Moissanite 9R (CSi) Structure: AB_hR6_160_3a_3a-001

This structure originally had the label `AB_hR6_160_3a_3a`. Calls to that address will be redirected here.

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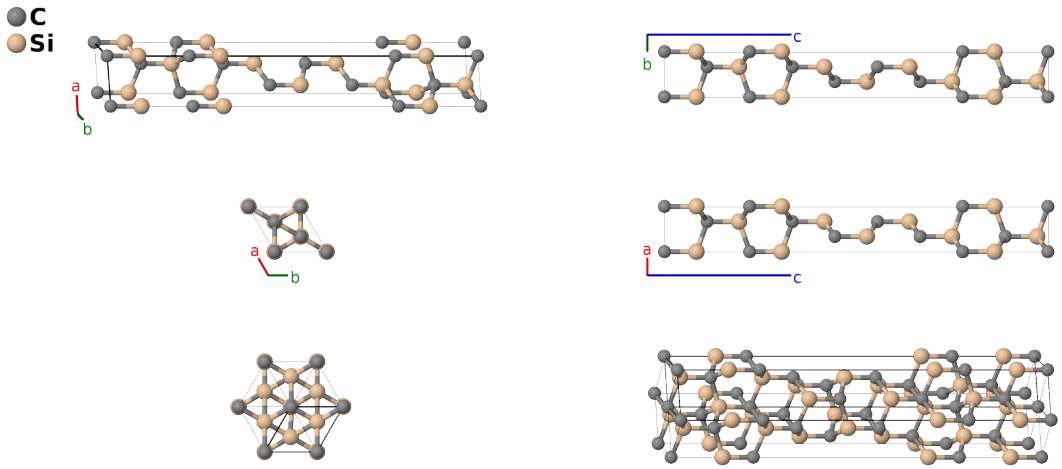
https://aflow.org/p/T8Y7

https://aflow.org/p/AB_hR6_160_3a_3a-001



Prototype	CSi
AFLOW prototype label	AB_hR6_160_3a_3a-001
Mineral name	moissanite
ICSD	37373
Pearson symbol	hR6
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB_hR6_160_3a_3a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, x_6$

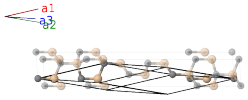
Other compounds with this structure
ZnS

- We will loosely use the name moissanite to describe any tetrahedrally bonded silicon carbide compound that does not have another name. The labels 4H, 6H, 9R, etc., refer to the repeat stacking distance in the hexagonal unit cell, while H and R refer to the primitive hexagonal and rhombohedral lattices, respectively. The label C refers to a cubic unit cell, which is a special case of R. Note that 2, 3, 6, 9, etc., refers to the number of C-Si dimers that are stacked in the conventional unit cell.
- Moissanite 9R is our hypothetical alternate stacking (ABCBCACAB) for tetrahedral structures. Compare this to hexagonal wurtzite (ABABAB, 2H, $B4$), cubic zincblende (ABCABC, 3C, $B3$), and the hexagonal 4H (ABAC,$B5$) and 6H (ABCACB, $B6$) moissanites.

- Some time after we proposed this structure we found the ICSD entry for 9-R ZnS, listing (Haussuehl, 1963) as the prototype. We have not been able to obtain this reference, so we continue to use 9-R CSi as the prototype. The ICSD entry is from (Haussuehl, 1963).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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)	Si I
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(1a)	Si II
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(1a)	Si III

References

[1] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

[2] S. Haussuehl and G. Mueller, *Neue ZnS-Polytypen (9R, 12R und 21R) in mesozoischen Sedimenten NW-Deutschland*, Beitraege zur Mineralogie und Petrographie **9**, 28–39 (1963).