

Hypothetical BCT5 Si Structure: A_tI4_139_e-001

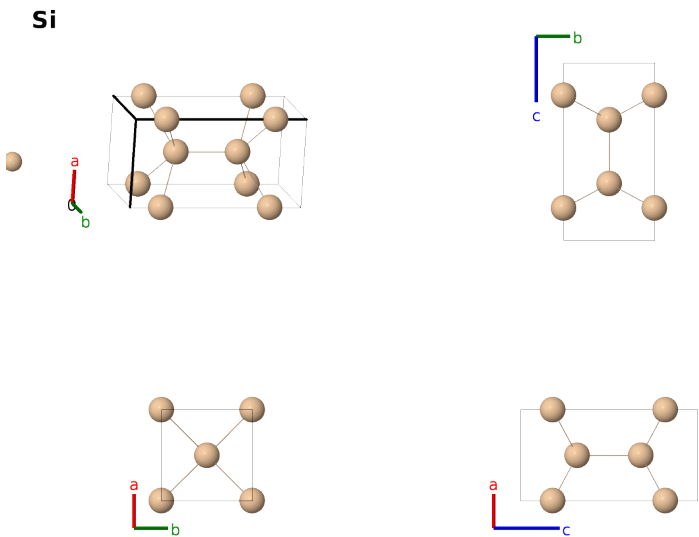
This structure previously used the label(s) **A.tI4.139.e**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/ZSDQ>

https://aflow.org/prototype-encyclopedia/A_tI4_139_e-001

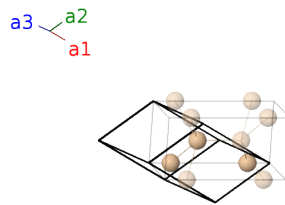


Prototype	Si
AFLOW prototype label	A.tI4_139_e-001
Pearson symbol	tI4
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A_tI4_139_e-001 --params=a, c/a, z₁</code>

- The bct5 structure is a tetragonal analog of the diamond (*A4*) structure, with 5-fold coordination. It was proposed in (Boyer, 1991) as a low-energy metastable phase of silicon, based on first-principles calculations and model potentials. (Gerbig, 2012) found evidence of this structure in strained silicon.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2$	$=$	$cz_1 \hat{\mathbf{z}}$	(4e) Si I
$\mathbf{B}_2$	$=$	$-z_1 \mathbf{a}_1 - z_1 \mathbf{a}_2$	$=$	$-cz_1 \hat{\mathbf{z}}$	(4e) Si I

References

- [1] L. L. Boyer, E. Kaxiras, J. L. Feldman, J. Q. Broughton, and M. J. Mehl, *New low-energy crystal structure for silicon*, Phys. Rev. Lett. **67**, 715–718 (1991), doi:10.1103/PhysRevLett.67.715.
- [2] Y. B. Gerbig, C. A. Michaels, A. M. Forster, and R. F. Cook, *In situ observation of the indentation-induced phase transformation of silicon thin films*, Phys. Rev. B **85**, 104102 (2012), doi:10.1103/PhysRevB.85.104102.

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