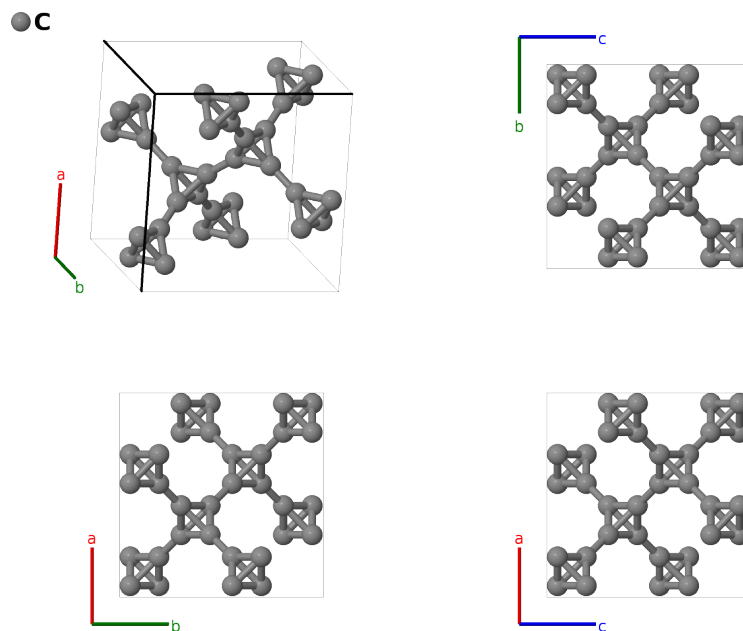


T-Carbon Structure: A_cF32_227_e-001

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<https://aflow.org/p/WPN9>

https://aflow.org/p/A_cF32_227_e-001



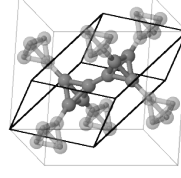
Prototype	C
AFLOW prototype label	A_cF32_227_e-001
ICSD	689215
Pearson symbol	cF32
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A_cF32_227_e-001 --params=a, x₁</code>

- 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

\hat{a}_2
 \hat{a}_1

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



Basis vectors

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

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