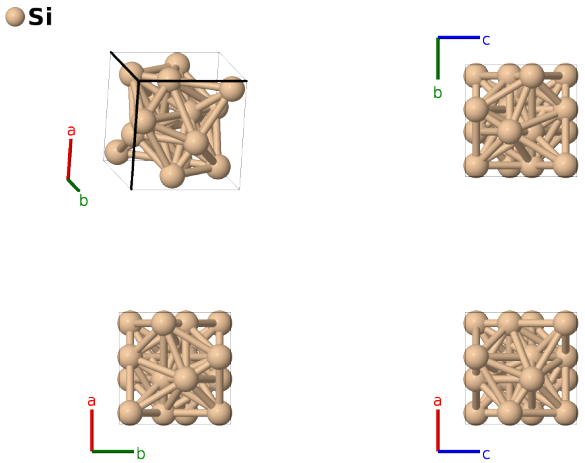
BC8 (Si) Structure: A_cI16_206_c-001

This structure originally had the label `A_cI16_206_c`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. 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

https://aflow.org/p/83MZ

https://aflow.org/p/A_cI16_206_c-001

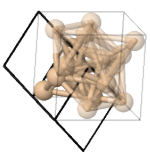


Prototype	Si
AFLOW prototype label	A_cI16_206_c-001
ICSD	none
Pearson symbol	cI16
Space group number	206
Space group symbol	$Ia\bar{3}$
AFLOW prototype command	`aflow --proto=A_cI16_206_c-001 --params=`a, x_1

- 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

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}a\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B_3}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B_4}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B_7}$	=	$\left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16c)	Si I
$\mathbf{B_8}$	=	$\left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.