

M-carbon Structure:

A_mC16_12_4i-001

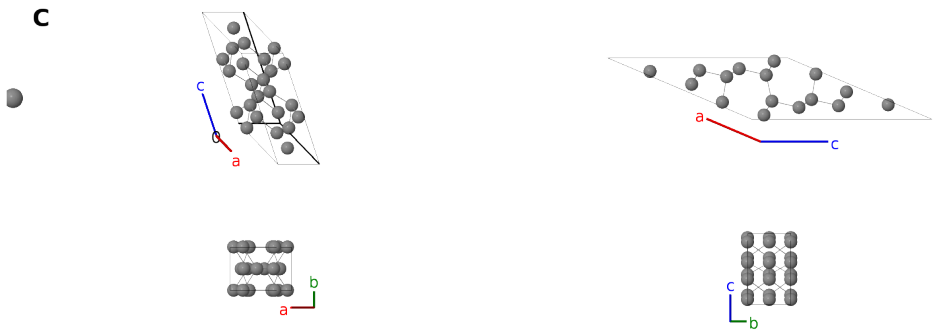
This structure previously used the label(s) **A_mC16_12_4i**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/MTF0>

https://aflow.org/prototype-encyclopedia/A_mC16_12_4i-001

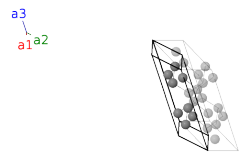


Prototype	C
AFLOW prototype label	A_mC16_12_4i-001
ICSD	182760
CCDC	1692097
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<code>aflow --proto=A_mC16_12_4i-001</code> <code>--params=a,b/a,c/a,β,x_1,z_1,x_2,z_2,x_3,z_3,x_4,z_4</code>

- This structure was originally found by (Oganov, 2006) and was refined and designated M-Carbon by (Li, 2009).

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	C II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	C III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	C III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	C IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	C IV

References

- [1] Q. Li, Y. Ma, A. R. Oganov, H. Wang, H. Wang, Y. Xu, T. Cui, H.-K. Mao, and G. Zou, *Superhard Monoclinic Polymorph of Carbon*, Phys. Rev. Lett. **102**, 175506 (2009), doi:10.1103/PhysRevLett.102.175506.
- [2] A. R. Oganov and C. W. Glass, *Crystal structure prediction using ab initio evolutionary techniques: Principles and applications*, J. Chem. Phys. **124**, 244704 (2006), doi:10.1063/1.2210932.

First cited in

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