Keatite (SiO_2) Structure: A2B_tP36_96_3b_ab-001

This structure originally had the label `A2B_tP36_96_3b_ab`. Calls to that address will be redirected here.

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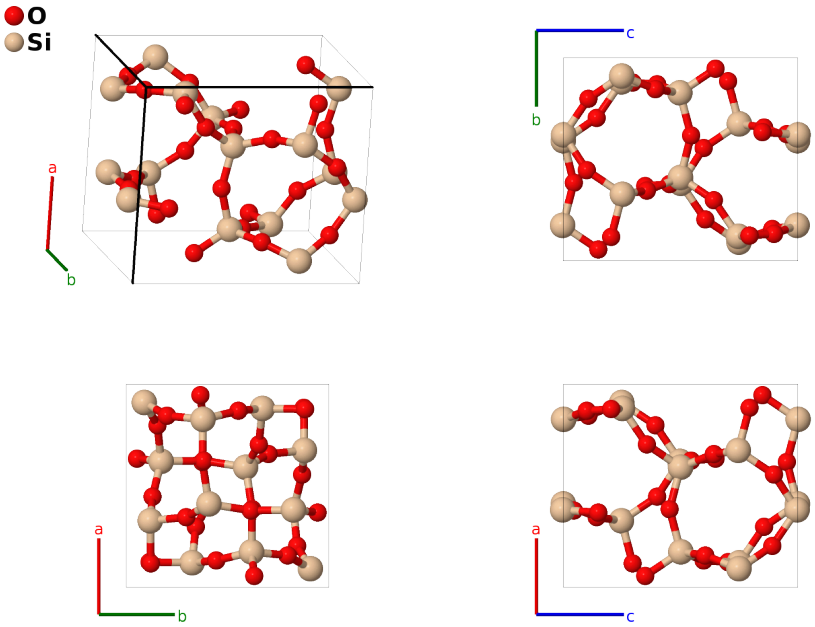
https://aflow.org/p/J0BF

https://aflow.org/p/A2B_tP36_96_3b_ab-001

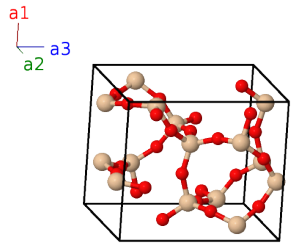


Prototype	O_2Si
AFLOW prototype label	A2B_tP36_96_3b_ab-001
Mineral name	keatite
ICSD	34889
Pearson symbol	tP36
Space group number	96
Space group symbol	$P4_32_12$
AFLOW prototype command	`aflow --proto=A2B_tP36_96_3b_ab-001 --params=`$a, c/a, x_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5,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

- 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. 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 place this structure in $P4_32_12$.

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
$\mathbf{B_{16}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{17}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{18}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{19}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{20}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O II
$\mathbf{B_{21}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{22}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O III

$\mathbf{B_{23}}$	=	$-\left(y_4-\frac{1}{2}\right)\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\mathbf{a}_2+\left(z_4+\frac{3}{4}\right)\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{3}{4}\right)\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{24}}$	=	$\left(y_4+\frac{1}{2}\right)\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\mathbf{a}_2+\left(z_4+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{25}}$	=	$-\left(x_4-\frac{1}{2}\right)\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\mathbf{a}_2-\left(z_4-\frac{3}{4}\right)\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{3}{4}\right)\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{26}}$	=	$\left(x_4+\frac{1}{2}\right)\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\mathbf{a}_2-\left(z_4-\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{27}}$	=	$y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{28}}$	=	$-y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{29}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{30}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{31}}$	=	$-\left(y_5-\frac{1}{2}\right)\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\mathbf{a}_2+\left(z_5+\frac{3}{4}\right)\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_5+\frac{3}{4}\right)\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{32}}$	=	$\left(y_5+\frac{1}{2}\right)\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\mathbf{a}_2+\left(z_5+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{33}}$	=	$-\left(x_5-\frac{1}{2}\right)\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\mathbf{a}_2-\left(z_5-\frac{3}{4}\right)\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{3}{4}\right)\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{34}}$	=	$\left(x_5+\frac{1}{2}\right)\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\mathbf{a}_2-\left(z_5-\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{35}}$	=	$y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{36}}$	=	$-y_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}}$	(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] R. W. G. Wyckoff, *Crystal Structure*, vol. 1 (Wiley, 1963), 2^{nd} edn.

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