FCC C$_{60}$ Buckminsterfullerene Structure: A_cF240_202_h2i-001

This structure originally had the label A_cF240_202_h2i. Calls to that address will be redirected here.

https://aflow.org/p/TV0E

https://aflow.org/p/A_cF240_202_h2i-001
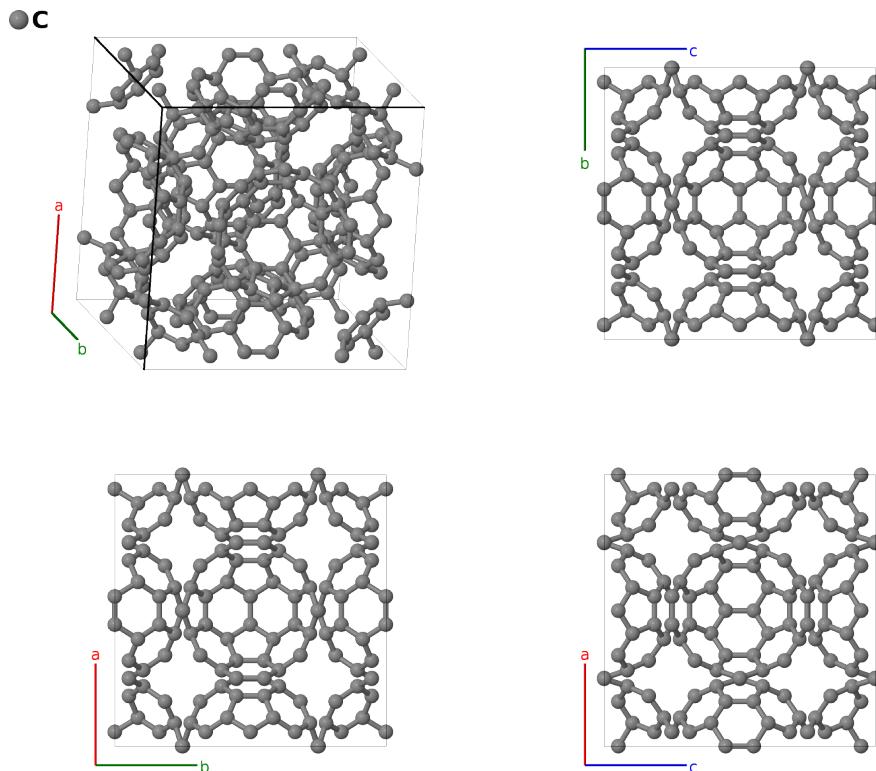
Prototype	C
AFLOW prototype label	A_cF240_202_h2i-001
Mineral name	buckminsterfullerene
ICSD	74523
Pearson symbol	cF240
Space group number	202
Space group symbol	$Fm\overline{3}$
AFLOW prototype command	aflow --proto=A_cF240_202_h2i-001 --params=$a, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

- This is an *approximate* representation of the structure of C_{60} 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 C_{60} molecules are centered on the sites of an fcc lattice.

- Below 249K there is a transition to a simple cubic phase of C_{60}.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}$$
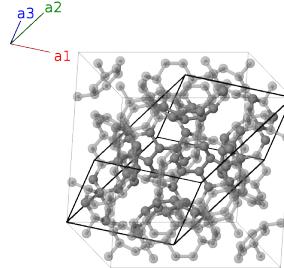
Basis vectors

		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
$\mathbf{B_{12}}$	$=$	$(y_1 - z_1)\,\mathbf{a_1} - (y_1 - z_1)\,\mathbf{a_2} - (y_1 + z_1)\,\mathbf{a_3}$	$=$	$-ay_1\,\hat{\mathbf{x}} - az_1\,\hat{\mathbf{y}}$	(48h)	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)	C II

$$\mathbf{B_{14}} = (x_2 - y_2 + z_2)\, \mathbf{a}_1 + (-x_2 + y_2 + z_2)\, \mathbf{a}_2 - (x_2 + y_2 + z_2)\, \mathbf{a}_3 = -ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{15}} = (x_2 + y_2 - z_2)\, \mathbf{a}_1 - (x_2 + y_2 + z_2)\, \mathbf{a}_2 + (-x_2 + y_2 + z_2)\, \mathbf{a}_3 = -ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{16}} = -(x_2 + y_2 + z_2)\, \mathbf{a}_1 + (x_2 + y_2 - z_2)\, \mathbf{a}_2 + (x_2 - y_2 + z_2)\, \mathbf{a}_3 = ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{17}} = (x_2 + y_2 - z_2)\, \mathbf{a}_1 + (-x_2 + y_2 + z_2)\, \mathbf{a}_2 + (x_2 - y_2 + z_2)\, \mathbf{a}_3 = az_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{18}} = -(x_2 + y_2 + z_2)\, \mathbf{a}_1 + (x_2 - y_2 + z_2)\, \mathbf{a}_2 + (-x_2 + y_2 + z_2)\, \mathbf{a}_3 = az_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{19}} = (-x_2 + y_2 + z_2)\, \mathbf{a}_1 + (x_2 + y_2 - z_2)\, \mathbf{a}_2 - (x_2 + y_2 + z_2)\, \mathbf{a}_3 = -az_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{20}} = (x_2 - y_2 + z_2)\, \mathbf{a}_1 - (x_2 + y_2 + z_2)\, \mathbf{a}_2 + (x_2 + y_2 - z_2)\, \mathbf{a}_3 = -az_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{21}} = (x_2 - y_2 + z_2)\, \mathbf{a}_1 + (x_2 + y_2 - z_2)\, \mathbf{a}_2 + (-x_2 + y_2 + z_2)\, \mathbf{a}_3 = ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{22}} = (-x_2 + y_2 + z_2)\, \mathbf{a}_1 - (x_2 + y_2 + z_2)\, \mathbf{a}_2 + (x_2 - y_2 + z_2)\, \mathbf{a}_3 = -ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{23}} = -(x_2 + y_2 + z_2)\, \mathbf{a}_1 + (-x_2 + y_2 + z_2)\, \mathbf{a}_2 + (x_2 + y_2 - z_2)\, \mathbf{a}_3 = ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{24}} = (x_2 + y_2 - z_2)\, \mathbf{a}_1 + (x_2 - y_2 + z_2)\, \mathbf{a}_2 - (x_2 + y_2 + z_2)\, \mathbf{a}_3 = -ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{25}} = (x_2 - y_2 - z_2)\, \mathbf{a}_1 - (x_2 - y_2 + z_2)\, \mathbf{a}_2 - (x_2 + y_2 - z_2)\, \mathbf{a}_3 = -ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{26}} = -(x_2 - y_2 + z_2)\, \mathbf{a}_1 + (x_2 - y_2 - z_2)\, \mathbf{a}_2 + (x_2 + y_2 + z_2)\, \mathbf{a}_3 = ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{27}} = -(x_2 + y_2 - z_2)\, \mathbf{a}_1 + (x_2 + y_2 + z_2)\, \mathbf{a}_2 + (x_2 - y_2 - z_2)\, \mathbf{a}_3 = ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{28}} = (x_2 + y_2 + z_2)\, \mathbf{a}_1 - (x_2 + y_2 - z_2)\, \mathbf{a}_2 - (x_2 - y_2 + z_2)\, \mathbf{a}_3 = -ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{29}} = -(x_2 + y_2 - z_2)\, \mathbf{a}_1 + (x_2 - y_2 - z_2)\, \mathbf{a}_2 - (x_2 - y_2 + z_2)\, \mathbf{a}_3 = -az_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$$\mathbf{B_{30}} = (x_2 + y_2 + z_2)\, \mathbf{a}_1 - (x_2 - y_2 + z_2)\, \mathbf{a}_2 + (x_2 - y_2 - z_2)\, \mathbf{a}_3 = -az_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \mathrm{C\ II}$$

$\mathbf{B_{31}}$	$=$	$(x_2 - y_2 - z_2)\,\mathbf{a}_1 - (x_2 + y_2 - z_2)\,\mathbf{a}_2 + (x_2 + y_2 + z_2)\,\mathbf{a}_3$	$=$	$az_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{32}}$	$=$	$-(x_2 - y_2 + z_2)\,\mathbf{a}_1 + (x_2 + y_2 + z_2)\,\mathbf{a}_2 - (x_2 + y_2 - z_2)\,\mathbf{a}_3$	$=$	$az_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{33}}$	$=$	$-(x_2 - y_2 + z_2)\,\mathbf{a}_1 - (x_2 + y_2 - z_2)\,\mathbf{a}_2 + (x_2 - y_2 - z_2)\,\mathbf{a}_3$	$=$	$-ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{34}}$	$=$	$(x_2 - y_2 - z_2)\,\mathbf{a}_1 + (x_2 + y_2 + z_2)\,\mathbf{a}_2 - (x_2 - y_2 + z_2)\,\mathbf{a}_3$	$=$	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{35}}$	$=$	$(x_2 + y_2 + z_2)\,\mathbf{a}_1 + (x_2 - y_2 - z_2)\,\mathbf{a}_2 - (x_2 + y_2 - z_2)\,\mathbf{a}_3$	$=$	$-ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{36}}$	$=$	$-(x_2 + y_2 - z_2)\,\mathbf{a}_1 - (x_2 - y_2 + z_2)\,\mathbf{a}_2 + (x_2 + y_2 + z_2)\,\mathbf{a}_3$	$=$	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(96i)	C II
$\mathbf{B_{37}}$	$=$	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 - y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{38}}$	$=$	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 - (x_3 + y_3 + z_3)\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{39}}$	$=$	$(x_3 + y_3 - z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{40}}$	$=$	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{41}}$	$=$	$(x_3 + y_3 - z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	$=$	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{42}}$	$=$	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 - y_3 + z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	$=$	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{43}}$	$=$	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3 + z_3)\,\mathbf{a}_3$	$=$	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{44}}$	$=$	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	$=$	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{45}}$	$=$	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{46}}$	$=$	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	$=$	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96i)	C III
$\mathbf{B_{47}}$	$=$	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	$=$	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96i)	C III

$$\mathbf{B_{48}} = \begin{aligned}&(x_3 + y_3 - z_3)\,\mathbf{a}_1 + \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_2 - \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{49}} = \begin{aligned}&(x_3 - y_3 - z_3)\,\mathbf{a}_1 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_2 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{50}} = \begin{aligned}&-(x_3 - y_3 + z_3)\,\mathbf{a}_1 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_2 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{51}} = \begin{aligned}&-(x_3 + y_3 - z_3)\,\mathbf{a}_1 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_2 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{52}} = \begin{aligned}&(x_3 + y_3 + z_3)\,\mathbf{a}_1 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_2 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{53}} = \begin{aligned}&-(x_3 + y_3 - z_3)\,\mathbf{a}_1 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_2 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{54}} = \begin{aligned}&(x_3 + y_3 + z_3)\,\mathbf{a}_1 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_2 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{55}} = \begin{aligned}&(x_3 - y_3 - z_3)\,\mathbf{a}_1 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_2 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{56}} = \begin{aligned}&-(x_3 - y_3 + z_3)\,\mathbf{a}_1 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_2 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{57}} = \begin{aligned}&-(x_3 - y_3 + z_3)\,\mathbf{a}_1 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_2 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{58}} = \begin{aligned}&(x_3 - y_3 - z_3)\,\mathbf{a}_1 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_2 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{59}} = \begin{aligned}&(x_3 + y_3 + z_3)\,\mathbf{a}_1 + \\ &(x_3 - y_3 - z_3)\,\mathbf{a}_2 - \\ &(x_3 + y_3 - z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad -ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

$$\mathbf{B_{60}} = \begin{aligned}&-(x_3 + y_3 - z_3)\,\mathbf{a}_1 - \\ &(x_3 - y_3 + z_3)\,\mathbf{a}_2 + \\ &(x_3 + y_3 + z_3)\,\mathbf{a}_3\end{aligned} \quad = \quad ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}} \qquad (96\mathrm{i}) \qquad \text{C III}$$

References

[1] D. L. Dorset and M. P. McCourt, *Disorder and the molecular packing of C_{60} buckminsterfullerene: a direct electron-crystallographic analysis*, Acta Crystallogr. Sect. A **50**, 344–351 (1994), doi:10.1107/S0108767393012607.