S-carbon Structure: A_mP8_10_2m2n-001

This structure previously used the label(s) `A_mP8_10_2m2n`. Calls to these addresses will be redirected here.

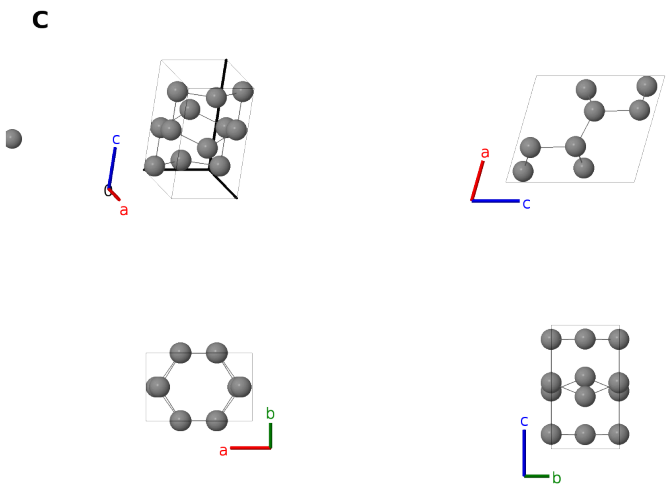
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/XRQ1

https://aflow.org/prototype-encyclopedia/A_mP8_10_2m2n-001

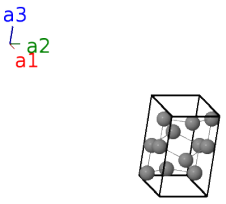


Prototype	C
AFLOW prototype label	A_mP8_10_2m2n-001
Pearson symbol	mP8
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=A_mP8_10_2m2n-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- This is a predicted "superhard" allotrope of iron. Shortly after this paper was published, two other papers predicted similar structures, differentiated mainly by an origin shift:
- F-carbon (Tian 2012): the origin is shifted by $\frac{1}{2}\,\mathbf{a_3}$.
- J-carbon (Wang, 2012): the origin is shifted by $\frac{1}{2}\,(\mathbf{a_1}+\mathbf{a_3})$.
- This is *not* the orthorhombic phase found by (He, 2012), which was also called S-carbon.

Simple Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2m)	C I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(2m)	C I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2m)	C II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2m)	C II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2n)	C III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2n)	C III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	C IV
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2n)	C IV

References

[1] H. Niu, X.-Q. Chen, S. Wang, D. Li, W. L. Mao, and Y. Li, *Families of Superhard Crystalline Carbon Allotropes Constructed via Cold Compression of Graphite and Nanotubes*, Phys. Rev. Lett. **108**, 135501 (2012), doi:10.1103/PhysRevLett.108.135501.

[2] F. Tian, X. Dong, Z. Zhao, J. He, and H.-T. Wang, *Superhard F-carbon predicted by ab initio particle-swarm optimization methodology*, J. Phys.: Condens. Matter **24**, 165504 (2012), doi:10.1088/0953-8984/24/16/165504.

[3] J.-T. Wang, C. Chen, and Y. Kawazoe, *Phase conversion from graphite toward a simple monoclinic sp^3-carbon allotrope*, Journal of Chemical Physics **137**, 024502 (2012), doi:10.1063/1.4732538.

[4] C. He, L. Sun, C. Zhang, X. Peng, K. Zhang, and J. Zhong, *New superhard carbon phases between graphite and diamond*, Solid State Commun. **152**, 1560–1563 (2012), doi:10.1016/j.ssc.2012.05.022.

[5] C. He, L. Z. Sun, and J. Zhong, *Prediction of superhard carbon allotropes from the segment combination method*, Journal of Superhard Materials **34**, 386–399 (2012), doi:10.3103/S1063457612060123.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043