Si_{34} Clathrate Structure: A_cF136_227_aeg-001

This structure previously used the label(s) `A_cF136_227_aeg`. 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.

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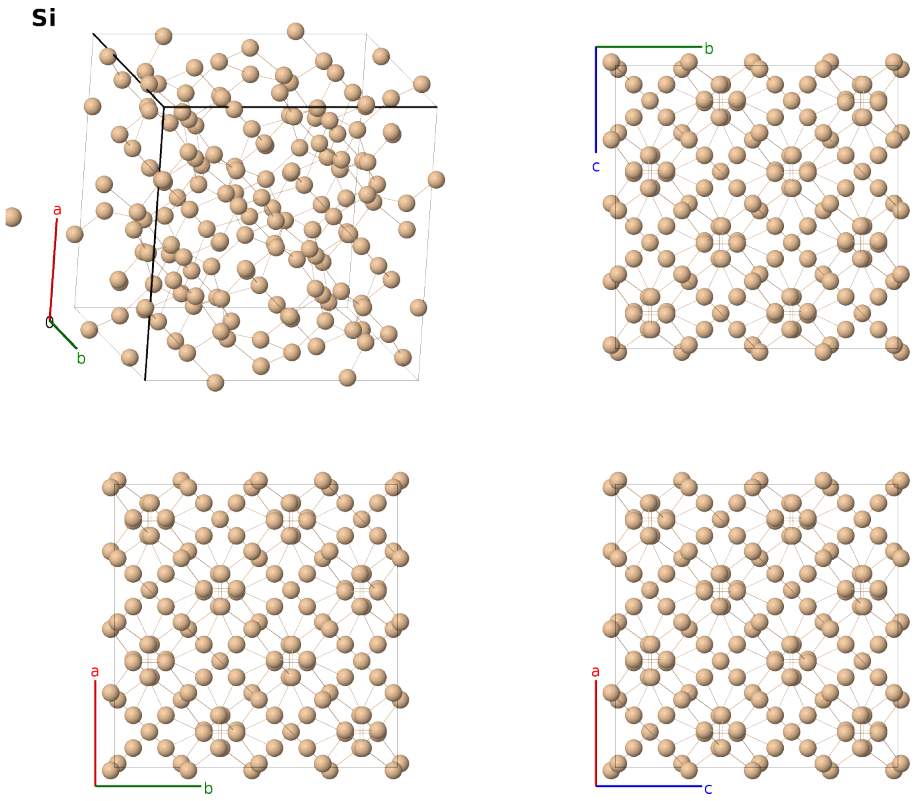
https://aflow.org/prototype-encyclopedia/U115

https://aflow.org/prototype-encyclopedia/A_cF136_227_aeg-001



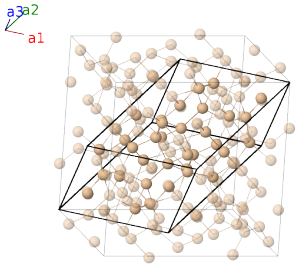
Prototype	Si
AFLOW prototype label	A_cF136_227_aeg-001
Pearson symbol	cF136
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A_cF136_227_aeg-001 --params=`a, x_2, x_3, z_3

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
$\mathbf{B_{11}}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2z_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(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

$$\mathbf{B_{17}} = z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 - \left(2x_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{18}} = z_3\,\mathbf{a}_1 - \left(2x_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3 = -a\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{19}} = z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{20}} = z_3\,\mathbf{a}_1 - \left(2x_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_3\,\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{21}} = -\left(2x_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}} - a\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{22}} = (2x_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(2x_3 + z_3 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(z_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{23}} = -z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{24}} = -z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{25}} = -(2x_3 - z_3)\,\mathbf{a}_1 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_3\,\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{26}} = \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{27}} = -(2x_3 - z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{28}} = \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - z_3\,\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} + a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{29}} = -z_3\,\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{30}} = -z_3\,\mathbf{a}_1 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_3\,\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{31}} = -z_3\,\mathbf{a}_1 - (2x_3 - z_3)\,\mathbf{a}_2 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{32}} = -z_3\,\mathbf{a}_1 + \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_2 - (2x_3 - z_3)\,\mathbf{a}_3 = a\left(z_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{33}} = \left(2x_3 + z_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - z_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -az_3\,\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

$$\mathbf{B_{34}} = -(2x_3 - z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \quad (96g) \quad \text{Si III}$$

References

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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