

Moissanite-6H SiC (*B6*) Structure: AB_hP12_186_a2b_a2b-001

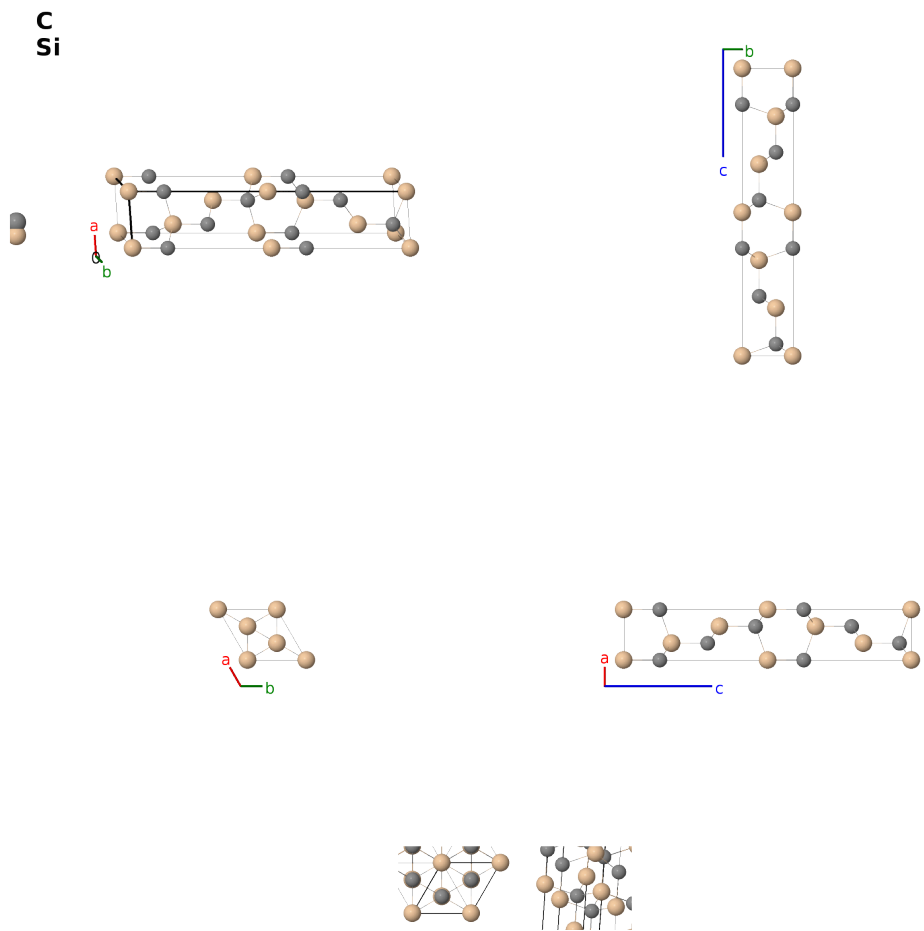
This structure previously used the label(s) **AB_hP12_186_a2b_a2b**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB_hP12_186_a2b_a2b-001



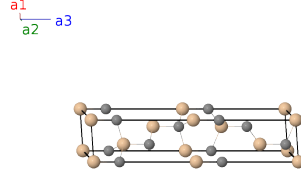
Prototype	SiC
AFLOW prototype label	AB_hP12_186_a2b_a2b-001
<i>Strukturbericht</i> designation	<i>B6</i>
Mineral name	moissanite
ICSD	156190
CCDC	1672758

Pearson symbol	hP12
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	<code>aflow --proto=AB_hP12_186_a2b_a2b-001</code> <code>--params=a, c/a, z₁, z₂, z₃, z₄, z₅, z₆</code>

- This is an alternate stacking (ABCACB) for tetrahedral structures. Compare this to zincblende ($B3$, ABCABC), moissanite-4H ($B5$, ABAC), and wurtzite ($B4$, ABABAB).
- The 6H refers to the fact that there are 6 CSi dimers in a hexagonal unit cell. Zincblende is denoted 3C, and wurtzite is 2H.
- Without loss of generality, we can take any of the z_i to be zero. Here we take $z_2 = 0$ for the silicon (2a) site.
- The ICSD entry is from the later work of (Capitani, 2007).

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(2b)	C III
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	C III
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(2b)	Si II
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Si II
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(2b)	Si III
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Si III

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).

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