Si_{34} Clathrate Structure: A_cF136_227_aeg-001

This structure originally had the label `A_cF136_227_aeg`. Calls to that address will be redirected here.

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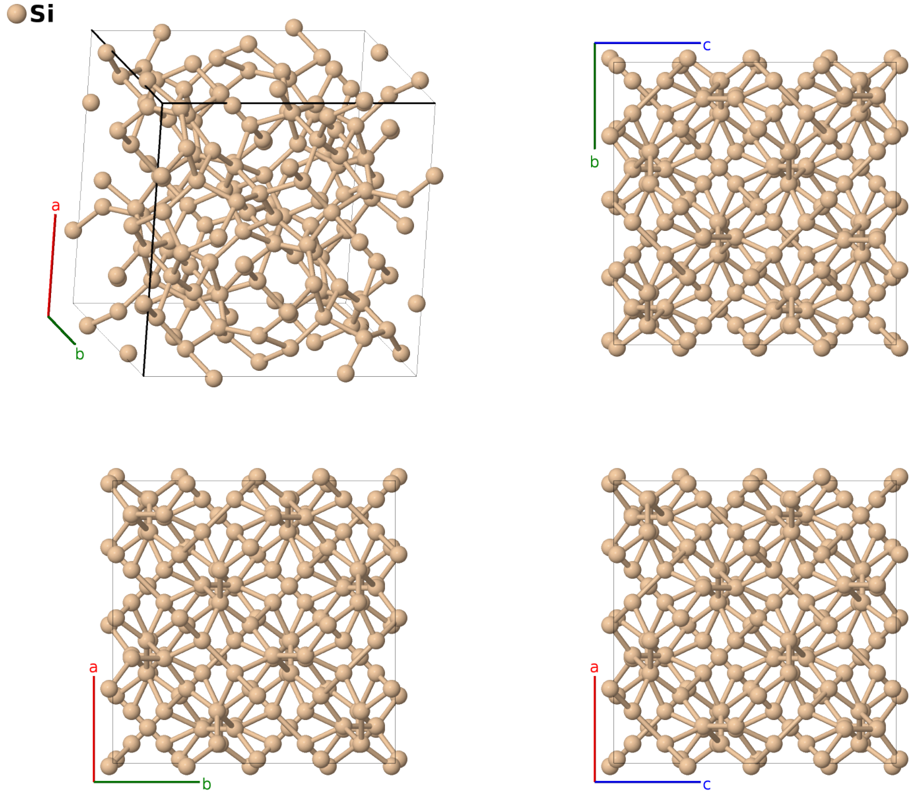
https://aflow.org/p/U115

https://aflow.org/p/A_cF136_227_aeg-001



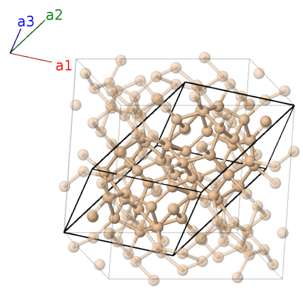
Prototype	Si
AFLOW prototype label	A_cF136_227_aeg-001
ICSD	none
Pearson symbol	cF136
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A_cF136_227_aeg-001` `--params=`a, x_2, x_3, z_3

Other compounds with this structure
Ge (high pressure)

- 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_{46} structure are proposed “pure” silicon clathrate structures.
- For more information about these structures and their possible stability, see (Adams, 1994).
- See (Gryko, 2000) for a possible experimental realization of this structure ($Si_{34}Na_x$, were x is very small).
- We have used the fact that all vectors of the form $(0, \pm a/2, \pm a/2)$, $(\pm a/2, 0, \pm a/2)$, and $(\pm a/2, \pm a/2, 0)$ are primitive vectors of the face-centered cubic lattice to simplify the positions of some atoms in both lattice and Cartesian coordinates.
- (Dong, 1999) study a similar, but not identical structure (ICSD 56271), and (Schwarz, 2008) find a similar high-pressure phase of germanium (ICSD 245948).

Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Si I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Si I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - \left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_6}$	=	$-\left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + \left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_{10}}$	=	$\left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Si II
$\mathbf{B_{11}}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96g)	Si III
$\mathbf{B_{12}}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96g)	Si III
$\mathbf{B_{13}}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Si III
$\mathbf{B_{14}}$	=	$-\left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Si III
$\mathbf{B_{15}}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96g)	Si III
$\mathbf{B_{16}}$	=	$-\left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(96g)	Si III

$\mathbf{B_{17}}$	=	$z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{18}}$	=	$z_3\,\mathbf{a}_1 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$-a\left(z_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + a x_3\,\mathbf{\hat{y}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{19}}$	=	$z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a x_3\,\mathbf{\hat{x}} + a z_3\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{20}}$	=	$z_3\,\mathbf{a}_1 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} + a z_3\,\mathbf{\hat{y}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{21}}$	=	$-\left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$a x_3\,\mathbf{\hat{x}} - a\left(z_3 - \frac{1}{4}\right)\,\mathbf{\hat{y}} - a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{22}}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(2x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\mathbf{\hat{x}} - a\left(z_3 - \frac{1}{4}\right)\,\mathbf{\hat{y}} + a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{23}}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - a z_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{24}}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3$	=	$-a x_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} - a z_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{25}}$	=	$-(2x_3 - z_3)\,\mathbf{a}_1 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} + a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{26}}$	=	$\left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a x_3\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{27}}$	=	$-(2x_3 - z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} + a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{28}}$	=	$\left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3$	=	$-a x_3\,\mathbf{\hat{x}} + a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{29}}$	=	$-z_3\,\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a x_3\,\mathbf{\hat{x}} - a z_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{30}}$	=	$-z_3\,\mathbf{a}_1 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} - a z_3\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{31}}$	=	$-z_3\,\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{32}}$	=	$-z_3\,\mathbf{a}_1 + \left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3$	=	$a\left(z_3 + \frac{1}{4}\right)\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{33}}$	=	$\left(2x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a z_3\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{y}} + a\left(x_3 + \frac{1}{4}\right)\,\mathbf{\hat{z}}$	(96g)	Si III
$\mathbf{B_{34}}$	=	$-(2x_3 - z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a z_3\,\mathbf{\hat{x}} - a x_3\,\mathbf{\hat{y}} - a x_3\,\mathbf{\hat{z}}$	(96g)	Si III

References

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