S-carbon Structure: A_mP8_10_2m2n-001

This structure originally had the label `A_mP8_10_2m2n`. Calls to that address will be redirected here.

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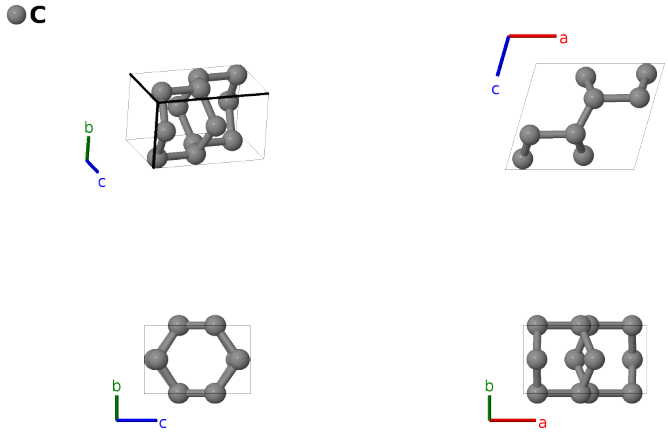
https://aflow.org/p/XRQ1

https://aflow.org/p/A_mP8_10_2m2n-001

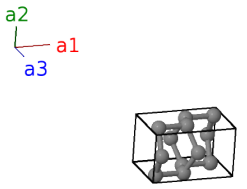


Prototype	C
AFLOW prototype label	A_mP8_10_2m2n-001
ICSD	None
Pearson symbol	mP8
Space group number	10
Space group symbol	$P2/m$
AFLOW prototype command	`aflow --proto=A_mP8_10_2m2n-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- 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

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