

Hypothetical Cubic SiO₂ Structure: A2B_cI72_211_hi_i-001

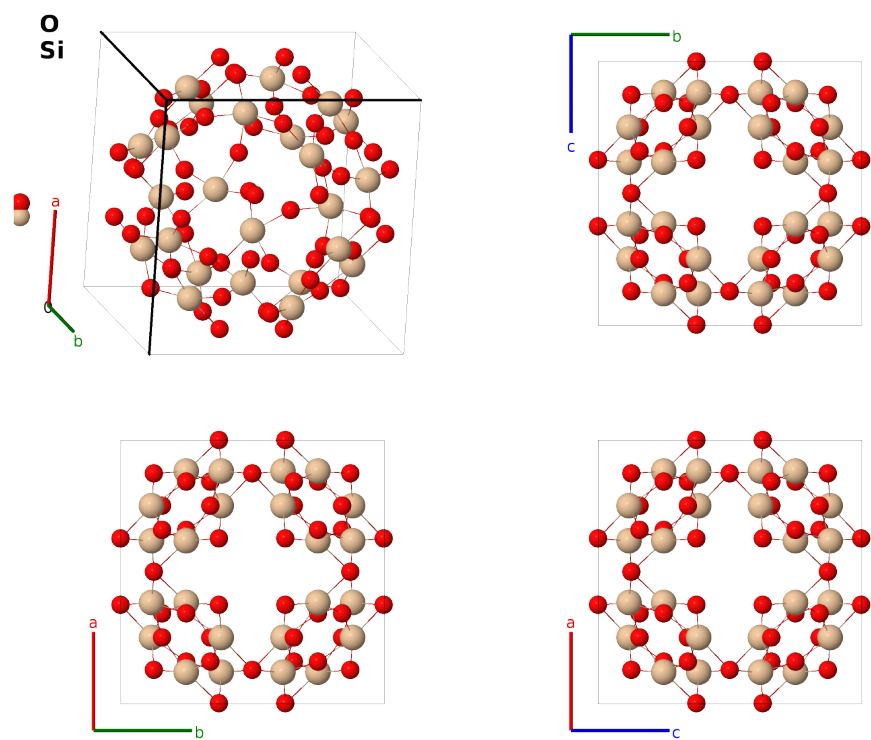
This structure previously used the label(s) **A2B_cI72.211_hi_i**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/NT1Y>

https://aflow.org/prototype-encyclopedia/A2B_cI72.211_hi_i-001

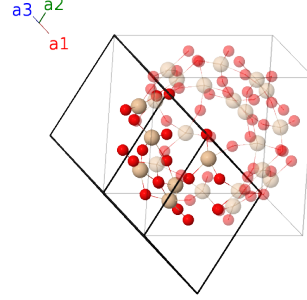


Prototype	O ₂ Si
AFLOW prototype label	A2B_cI72_211_hi_i-001
ICSD	170506
CCDC	1685978
Pearson symbol	cI72
Space group number	211
Space group symbol	I432
AFLOW prototype command	<code>aflow --proto=A2B_cI72_211_hi_i-001 --params=a, y₁, y₂, y₃</code>

- This is a hypothetical cubic structure for SiO₂. We use the data from the 1_158.cif file provided in the supplementary information of (Foster, 2004).
- More information about other real and proposed SiO₂ and related structures can be found in our article on SiO₂ and AlPO₄.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 2y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_3$	$= -y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_4$	$= -2y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_5$	$= y_1 \mathbf{a}_1 + 2y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_6$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_7$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_8$	$= -y_1 \mathbf{a}_1 - 2y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{z}}$	(24h)	O I
$\mathbf{B}_9$	$= y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + 2y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{10}$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-ay_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{11}$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$ay_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{12}$	$= -y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - 2y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}}$	(24h)	O I
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_1 - (y_2 - \frac{3}{4}) \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{14}$	$= -(2y_2 - \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{4}) \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{15}$	$= (2y_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{4}) \mathbf{a}_2 + (y_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{16}$	$= \frac{1}{2} \mathbf{a}_1 + (y_2 + \frac{3}{4}) \mathbf{a}_2 - (y_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{17}$	$= (y_2 + \frac{1}{4}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{18}$	$= -(y_2 - \frac{3}{4}) \mathbf{a}_1 - (2y_2 - \frac{1}{2}) \mathbf{a}_2 - (y_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{19}$	$= (y_2 + \frac{3}{4}) \mathbf{a}_1 + (2y_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B}_{20}$	$= -(y_2 - \frac{1}{4}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (y_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(24i)	O II

$$\begin{aligned}
\mathbf{B}_{21} &= -\left(y_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = ay_2 \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{22} &= -\left(y_2 - \frac{1}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right) \mathbf{a}_2 - \left(2y_2 - \frac{1}{2}\right) \mathbf{a}_3 = -a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{23} &= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \left(2y_2 + \frac{1}{2}\right) \mathbf{a}_3 = a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{24} &= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -ay_2 \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{O II} \\
\mathbf{B}_{25} &= \frac{1}{2} \mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{26} &= -\left(2y_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{27} &= \left(2y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{28} &= \frac{1}{2} \mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_3 = \frac{1}{4}a \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{29} &= \left(y_3 + \frac{1}{4}\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_3 = -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{30} &= -\left(y_3 - \frac{3}{4}\right) \mathbf{a}_1 - \left(2y_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{31} &= \left(y_3 + \frac{3}{4}\right) \mathbf{a}_1 + \left(2y_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{32} &= -\left(y_3 - \frac{1}{4}\right) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_3 = a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{33} &= -\left(y_3 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{34} &= -\left(y_3 - \frac{1}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right) \mathbf{a}_2 - \left(2y_3 - \frac{1}{2}\right) \mathbf{a}_3 = -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{35} &= \left(y_3 + \frac{1}{4}\right) \mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right) \mathbf{a}_2 + \left(2y_3 + \frac{1}{2}\right) \mathbf{a}_3 = a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{Si I} \\
\mathbf{B}_{36} &= \left(y_3 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}} & (24i) & \text{Si I}
\end{aligned}$$

References

- [1] M. D. Foster, O. D. Friedrichs, R. G. Bell, F. A. A. Paz, and J. Klinowski, *Chemical Evaluation of Hypothetical Uninodal Zeolites*, J. Am. Chem. Soc. **126**, 9769–9775 (2004), doi:10.1021/ja037334j.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043