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

This structure originally had the label `AB_hR10_160_5a_5a`. Calls to that address will be redirected here.

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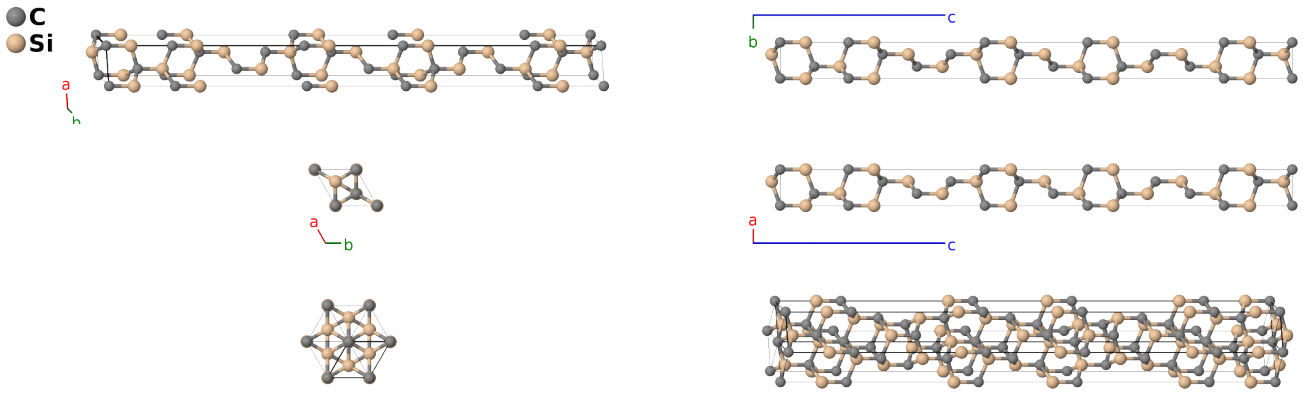
https://aflow.org/p/KX5G

https://aflow.org/p/AB_hR10_160_5a_5a-001

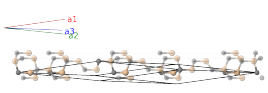


Prototype	CSi
AFLOW prototype label	AB_hR10_160_5a_5a-001
***Strukturbericht* designation**	$B7$
Mineral name	moissanite
ICSD	24168
Pearson symbol	hR10
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB_hR10_160_5a_5a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}$

- (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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		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).