M-carbon Structure: A_mC16_12_4i-001

This structure originally had the label `A_mC16_12_4i`. Calls to that address will be redirected here.

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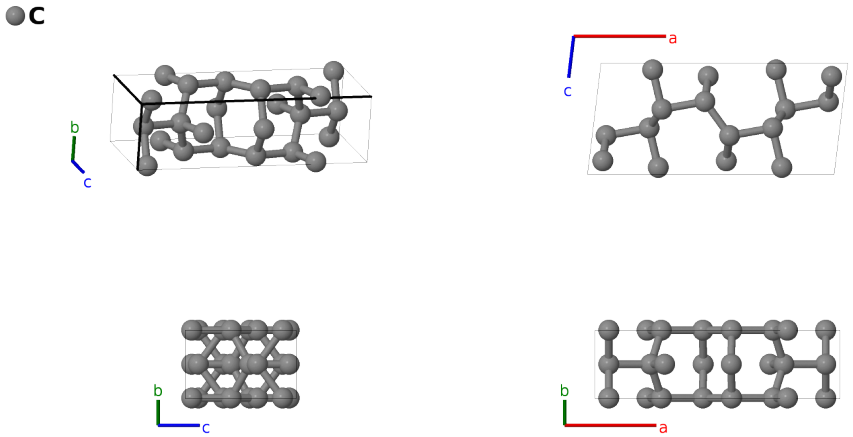
https://aflow.org/p/MTF0

https://aflow.org/p/A_mC16_12_4i-001

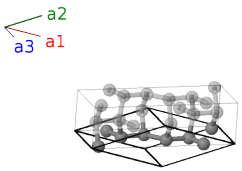


Prototype	C
AFLOW prototype label	A_mC16_12_4i-001
ICSD	182760
Pearson symbol	mC16
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A_mC16_12_4i-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

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

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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.