

BC8 (Si) Structure: A_cI16_206_c-001

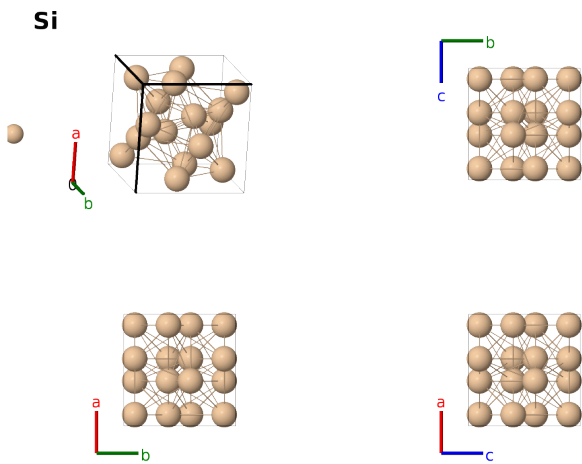
This structure previously used the label(s) **A_cI16_206_c**. Calls to these addresses will be redirected here.

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.

<https://aflow.org/prototype-encyclopedia/83MZ>

https://aflow.org/prototype-encyclopedia/A_cI16_206_c-001



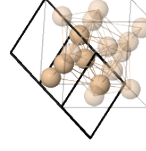
Prototype	Si
AFLOW prototype label	A_cI16_206_c-001
Pearson symbol	cI16
Space group number	206
Space group symbol	$Ia\bar{3}$
AFLOW prototype command	<code>aflow --proto=A_cI16_206_c-001</code> <code>--params=a, x₁</code>

- This is a tetragonally bonded structure which packs more efficiently than diamond. See (Crain, 1995) and references therein. The reference compound chosen here, found in (Wentorf, 1963), is stable in the range 11-16 GPa.

Body-centered Cubic primitive vectors

a3
a2
a1

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (2x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_3$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_4$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_5$	$= -2x_1 \mathbf{a}_1 - 2x_1 \mathbf{a}_2 - 2x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + (2x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_7$	$= (2x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B}_8$	$= (2x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(16c)	Si I

References

- [1] J. R. H. Wentorf and J. S. Kasper, *Two New Forms of Silicon*, Science **139**, 338–339 (1963), doi:10.1126/science.139.3552.338.b.
- [2] 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.

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