Hypothetical Cubic SiO_2 Structure: A2B_cI72_211_hi_i-001

This structure originally had the label `A2B_cI72_211_hi_i`. Calls to that address will be redirected here.

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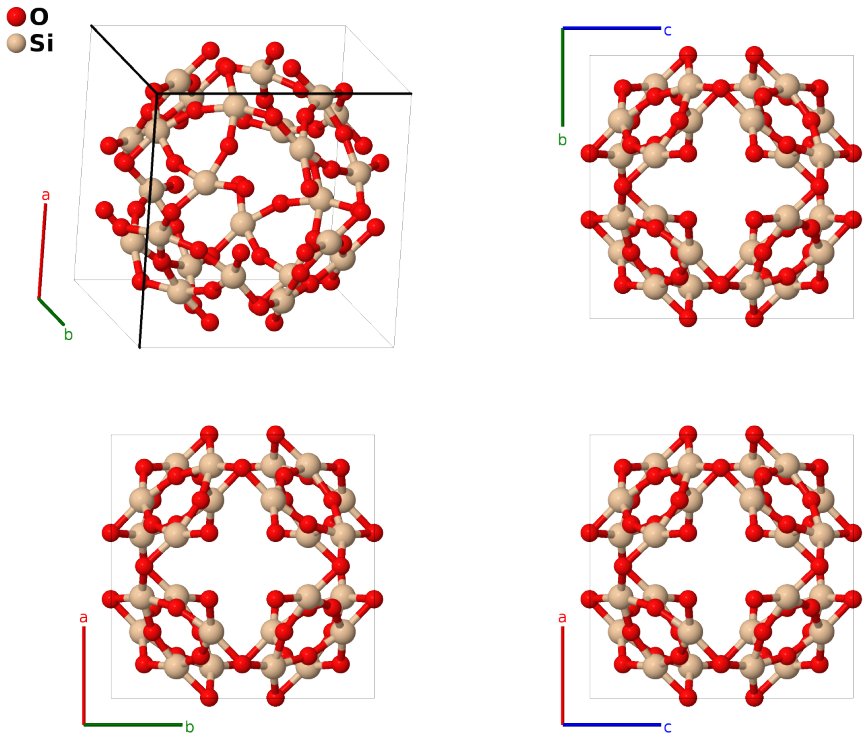
https://aflow.org/p/NT1Y

https://aflow.org/p/A2B_cI72_211_hi_i-001

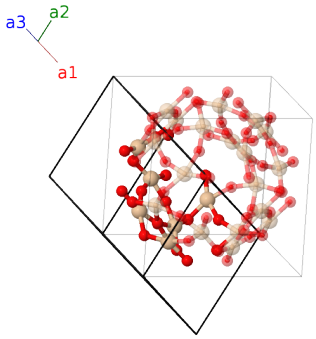


Prototype	O_2Si
AFLOW prototype label	A2B_cI72_211_hi_i-001
ICSD	170506
Pearson symbol	cI72
Space group number	211
Space group symbol	$I432$
AFLOW prototype command	`aflow --proto=A2B_cI72_211_hi_i-001 --params=`a, y_1, y_2, y_3

- This is a hypothetical cubic structure for SiO_2. We use the data from the 1_158.cif file provided in the supplementary information of (Foster, 2004).

Body-centered Cubic primitive vectors

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



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
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{14}}$	=	$-\left(2y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{15}}$	=	$\left(2y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{17}}$	=	$\left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{18}}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(2y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{19}}$	=	$\left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(2y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{20}}$	=	$-\left(y_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(y_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24i)	O II
$\mathbf{B_{21}}$	=	$-\left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24i)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	Si I

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.