Keatite (SiO_2) Structure: A2B_tP36_96_3b_ab-001

This structure previously used the label(s) `A2B_tP36_96_3b_ab`. Calls to these addresses will be redirected here.

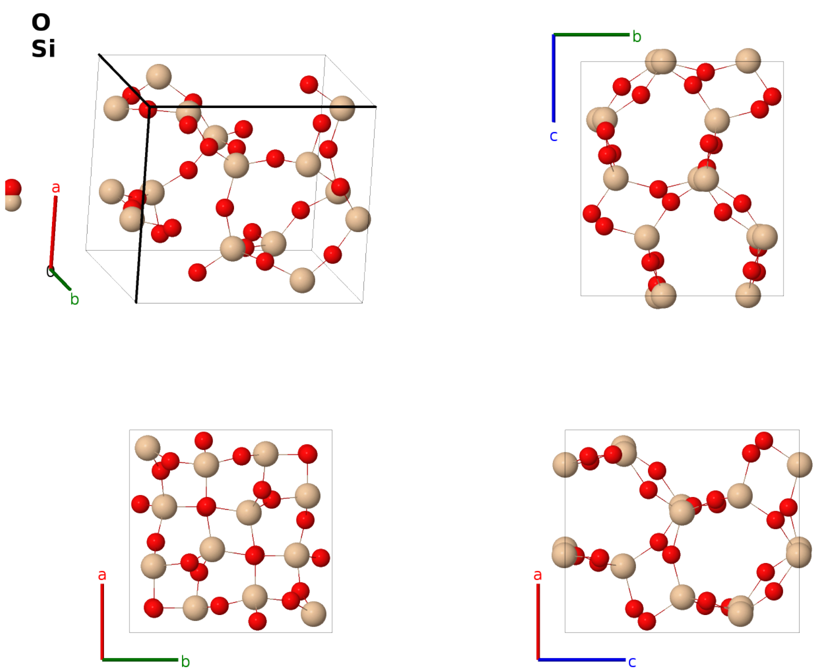
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/J0BF

https://aflow.org/prototype-encyclopedia/A2B_tP36_96_3b_ab-001

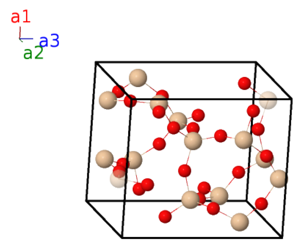


Prototype	O_2Si
AFLOW prototype label	A2B_tP36_96_3b_ab-001
Mineral name	keatite
ICSD	34889
CCDC	1607160
Pearson symbol	tP36
Space group number	96
Space group symbol	$P4_32_12$
AFLOW prototype command	`aflow --proto=A2B_tP36_96_3b_ab-001` `--params=`$a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

- Keatite was originally synthesized by Paul Keat in 1954 (Keat, 1954). All references, including (Wyckoff, 1963), (Shropshire, 1959) and (Demuth, 1999) note that keatite can exist in both space group $P4_12_12$ #92 and its enantiomorph $P4_32_12$ #96 and so is chiral, Sohncke Class II.
- Wyckoff uses the coordinates proposed by Shropshire and assumes the space group is $P4_12_12$. He then notes that one of the Si-O bonds in this structure is very long (3.69 Å), and is "so probable that there is something wrong either with the parameters as stated or the structure itself." If we use space group $P4_32_12$ while retaining Shropshire's coordinates we obtain a much more convincing structure, one that looks much like the structure in Shropshire's Fig. 3. For this reason we and the ICSD place this structure in $P4_32_12$, with the mirror image structure in $P4_12_12$.
- More information about other SiO_2 and related structures can be found in our article on SiO_2 and $AlPO_4$.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(4a)	Si I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_7}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_8}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_9}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{11}}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{15}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O II

$\mathbf{B_{16}}$	=	$\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_3+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_3-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_3+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O II
$\mathbf{B_{17}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_3-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(y_3+\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_3-\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O II
$\mathbf{B_{18}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_3-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(y_3-\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_3-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O II
$\mathbf{B_{19}}$	=	$y_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$ay_3\,\mathbf{\hat{x}}+ax_3\,\mathbf{\hat{y}}-cz_3\,\mathbf{\hat{z}}$	(8b)	O II
$\mathbf{B_{20}}$	=	$-y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\mathbf{\hat{x}}-ax_3\,\mathbf{\hat{y}}-c\left(z_3-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O II
$\mathbf{B_{21}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}}+ay_4\,\mathbf{\hat{y}}+cz_4\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}}-ay_4\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{23}}$	=	$-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_4+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_4+\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{24}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_4-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_4+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{25}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(y_4+\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_4-\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{26}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(y_4-\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{27}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{x}}+ax_4\,\mathbf{\hat{y}}-cz_4\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{28}}$	=	$-y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}}-ax_4\,\mathbf{\hat{y}}-c\left(z_4-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{29}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\mathbf{\hat{x}}+ay_5\,\mathbf{\hat{y}}+cz_5\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{30}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\mathbf{\hat{x}}-ay_5\,\mathbf{\hat{y}}+c\left(z_5+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{31}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(x_5+\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_5+\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{32}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(x_5-\frac{1}{2}\right)\,\mathbf{\hat{y}}+c\left(z_5+\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{33}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\mathbf{\hat{x}}+a\left(y_5+\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_5-\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{34}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(y_5-\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_5-\frac{1}{4}\right)\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{35}}$	=	$y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$ay_5\,\mathbf{\hat{x}}+ax_5\,\mathbf{\hat{y}}-cz_5\,\mathbf{\hat{z}}$	(8b)	Si II
$\mathbf{B_{36}}$	=	$-y_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\mathbf{\hat{x}}-ax_5\,\mathbf{\hat{y}}-c\left(z_5-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	Si II

References

[1] J. Shropshire, P. P. Keat, and P. A. Vaughan, *The crystal structure of keatite, a new form of silica*, Z. Krystallogr. **112**, 409–413 (1959), doi:10.1524/zkri.1959.112.jg.409.

[2] P. P. Keat, *A New Crystalline Silica*, Science **120**, 328–330 (1954), doi:10.1126/science.120.3113.328.

[3] R. W. G. Wyckoff, *Crystal Structure*, vol. 1 (Wiley, 1963), 2^{nd} edn.

Found in

[1] T. Demuth, Y. Jeanvoine, J. Hafner, and J. G. Ángyán, *Polymorphism in silica studied in the local density and generalized-gradient approximations*, J. Phys.: Condens. Matter **11**, 3833–3874 (1999), doi:10.1088/0953-8984/11/19/306.

First cited in

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**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017