

Moissanite-15R (SiC, *B7*) Structure: AB_hR10_160_5a_5a-001

This structure previously used the label(s) **AB_hR10_160_5a_5a**. 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. Osos, 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/KX5G>

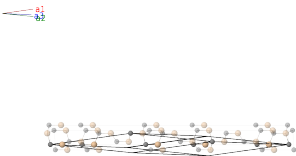
https://aflow.org/prototype-encyclopedia/AB_hR10_160_5a_5a-001

Prototype	CSi
AFLOW prototype label	AB_hR10_160_5a_5a-001
<i>Strukturbericht</i> designation	<i>B7</i>
Mineral name	moissanite
ICSD	24168
CCDC	1600216
Pearson symbol	hR10
Space group number	160
Space group symbol	<i>R3m</i>
AFLOW prototype command	<code>aflow --proto=AB_hR10_160_5a_5a-001</code> <code>--params=<i>a</i>, <i>c</i>/<i>a</i>, <i>x</i>₁, <i>x</i>₂, <i>x</i>₃, <i>x</i>₄, <i>x</i>₅, <i>x</i>₆, <i>x</i>₇, <i>x</i>₈, <i>x</i>₉, <i>x</i>₁₀</code>

- (Ewald, 1931) and (Thibault, 1944) both call this structure “Type I α -silicon carbide.” The atomic positions are not well determined. We follow (Thibault, 1944) and assume that the (0001) planes of carbon atoms are equally spaced, and that each carbon atom has a silicon atom at a distance of $c/20$ along the z axis.

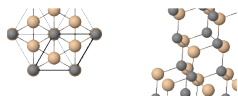
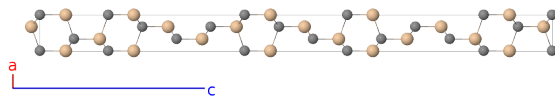
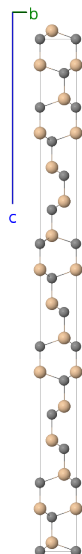
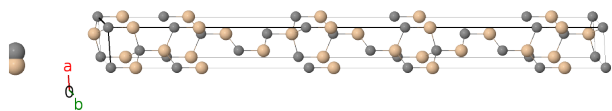
Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

C
Si



	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a) C I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a) C II
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(1a) C III
$\mathbf{B}_4$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(1a) C IV
$\mathbf{B}_5$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$cx_5 \hat{\mathbf{z}}$	(1a) C V
$\mathbf{B}_6$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$cx_6 \hat{\mathbf{z}}$	(1a) Si I
$\mathbf{B}_7$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$cx_7 \hat{\mathbf{z}}$	(1a) Si II
$\mathbf{B}_8$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$cx_8 \hat{\mathbf{z}}$	(1a) Si III
$\mathbf{B}_9$	$=$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$cx_9 \hat{\mathbf{z}}$	(1a) Si IV
$\mathbf{B}_{10}$	$=$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$cx_{10} \hat{\mathbf{z}}$	(1a) Si V

References

- [1] 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).
- [2] P. P. Ewald and K. Herrman, eds., *Strukturbericht 1913-1928*, vol. I (Akademische Verlagsgesellschaft M. B. H., 1931).

Found in

- [1] G. L. Harris, ed., *Properties of Silicon Carbide* (INSPEC, London, 1995).

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043