Si_{46} Clathrate Structure: A_cP46_223_cik-001

This structure originally had the label `A_cP46_223_dik`. Calls to that address will be redirected here.

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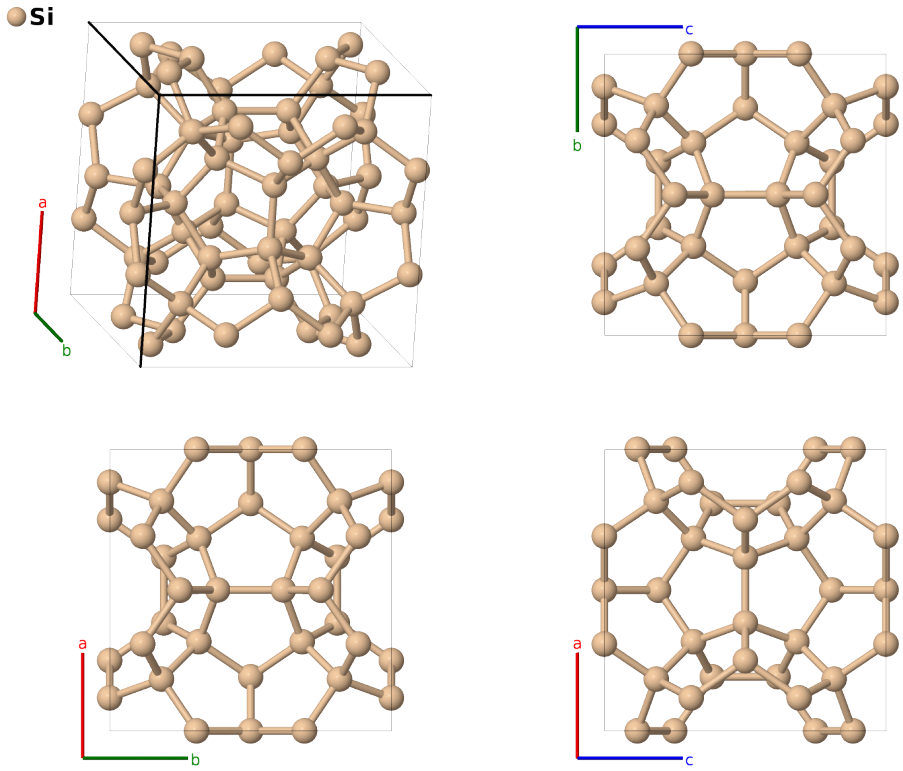
https://aflow.org/p/VFEB

https://aflow.org/p/A_cP46_223_cik-001



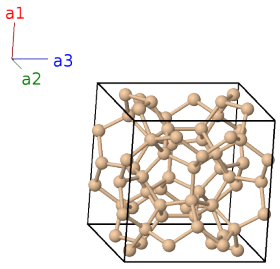
Prototype	Si
AFLOW prototype label	A_cP46_223_cik-001
Mineral name	clathrate
ICSD	none
Pearson symbol	cP46
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	`aflow --proto=A_cP46_223_cik-001 --params=`a, x_2, y_3, z_3

- Silicon clathrates are open structures of pentagonal dodecahedra connected so that all of the silicon atoms have sp3 bonding. In nature these structures are stabilized by alkali impurity atoms. This structure and the Si_{34} structure are proposed "pure" silicon clathrate structures.

- For more information about these structures and their possible stability, see (Adams, 1994).
- This is a theoretical description of a possible silicon clathrate crystal. (Pauling, 1952) showed that the oxygen atoms in $Cl_2{\cdot}10H_2O$ (ICSD 29340) have similar positions to the chlorine atoms in this structure.

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(6c)	Si I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(6c)	Si I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	Si I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{11}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{12}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{13}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{14}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{15}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{16}}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{17}}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{18}}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{19}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{20}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II

$\mathbf{B_{21}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{22}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16i)	Si II
$\mathbf{B_{23}}$	=	$y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}}+az_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{24}}$	=	$-y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}}+az_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{25}}$	=	$y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}}-az_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{26}}$	=	$-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}}-az_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{27}}$	=	$z_3\,\mathbf{a}_1+y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{28}}$	=	$z_3\,\mathbf{a}_1-y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{29}}$	=	$-z_3\,\mathbf{a}_1+y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{30}}$	=	$-z_3\,\mathbf{a}_1-y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{31}}$	=	$y_3\,\mathbf{a}_1+z_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}$	(24k)	Si III
$\mathbf{B_{32}}$	=	$-y_3\,\mathbf{a}_1+z_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}}+az_3\,\hat{\mathbf{y}}$	(24k)	Si III
$\mathbf{B_{33}}$	=	$y_3\,\mathbf{a}_1-z_3\,\mathbf{a}_2$	=	$ay_3\,\hat{\mathbf{x}}-az_3\,\hat{\mathbf{y}}$	(24k)	Si III
$\mathbf{B_{34}}$	=	$-y_3\,\mathbf{a}_1-z_3\,\mathbf{a}_2$	=	$-ay_3\,\hat{\mathbf{x}}-az_3\,\hat{\mathbf{y}}$	(24k)	Si III
$\mathbf{B_{35}}$	=	$\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{36}}$	=	$-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{37}}$	=	$\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{38}}$	=	$-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{39}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{40}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{41}}$	=	$\frac{1}{2}\,\mathbf{a}_1-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{42}}$	=	$\frac{1}{2}\,\mathbf{a}_1-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{43}}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{44}}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{45}}$	=	$-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24k)	Si III
$\mathbf{B_{46}}$	=	$-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}a\,\hat{\mathbf{z}}$	(24k)	Si III

References

[1] G. B. Adams, M. O'Keeffe, A. A. Demkov, O. F. Sankey, and Y.-M. Huang, *Wide-band-gap Si in open fourfold-coordinated clathrate structures*, Phys. Rev. B **49**, 8048–8053 (1994), doi:10.1103/PhysRevB.49.8048.

[2] L. Pauling and R. E. Marsh, *The Structure of Chlorine Hydrate*, Proceedings of the National Academy of Sciences **38**, 112–118 (1952), doi:10.1073/pnas.38.2.11.