

Hypothetical Tetrahedrally Bonded Carbon with 3-Member Rings

Model Structure:

A_hP6_194_h-001

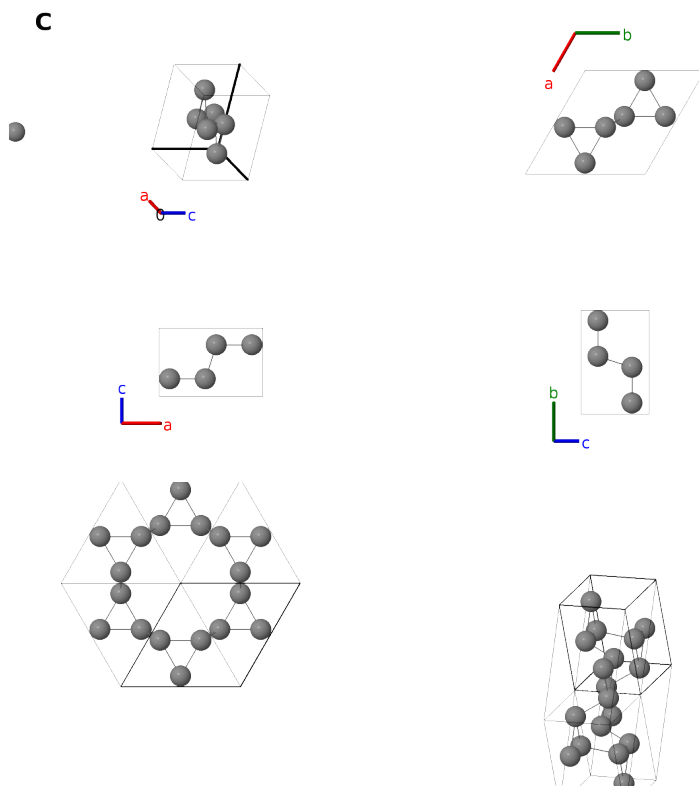
This structure previously used the label(s) **A_hP6_194_h**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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. Oses, 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/1BYJ>

https://aflow.org/prototype-encyclopedia/A_hP6_194_h-001



Prototype	C
AFLOW prototype label	A_hP6_194_h-001
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A_hP6_194_h-001 --params=a, c/a, x₁</code>

- 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

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

$\mathbf{a}_1$ $\mathbf{a}_2$
 $\mathbf{a}_3$



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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017