Hypothetical Tetrahedrally Bonded Carbon with 3-Member Rings Model Structure: A_hP6_194_h-001

This structure originally had the label `A_hP6_194_h`. Calls to that address will be redirected here.

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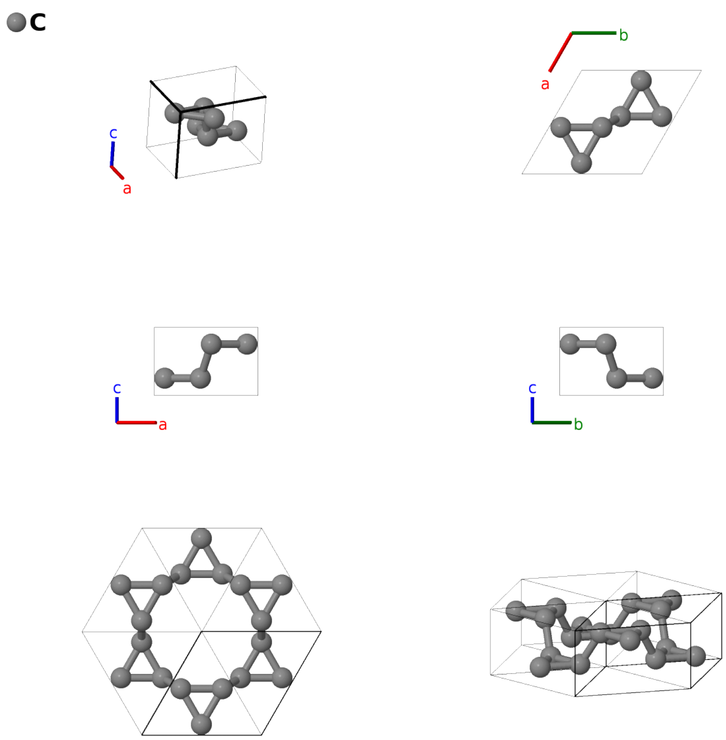
https://aflow.org/p/1BYJ

https://aflow.org/p/A_hP6_194_h-001

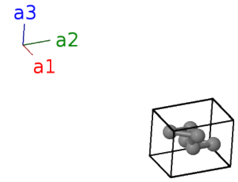


Prototype	C
AFLOW prototype label	A_hP6_194_h-001
ICSD	None
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A_hP6_194_h-001` `--params=`$a, c/a, x_1$

- This structure was proposed in (Schultz, 1999) to show that it was energetically possible to form three-member rings in amorphous sp^3 carbon structures.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_2}$	=	$-2x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - 2x_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_5}$	=	$2x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_6}$	=	$-x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I

References

[1] P. A. Schultz, K. Leung, and E. B. Stechel, *Small rings and amorphous tetrahedral carbon*, Phys. Rev. B **59**, 733–741 (1999), doi:10.1103/PhysRevB.59.733.