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

This structure originally had the label `AB_hP8_186_ab_ab`. Calls to that address will be redirected here.

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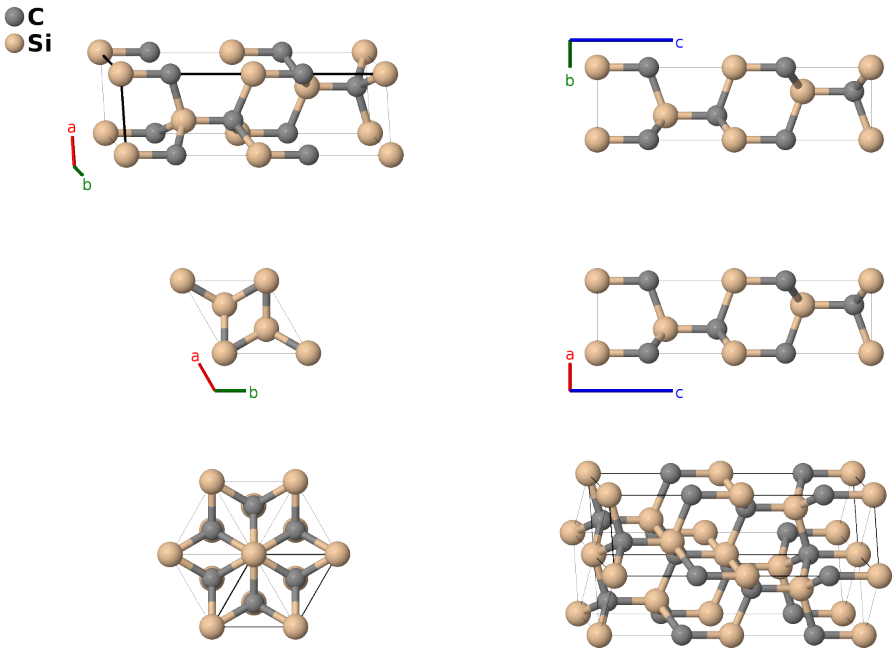
https://aflow.org/p/FSH2

https://aflow.org/p/AB_hP8_186_ab_ab-001



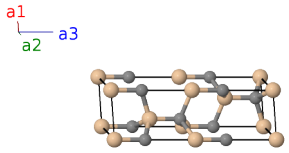
Prototype	CSi
AFLOW prototype label	AB_hP8_186_ab_ab-001
***Strukturbericht* designation**	$B5$
Mineral name	moissanite
ICSD	24170
Pearson symbol	hP8
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=AB_hP8_186_ab_ab-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

- 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 $P6_3mc$ #186 allows us to take any one of the z_i to be zero. 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

$$\begin{aligned} \mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}} \end{aligned}$$



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
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Si I
$\mathbf{B_4}$	=	$\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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).