"ST12" Structure of Si: A_tP12_96_ab-001

This structure originally had the label `A_tP12_96_ab`. Calls to that address will be redirected here.

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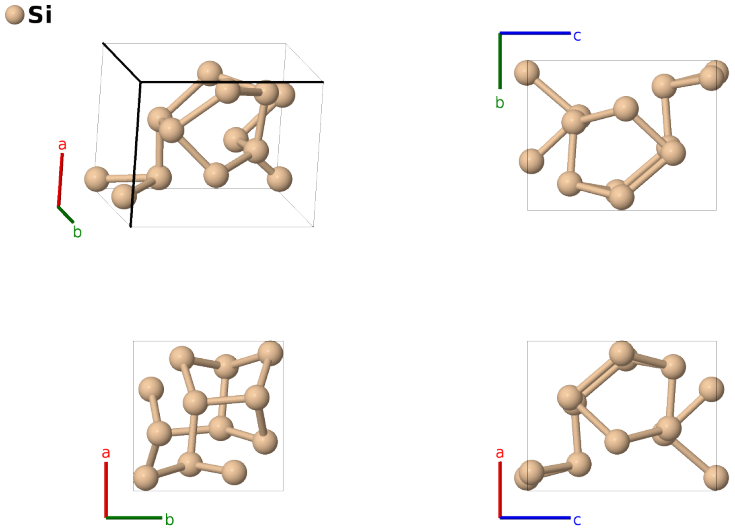
https://aflow.org/p/YUU3

https://aflow.org/p/A_tP12_96_ab-001



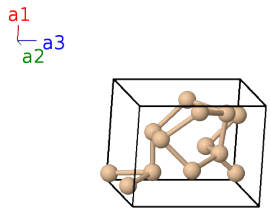
Prototype	Si
AFLOW prototype label	A_tP12_96_ab-001
ICSD	16954
Pearson symbol	tP12
Space group number	96
Space group symbol	$P4_32_12$
AFLOW prototype command	`aflow --proto=A_tP12_96_ab-001 --params=`$a, c/a, x_1, x_2, y_2, z_2$

Other compounds with this structure
γ-Ge

- This is a tetragonally bonded structure which packs more efficiently than diamond. It is seen experimentally in some silicon and germanium samples and is a staple for testing silicon potentials and first-principles calculations. The structure shown here is taken from the calculations in (Crain, 1994), but the ICSD entry is an experimental entry for germanium (Bundy, 1963).

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)	Si II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_7}$	=	$-\left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_8}$	=	$\left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_9}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{11}}$	=	$y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	Si II

References

[1] J. Crain, S. J. Clark, G. J. Ackland, M. C. Payne, V. Milman, P. D. Hatton, and B. J. Reid, *Theoretical study of high-density phases of covalent semiconductors. I.* Ab initio treatment, Phys. Rev. B **49**, 5329–5340 (1994), doi:10.1103/PhysRevB.49.5329.

[2] F. P. Bundy and J. S. Kasper, *A New Dense Form of Solid Germanium*, Science **139**, 340–341 (1963), doi:10.1126/science.139.3552.340.