Hypothetical Hexagonal SiO_2 Structure: A2B_hP36_177_j2lm_n-001

This structure originally had the label `A2B_hP36_177_j2lm_n`. Calls to that address will be redirected here.

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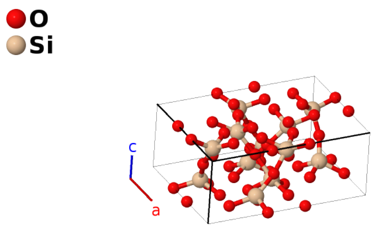
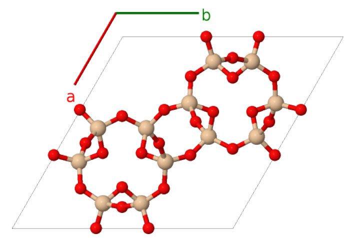
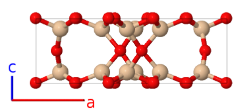
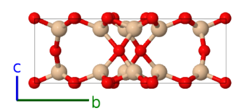
https://aflow.org/p/XNAH

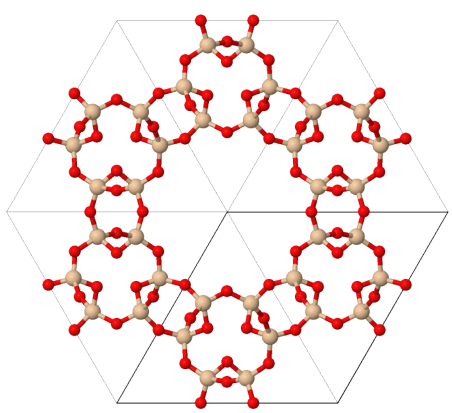
https://aflow.org/p/A2B_hP36_177_j2lm_n-001

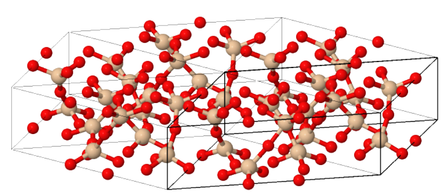












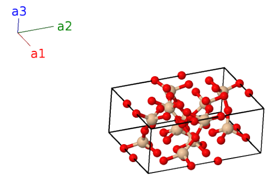
Prototype	O_2Si
AFLOW prototype label	A2B_hP36_177_j2lm_n-001
ICSD	170519
Pearson symbol	hP36
Space group number	177
Space group symbol	$P622$

AFLOW prototype command `aflow --proto=A2B_hP36_177_j2lm_n-001`
`--params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, y_5, z_5$

- This is a hypothetical hexagonal structure for SiO_2. We use the data from the 1_200.cif file provided in the supplementary information of (Foster, 2004).

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(6j)	O I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6j)	O I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(6j)	O I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_9}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{12}}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{14}}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{15}}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{17}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{18}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O III
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{20}}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{21}}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{23}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{24}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6m)	O IV
$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I

$\mathbf{B_{26}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{27}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{28}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{29}}$	=	$y_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{30}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{31}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{32}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{33}}$	=	$-x_5\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{34}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{35}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5 + 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{36}}$	=	$x_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(12n)	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.