

R-carbon Structure: A_oP16_55_2g2h-001

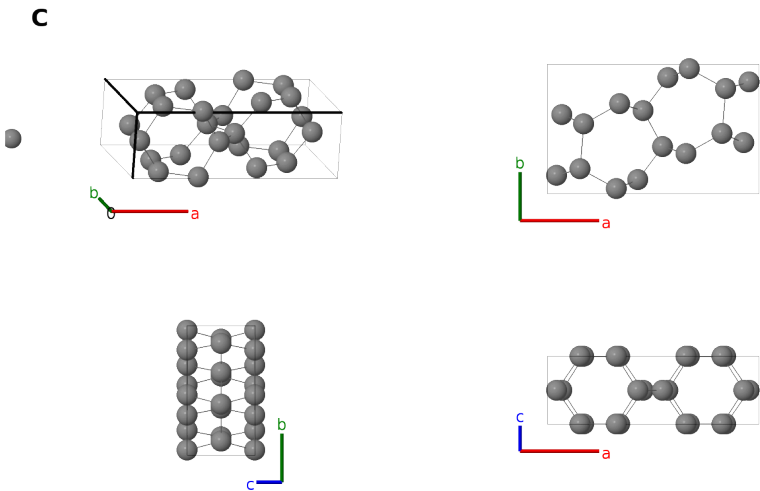
This structure previously used the label(s) **A_oP16_55_2g2h**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A_oP16_55_2g2h-001



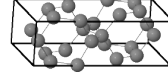
Prototype	C
AFLOW prototype label	A_oP16_55_2g2h-001
Pearson symbol	oP16
Space group number	55
Space group symbol	<i>Pbam</i>
AFLOW prototype command	<code>aflow --proto=A_oP16_55_2g2h-001</code> <code>--params=a, b/a, c/a, x₁, y₁, x₂, y₂, x₃, y₃, x₄, y₄</code>

- This is a predicted “superhard” allotrope of carbon. Shortly after this paper was published, another paper predicted a similar phase, called “H-Carbon” (He, 2012a; He, 2012b). The similarity between the two structures can be seen by shifting the origin by $\frac{1}{2}\mathbf{a}_1$. Other sources (Zhao, 2012) refer to this structure as “O-Carbon.”

Simple Orthorhombic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_3$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}}$	(4g)	C II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}}$	(4g)	C II
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	C II
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	C II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C III
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C III
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C IV
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C IV
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C IV
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4h)	C IV

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