Hypothetical Tetrahedrally Bonded Carbon with 4-Member Rings Model Structure:
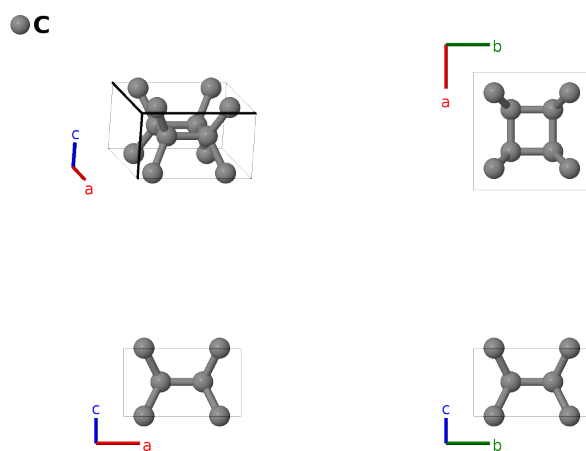# A_tI8_139_h-001

This structure originally had the label `A_tI8_139_h`. Calls to that address will be redirected here.

https://aflow.org/p/TE0L

https://aflow.org/p/A_tI8_139_h-001

Prototype	C
AFLOW prototype label	A_tI8_139_h-001
ICSD	None
Pearson symbol	tI8
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	aflow --proto=A_tI8_139_h-001 --params=$a, c/a, x_1$

- 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
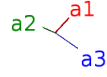
$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
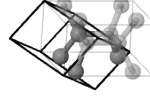
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + 2x_1\,\mathbf{a_3}$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(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.