Si_{24} Clathrate Structure: A_oC24_63_3f-001

This structure originally had the label `A_oC24_63_3f`. Calls to that address will be redirected here.

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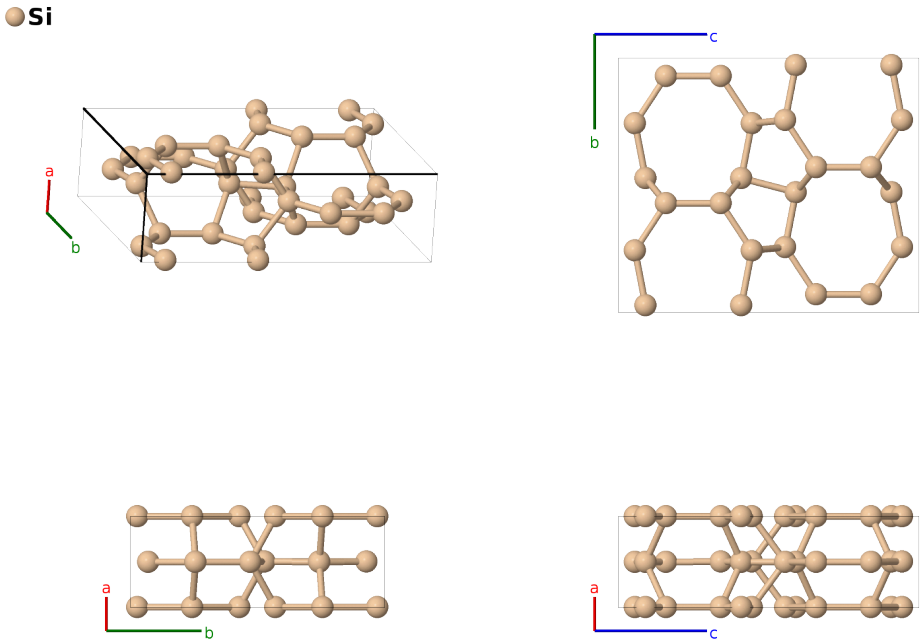
https://aflow.org/p/TPXT

https://aflow.org/p/A_oC24_63_3f-001



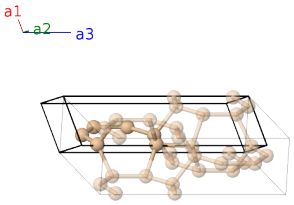
Prototype	Si_{24}
AFLOW prototype label	A_oC24_63_3f-001
Mineral name	clathrate
ICSD	291479
Pearson symbol	oC24
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A_oC24_63_3f-001 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3$

- Unlike the Si_{34} and Si_{46} clathrates, this is an experimentally determined structure, prepared by removing sodium atoms from an Na_4Si_{24} predecessor.

- There is no consistency in the naming of these clathrate structures. Si_{34} and Si_{46} were named by their authors based on the size of the primitive unit cell. Here (Kim, 2015) has chosen to name the structure based on the size of the conventional cell. For now, at least, we will follow the authors' naming schemes for these structures.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_4}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8f)	Si I
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_6}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_7}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8f)	Si II
$\mathbf{B_9}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Si III
$\mathbf{B_{10}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si III
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Si III
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Si III

References

[1] D. Y. Kim, S. Stefanoski, O. O. Kurakevych, and T. A. Strobel, *Synthesis of an open-framework allotrope of silicon*, Nat. Mater. **14**, 169–173 (2015), doi:10.1038/NMAT4140.