# Hypothetical Hexagonal $SiO_2$ Structure: A2B_hP36_177_j2lm_n-001

This structure previously used the label(s) `A2B_hP36_177_j2lm_n`. Calls to these addresses will be redirected here.

Cite this page as:


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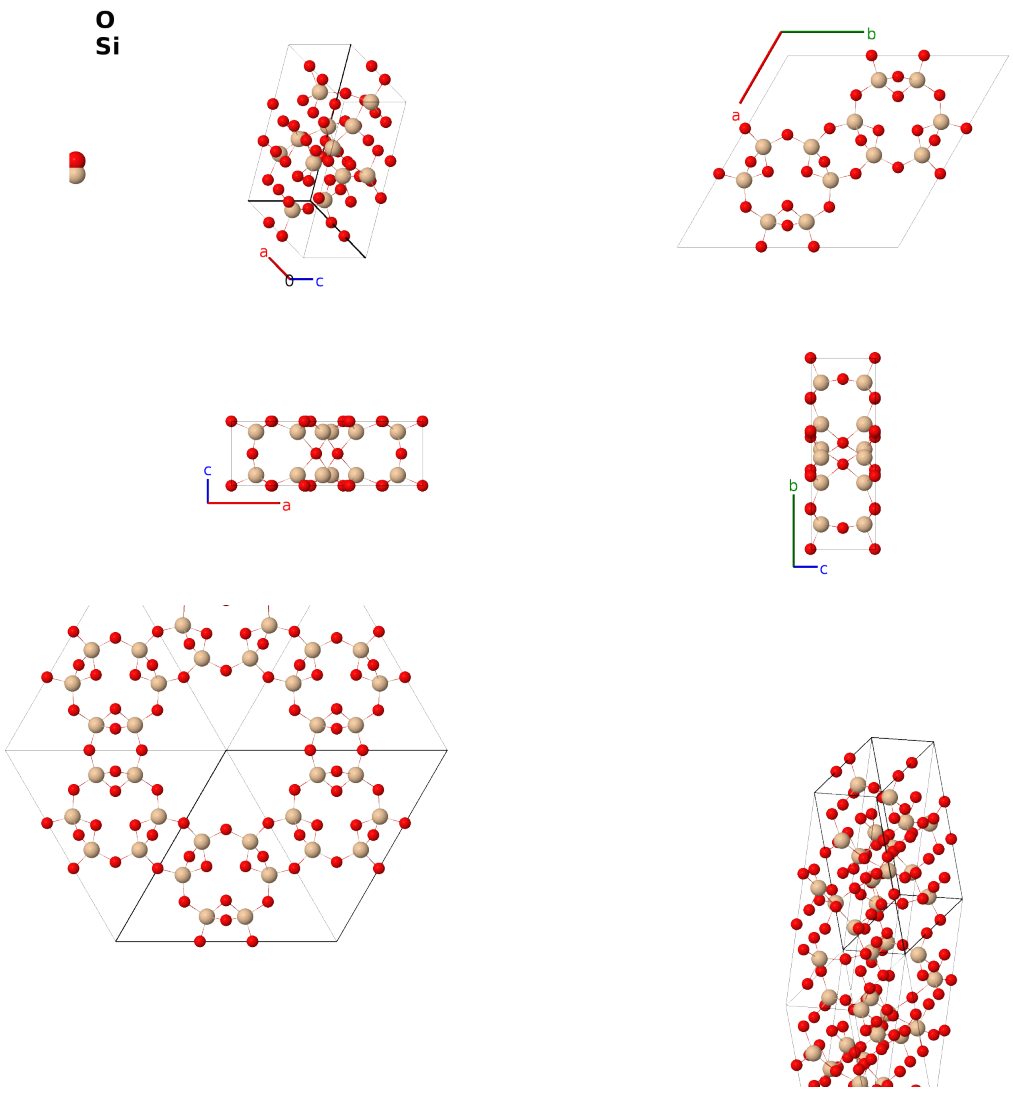
https://aflow.org/prototype-encyclopedia/XNAH

https://aflow.org/prototype-encyclopedia/A2B_hP36_177_j2lm_n-001




| | |
|---|---|
| **Prototype** | $O_2Si$ |
| **AFLOW prototype label** | A2B_hP36_177_j2lm_n-001 |
| **ICSD** | 170519 |

| | |
|---|---|
| **CCDC** | 1685991 |
| **Pearson symbol** | hP36 |
| **Space group number** | 177 |
| **Space group symbol** | $P622$ |
| **AFLOW prototype command** | `aflow --proto=A2B_hP36_177_j2lm_n-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, y_5, z_5$ |

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- 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).
- More information about other real and proposed $SiO_2$ and related structures can be found in our article on $SiO_2$ and $AlPO_4$.

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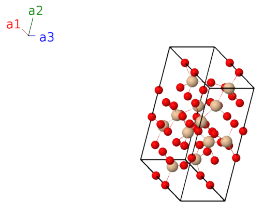
**Hexagonal primitive vectors**

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

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**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.


## 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