

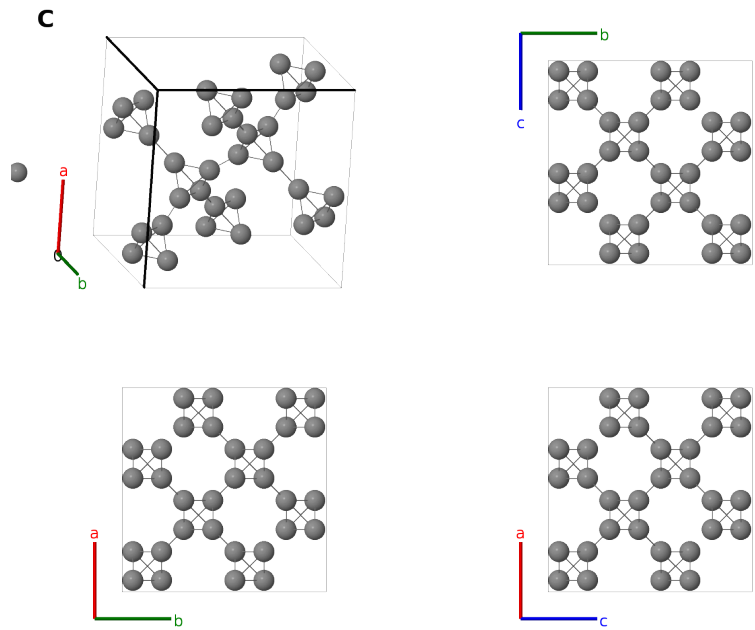
T-Carbon Structure: A_cF32_227_e-001

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<https://aflow.org/prototype-encyclopedia/WPN9>

https://aflow.org/prototype-encyclopedia/A_cF32_227_e-001

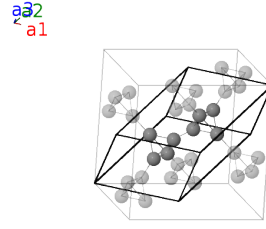


Prototype	C
AFLOW prototype label	A_cF32_227_e-001
ICSD	689215
CCDC	2276938
Pearson symbol	cF32
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A_cF32_227_e-001 --params=a, x₁</code>

- This was predicted by (Sheng, 2011) and found experimentally by (Xu, 2020) and others.
- The ICSD entry is from (Kang, 2020), who gave the atomic positions in terms of setting 1 of space group $Fd\bar{3}m$ #227. We used FINDSYM to change this to the standard setting 2.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - (3x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - (3x_1 - \frac{1}{2}) \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_4$	$= -(3x_1 - \frac{1}{2}) \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (3x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_6$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_7$	$= -x_1 \mathbf{a}_1 + (3x_1 + \frac{1}{2}) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	C I
$\mathbf{B}_8$	$= (3x_1 + \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(32e)	C I

References

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- [3] K. Xu, H. Liu, Y.-C. Shi, J.-Y. You, X.-Y. Ma, H.-J. Cui, Q.-B. Yan, G.-C. Chen, and G. Su, *Preparation of T-carbon by plasma enhanced chemical vapor deposition*, Carbon **157**, 270–276 (2020), doi:10.1016/j.carbon.2019.10.032.

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