

Hypothetical Tetrahedrally Bonded Carbon with 4-Member Rings

Model Structure:

A_tI8_139_h-001

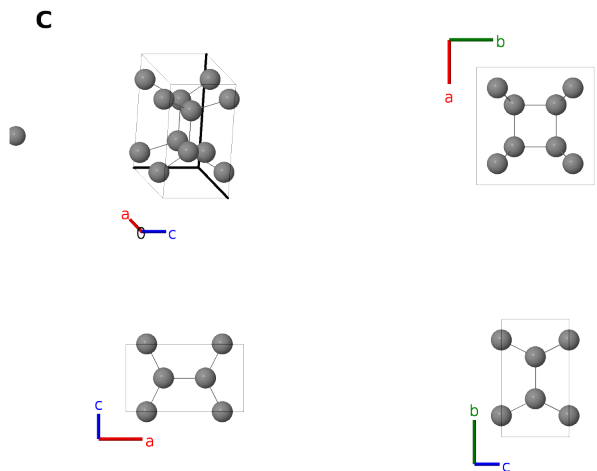
This structure previously used the label(s) **A.tI8-139-h**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/TE0L>

https://aflow.org/prototype-encyclopedia/A.tI8_139_h-001



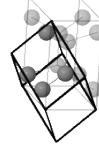
Prototype	C
AFLOW prototype label	A_tI8_139_h-001
Pearson symbol	tI8
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A_tI8_139_h-001 --params=a, c/a, x₁</code>

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

Body-centered Tetragonal primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}}$	(8h) C I
$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - 2x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}}$	(8h) C I
$\mathbf{B}_3$	$=$	$x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}}$	(8h) C I
$\mathbf{B}_4$	$=$	$-x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}}$	(8h) 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

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