

FCC C₆₀ Buckminsterfullerene Structure: A_cF240_202_h2i-001

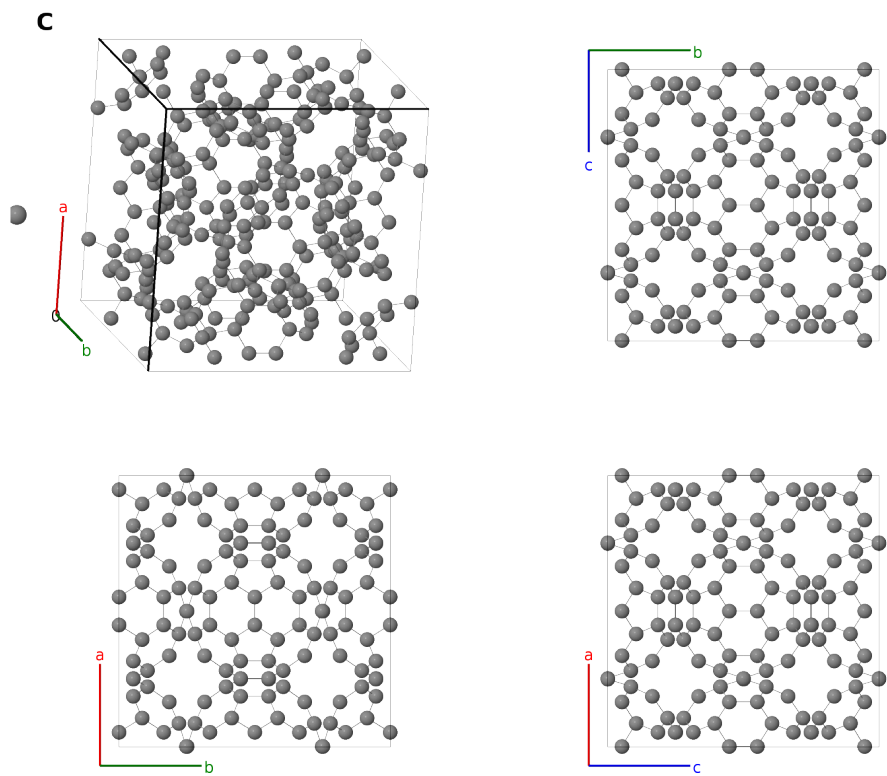
This structure previously used the label(s) **A_cF240_202_h2i**. Calls to these addresses will be redirected here.

Cite this page as:

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- 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/TV0E>

https://aflow.org/prototype-encyclopedia/A_cF240_202_h2i-001



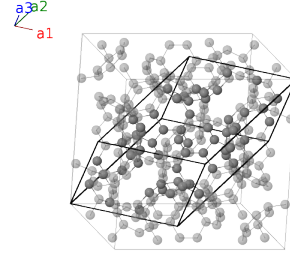
Prototype	C
AFLOW prototype label	A_cF240_202_h2i-001
Mineral name	buckminsterfullerene
ICSD	74523
CCDC	1635233
Pearson symbol	cF240
Space group number	202
Space group symbol	$Fm\bar{3}$

AFLOW prototype command `aflow --proto=A_cF240_202_h2i-001`
 `--params=a, y1, z1, x2, y2, z2, x3, y3, z3`

- This is an *approximate* representation of the structure of C₆₀ buckminsterfullerene. As noted by the authors, “a careful analysis of the intensity data reveals that the molecules must pack in an uncorrelated array, in full agreement with the results from most previous diffraction and spectroscopic determinations.”
- The C₆₀ molecules are centered on the sites of an fcc lattice.
- Below 249K there is a transition to a simple cubic phase of C₆₀.

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
$\mathbf{B}_1$	$= (y_1 + z_1) \mathbf{a}_1 - (y_1 - z_1) \mathbf{a}_2 + (y_1 - z_1) \mathbf{a}_3$	$= ay_1 \hat{\mathbf{y}} + az_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_2$	$= -(y_1 - z_1) \mathbf{a}_1 + (y_1 + z_1) \mathbf{a}_2 - (y_1 + z_1) \mathbf{a}_3$	$= -ay_1 \hat{\mathbf{y}} + az_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_3$	$= (y_1 - z_1) \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3$	$= ay_1 \hat{\mathbf{y}} - az_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_4$	$= -(y_1 + z_1) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 - (y_1 - z_1) \mathbf{a}_3$	$= -ay_1 \hat{\mathbf{y}} - az_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_5$	$= (y_1 - z_1) \mathbf{a}_1 + (y_1 + z_1) \mathbf{a}_2 - (y_1 - z_1) \mathbf{a}_3$	$= az_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_6$	$= -(y_1 + z_1) \mathbf{a}_1 - (y_1 - z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3$	$= az_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_7$	$= (y_1 + z_1) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 - (y_1 + z_1) \mathbf{a}_3$	$= -az_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_8$	$= -(y_1 - z_1) \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 + (y_1 - z_1) \mathbf{a}_3$	$= -az_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{z}}$	(48h)	C I
$\mathbf{B}_9$	$= -(y_1 - z_1) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 + (y_1 + z_1) \mathbf{a}_3$	$= ay_1 \hat{\mathbf{x}} + az_1 \hat{\mathbf{y}}$	(48h)	C I
$\mathbf{B}_{10}$	$= (y_1 + z_1) \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 - (y_1 - z_1) \mathbf{a}_3$	$= -ay_1 \hat{\mathbf{x}} + az_1 \hat{\mathbf{y}}$	(48h)	C I
$\mathbf{B}_{11}$	$= -(y_1 + z_1) \mathbf{a}_1 + (y_1 + z_1) \mathbf{a}_2 + (y_1 - z_1) \mathbf{a}_3$	$= ay_1 \hat{\mathbf{x}} - az_1 \hat{\mathbf{y}}$	(48h)	C I

$$\begin{aligned}
\mathbf{B}_{12} &= (y_1 - z_1) \mathbf{a}_1 - (y_1 - z_1) \mathbf{a}_2 - (y_1 + z_1) \mathbf{a}_3 &= & -ay_1 \hat{\mathbf{x}} - az_1 \hat{\mathbf{y}} & (48h) & \text{C I} \\
\mathbf{B}_{13} &= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3 &= & ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{14} &= (x_2 - y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3 &= & -ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{15} &= (x_2 + y_2 - z_2) \mathbf{a}_1 - (x_2 + y_2 + z_2) \mathbf{a}_2 + (-x_2 + y_2 + z_2) \mathbf{a}_3 &= & -ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{16} &= -(x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 + y_2 - z_2) \mathbf{a}_2 + (x_2 - y_2 + z_2) \mathbf{a}_3 &= & ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{17} &= (x_2 + y_2 - z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2 + z_2) \mathbf{a}_3 &= & az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{18} &= -(x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (-x_2 + y_2 + z_2) \mathbf{a}_3 &= & az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{19} &= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 + y_2 - z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3 &= & -az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{20} &= (x_2 - y_2 + z_2) \mathbf{a}_1 - (x_2 + y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3 &= & -az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{21} &= (x_2 - y_2 + z_2) \mathbf{a}_1 + (x_2 + y_2 - z_2) \mathbf{a}_2 + (-x_2 + y_2 + z_2) \mathbf{a}_3 &= & ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{22} &= (-x_2 + y_2 + z_2) \mathbf{a}_1 - (x_2 + y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2 + z_2) \mathbf{a}_3 &= & -ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{23} &= -(x_2 + y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3 &= & ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{24} &= (x_2 + y_2 - z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3 &= & -ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{25} &= (x_2 - y_2 - z_2) \mathbf{a}_1 - (x_2 - y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 - z_2) \mathbf{a}_3 &= & -ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{26} &= -(x_2 - y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 - z_2) \mathbf{a}_2 + (x_2 + y_2 + z_2) \mathbf{a}_3 &= & ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{27} &= -(x_2 + y_2 - z_2) \mathbf{a}_1 + (x_2 + y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2 - z_2) \mathbf{a}_3 &= & ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96i) & \text{C II} \\
\mathbf{B}_{28} &= (x_2 + y_2 + z_2) \mathbf{a}_1 - (x_2 + y_2 - z_2) \mathbf{a}_2 - (x_2 - y_2 + z_2) \mathbf{a}_3 &= & -ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96i) & \text{C II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{46} &= \begin{pmatrix} (-x_3 + y_3 + z_3) \mathbf{a}_1 - \\ (x_3 + y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{47} &= \begin{pmatrix} -(x_3 + y_3 + z_3) \mathbf{a}_1 + \\ (-x_3 + y_3 + z_3) \mathbf{a}_2 + \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{48} &= \begin{pmatrix} (x_3 + y_3 - z_3) \mathbf{a}_1 + \\ (x_3 - y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{49} &= \begin{pmatrix} (x_3 - y_3 - z_3) \mathbf{a}_1 - \\ (x_3 - y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(x_3 - y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 - z_3) \mathbf{a}_2 + \\ (x_3 + y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{51} &= \begin{pmatrix} -(x_3 + y_3 - z_3) \mathbf{a}_1 + \\ (x_3 + y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{52} &= \begin{pmatrix} (x_3 + y_3 + z_3) \mathbf{a}_1 - \\ (x_3 + y_3 - z_3) \mathbf{a}_2 - \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{53} &= \begin{pmatrix} -(x_3 + y_3 - z_3) \mathbf{a}_1 + \\ (x_3 - y_3 - z_3) \mathbf{a}_2 - \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{54} &= \begin{pmatrix} (x_3 + y_3 + z_3) \mathbf{a}_1 - \\ (x_3 - y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{55} &= \begin{pmatrix} (x_3 - y_3 - z_3) \mathbf{a}_1 - \\ (x_3 + y_3 - z_3) \mathbf{a}_2 + \\ (x_3 + y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{56} &= \begin{pmatrix} -(x_3 - y_3 + z_3) \mathbf{a}_1 + \\ (x_3 + y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{57} &= \begin{pmatrix} -(x_3 - y_3 + z_3) \mathbf{a}_1 - \\ (x_3 + y_3 - z_3) \mathbf{a}_2 + \\ (x_3 - y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{58} &= \begin{pmatrix} (x_3 - y_3 - z_3) \mathbf{a}_1 + \\ (x_3 + y_3 + z_3) \mathbf{a}_2 - \\ (x_3 - y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{59} &= \begin{pmatrix} (x_3 + y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 - z_3) \mathbf{a}_2 - \\ (x_3 + y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96i) & \text{C III} \\
\mathbf{B}_{60} &= \begin{pmatrix} -(x_3 + y_3 - z_3) \mathbf{a}_1 - \\ (x_3 - y_3 + z_3) \mathbf{a}_2 + \\ (x_3 + y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96i) & \text{C III}
\end{aligned}$$

References

- [1] D. L. Dorset and M. P. McCourt, *Disorder and the molecular packing of C₆₀ buckminsterfullerene: a direct electron-crystallographic analysis*, Acta Crystallogr. Sect. A **50**, 344–351 (1994), doi:10.1107/S0108767393012607.

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