is corrected here.
 - More information about other SiO₂ and related structures can be found in our article on SiO₂ and AlPO₄.
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Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(4a)	O I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_4$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \sin \beta \hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_6$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_7$	$-(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_8$	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_9$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{10}$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{11}$	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	O IV
$\mathbf{B}_{12}$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	O IV

$$\begin{aligned}
\mathbf{B}_{13} &= \begin{matrix} (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \\ z_5 \mathbf{a}_3 \end{matrix} = (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}} & (8f) & \text{O V} \\
\mathbf{B}_{14} &= \begin{matrix} -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - \\ (z_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -\left(ax_5 + c\left(z_5 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - \\ & \quad c\left(z_5 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{O V} \\
\mathbf{B}_{15} &= \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} & (8f) & \text{O V} \\
\mathbf{B}_{16} &= \begin{matrix} (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \\ (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \left(ax_5 + c\left(z_5 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \\ & \quad c\left(z_5 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{O V} \\
\mathbf{B}_{17} &= \begin{matrix} (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si I} \\
\mathbf{B}_{18} &= \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -\left(ax_6 + c\left(z_6 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - \\ & \quad c\left(z_6 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si I} \\
\mathbf{B}_{19} &= \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si I} \\
\mathbf{B}_{20} &= \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \left(ax_6 + c\left(z_6 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \\ & \quad c\left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si I} \\
\mathbf{B}_{21} &= \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{22} &= \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -\left(ax_7 + c\left(z_7 - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - \\ & \quad c\left(z_7 - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{23} &= \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si II} \\
\mathbf{B}_{24} &= \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \left(ax_7 + c\left(z_7 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \\ & \quad c\left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} & (8f) & \text{Si II}
\end{aligned}$$

References

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- [2] L. Coes Jr., *A New Dense Crystalline Silica*, Science **118**, 131–132 (1953), doi:10.1126/science.118.3057.131.
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- [4] 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–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

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