

Moissanite-4H SiC (*B5*) Structure: AB_hP8_186_ab_ab-001

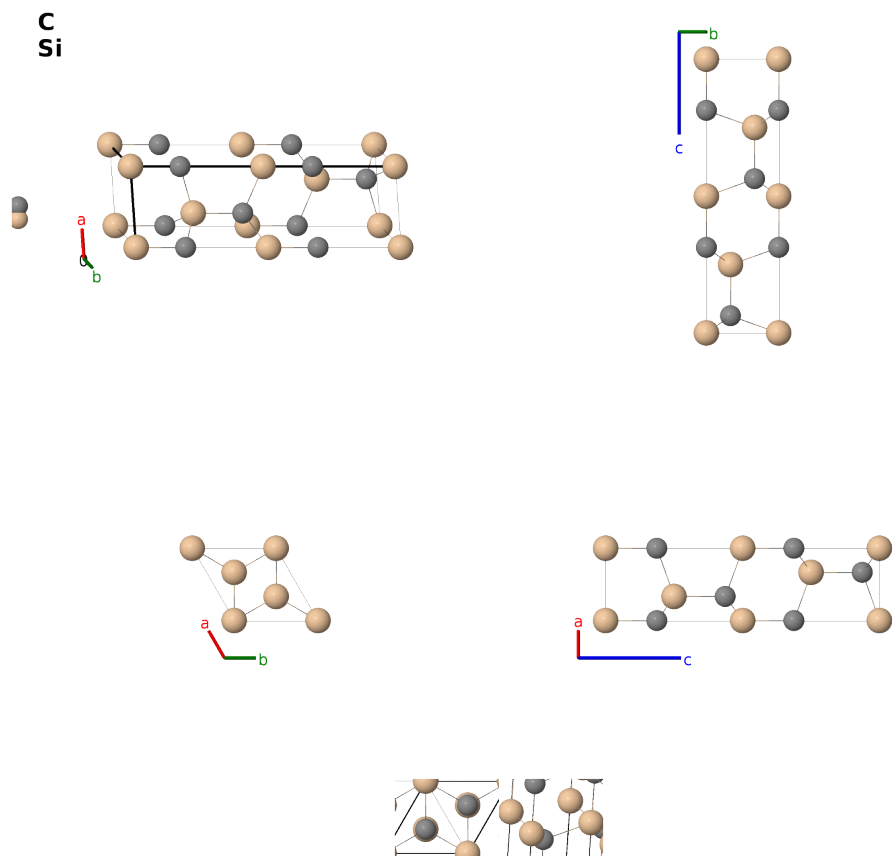
This structure previously used the label(s) **AB_hP8_186_ab_ab**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/FSH2>

https://aflow.org/prototype-encyclopedia/AB_hP8_186_ab_ab-001



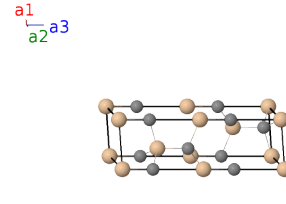
Prototype	CSi
AFLOW prototype label	AB_hP8_186_ab_ab-001
<i>Strukturbericht</i> designation	<i>B5</i>
Mineral name	moissanite
ICSD	24170
CCDC	1600218
Pearson symbol	hP8
Space group number	186

Space group symbol $P6_3mc$

AFLOW prototype command `aflow --proto=AB_hP8_186_ab_ab-001`
`--params=a, c/a, z1, z2, z3, z4`

- This is one possible stacking (ABAC) for tetrahedral structures. Compare this to zincblende ($B3$, ABCABC), wurtzite ($B4$, ABABAB), 6H (ABCACB), and 9R (ABCBCACAB). The 4H refers to the fact that there are 4 CSi dimers in a hexagonal unit cell. Zincblende is denoted 3C and wurtzite is 2H. This structure is related to the α -La ($A3'$) structure in the same way that zincblende ($B3$) is related to the fcc ($A1$) lattice.
- Space group $P6_3$ #186 is polar, so there is no fixed origin for the z axis. In the pictures here we take $z_2 = 0$ for the silicon (2a) site.
- We did not find an ICSD or CCDC entry for (Bauer, 2001). The ICSD entry here is from (Thibault, 1944).

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_2$	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_3$	$z_2 \mathbf{a}_3$	=	$cz_2 \hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B}_4$	$(z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B}_5$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	C II
$\mathbf{B}_6$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	C II
$\mathbf{B}_7$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Si II
$\mathbf{B}_8$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Si II

References

- [1] A. Bauer, P. Reischauer, J. Kräusslich, N. Schell, W. Matz, and K. Goetz, *Structure refinement of the silicon carbide polytypes 4H and 6H: unambiguous determination of the refinement parameters*, Acta Crystallogr. Sect. A **57**, 60–67 (2001), doi:10.1107/S0108767300012915.
- [2] N. W. Thibault, *Morphological and Structural Crystallography and Optical Properties of Silicon Carbide (SiC) Part II: Structural Crystallography and Optical Properties*, Am. Mineral. **29**, 327–362 (1944).
- [3] G. C. Capitani, S. D. Pierro, and G. Tempesta, *The 6H-SiC structure model: Further refinement from SCXRD data from a terrestrial moissanite*, Am. Mineral. **92**, 403–407 (2007).

First cited in

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