Orthorhombic Fullerene (Cs_3C_{60}) Structure: A15B_oI128_71_lmn6o_eg-001

https://aflow.org/p/88NV

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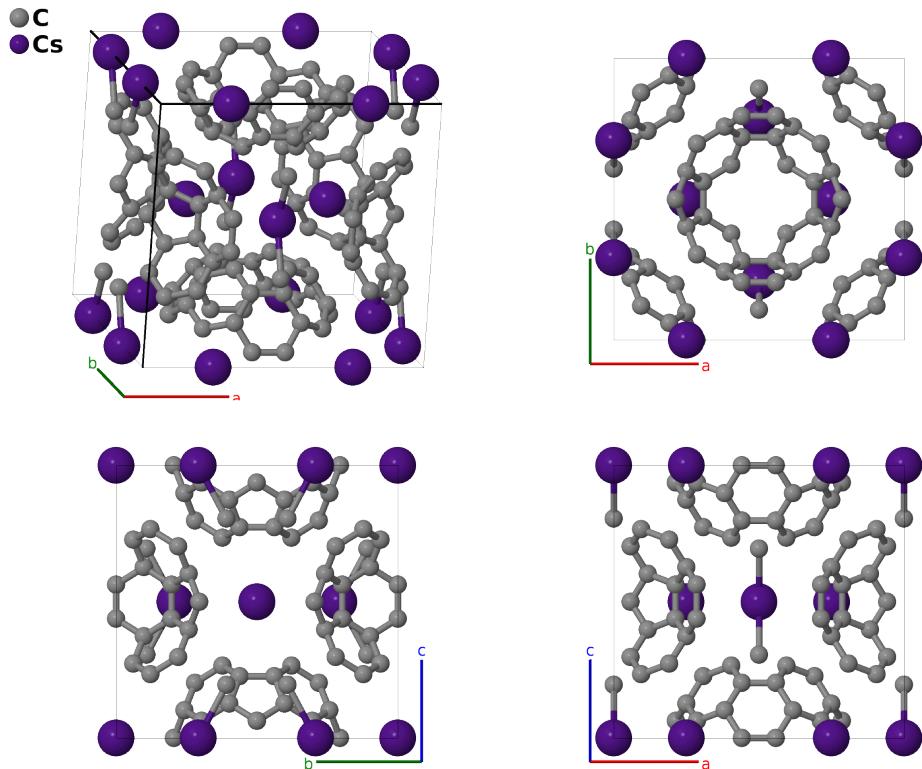
| Prototype	$C_{60}Cs_3$
AFLOW prototype label	A15B_oI128_71_lmn6o_eg-001
ICSD	None
Pearson symbol	oI128
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A15B_oI128_71_lmn6o_eg-001` `--params=`$a, b/a, c/a, x_1, y_2, y_3, z_3, x_4, z_4, x_5, y_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- The Cesium (4e) and (4g) sites each have 75% occupancy.

Body-centered Orthorhombic primitive vectors

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

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

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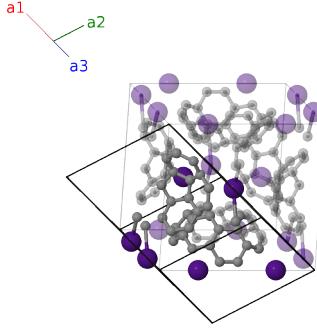
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_2} + x_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_2} - x_1\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Cs I
$\mathbf{B_3}$	$=$	$y_2\,\mathbf{a_1} + y_2\,\mathbf{a_3}$	$=$	$by_2\,\hat{\mathbf{y}}$	(4g)	Cs II
$\mathbf{B_4}$	$=$	$-y_2\,\mathbf{a_1} - y_2\,\mathbf{a_3}$	$=$	$-by_2\,\hat{\mathbf{y}}$	(4g)	Cs II
$\mathbf{B_5}$	$=$	$(y_3 + z_3)\,\mathbf{a_1} + z_3\,\mathbf{a_2} + y_3\,\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8l)	C I
$\mathbf{B_6}$	$=$	$-(y_3 - z_3)\,\mathbf{a_1} + z_3\,\mathbf{a_2} - y_3\,\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8l)	C I
$\mathbf{B_7}$	$=$	$(y_3 - z_3)\,\mathbf{a_1} - z_3\,\mathbf{a_2} + y_3\,\mathbf{a_3}$	$=$	$by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8l)	C I
$\mathbf{B_8}$	$=$	$-(y_3 + z_3)\,\mathbf{a_1} - z_3\,\mathbf{a_2} - y_3\,\mathbf{a_3}$	$=$	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8l)	C I
$\mathbf{B_9}$	$=$	$z_4\,\mathbf{a_1} + (x_4 + z_4)\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8m)	C II
$\mathbf{B_{10}}$	$=$	$z_4\,\mathbf{a_1} - (x_4 - z_4)\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8m)	C II
$\mathbf{B_{11}}$	$=$	$-z_4\,\mathbf{a_1} - (x_4 + z_4)\,\mathbf{a_2} - x_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8m)	C II
$\mathbf{B_{12}}$	$=$	$-z_4\,\mathbf{a_1} + (x_4 - z_4)\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8m)	C II
$\mathbf{B_{13}}$	$=$	$y_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + (x_5 + y_5)\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}}$	(8n)	C III
$\mathbf{B_{14}}$	$=$	$-y_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - (x_5 + y_5)\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}}$	(8n)	C III
$\mathbf{B_{15}}$	$=$	$y_5\,\mathbf{a_1} - x_5\,\mathbf{a_2} - (x_5 - y_5)\,\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}}$	(8n)	C III
$\mathbf{B_{16}}$	$=$	$-y_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + (x_5 - y_5)\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}}$	(8n)	C III
$\mathbf{B_{17}}$	$=$	$(y_6 + z_6)\,\mathbf{a_1} + (x_6 + z_6)\,\mathbf{a_2} + (x_6 + y_6)\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{18}}$	$=$	$-(y_6 - z_6)\,\mathbf{a_1} - (x_6 - z_6)\,\mathbf{a_2} - (x_6 + y_6)\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{19}}$	$=$	$(y_6 - z_6)\,\mathbf{a_1} - (x_6 + z_6)\,\mathbf{a_2} - (x_6 - y_6)\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{20}}$	$=$	$-(y_6 + z_6)\,\mathbf{a_1} + (x_6 - z_6)\,\mathbf{a_2} + (x_6 - y_6)\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{21}}$	$=$	$-(y_6 + z_6)\,\mathbf{a_1} - (x_6 + z_6)\,\mathbf{a_2} - (x_6 + y_6)\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{22}}$	$=$	$(y_6 - z_6)\,\mathbf{a_1} + (x_6 - z_6)\,\mathbf{a_2} + (x_6 + y_6)\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(16o)	C IV
$\mathbf{B_{23}}$	$=$	$-(y_6 - z_6)\,\mathbf{a_1} + (x_6 + z_6)\,\mathbf{a_2} + (x_6 - y_6)\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(16o)	C IV

$$\mathbf{B_{24}} = \quad (y_6 + z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - \qquad = \qquad -ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IV}$$
$$(x_6 - y_6)\,\mathbf{a}_3$$

$$\mathbf{B_{25}} = \quad (y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + \qquad = \qquad ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 + y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{26}} = \quad -(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \qquad = \qquad -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 + y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{27}} = \quad (y_7 - z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - \qquad = \qquad -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 - y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{28}} = \quad -(y_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \qquad = \qquad ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 - y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{29}} = \quad -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - \qquad = \qquad -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 + y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{30}} = \quad (y_7 - z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \qquad = \qquad ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 + y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{31}} = \quad -(y_7 - z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + \qquad = \qquad ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 - y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{32}} = \quad (y_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \qquad = \qquad -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C V}$$
$$(x_7 - y_7)\,\mathbf{a}_3$$

$$\mathbf{B_{33}} = \quad (y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + \qquad = \qquad ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 + y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{34}} = \quad -(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - \qquad = \qquad -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 + y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{35}} = \quad (y_8 - z_8)\,\mathbf{a}_1 - (x_8 + z_8)\,\mathbf{a}_2 - \qquad = \qquad -ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 - y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{36}} = \quad -(y_8 + z_8)\,\mathbf{a}_1 + (x_8 - z_8)\,\mathbf{a}_2 + \qquad = \qquad ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 - y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{37}} = \quad -(y_8 + z_8)\,\mathbf{a}_1 - (x_8 + z_8)\,\mathbf{a}_2 - \qquad = \qquad -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 + y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{38}} = \quad (y_8 - z_8)\,\mathbf{a}_1 + (x_8 - z_8)\,\mathbf{a}_2 + \qquad = \qquad ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 + y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{39}} = \quad -(y_8 - z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + \qquad = \qquad ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 - y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{40}} = \quad (y_8 + z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - \qquad = \qquad -ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VI}$$
$$(x_8 - y_8)\,\mathbf{a}_3$$

$$\mathbf{B_{41}} = \quad (y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + \qquad = \qquad ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 + y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{42}} = \quad -(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - \qquad = \qquad -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 + y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{43}} = \quad (y_9 - z_9)\,\mathbf{a}_1 - (x_9 + z_9)\,\mathbf{a}_2 - \qquad = \qquad -ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 - y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{44}} = \quad -(y_9 + z_9)\,\mathbf{a}_1 + (x_9 - z_9)\,\mathbf{a}_2 + \qquad = \qquad ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 - y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{45}} = \quad -(y_9 + z_9)\,\mathbf{a}_1 - (x_9 + z_9)\,\mathbf{a}_2 - \qquad = \qquad -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 + y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{46}} = \quad (y_9 - z_9)\,\mathbf{a}_1 + (x_9 - z_9)\,\mathbf{a}_2 + \qquad = \qquad ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 + y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{47}} = \quad -(y_9 - z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + \qquad = \qquad ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$
$$(x_9 - y_9)\,\mathbf{a}_3$$

$$\mathbf{B_{48}} = (y_9 + z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VII}$$

$$\mathbf{B_{49}} = (y_{10} + z_{10})\,\mathbf{a}_1 + (x_{10} + z_{10})\,\mathbf{a}_2 + (x_{10} + y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{50}} = -(y_{10} - z_{10})\,\mathbf{a}_1 - (x_{10} - z_{10})\,\mathbf{a}_2 - (x_{10} + y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{51}} = (y_{10} - z_{10})\,\mathbf{a}_1 - (x_{10} + z_{10})\,\mathbf{a}_2 - (x_{10} - y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{52}} = -(y_{10} + z_{10})\,\mathbf{a}_1 + (x_{10} - z_{10})\,\mathbf{a}_2 + (x_{10} - y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{53}} = -(y_{10} + z_{10})\,\mathbf{a}_1 - (x_{10} + z_{10})\,\mathbf{a}_2 - (x_{10} + y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{54}} = (y_{10} - z_{10})\,\mathbf{a}_1 + (x_{10} - z_{10})\,\mathbf{a}_2 + (x_{10} + y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{55}} = -(y_{10} - z_{10})\,\mathbf{a}_1 + (x_{10} + z_{10})\,\mathbf{a}_2 + (x_{10} - y_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{56}} = (y_{10} + z_{10})\,\mathbf{a}_1 - (x_{10} - z_{10})\,\mathbf{a}_2 - (x_{10} - y_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C VIII}$$

$$\mathbf{B_{57}} = (y_{11} + z_{11})\,\mathbf{a}_1 + (x_{11} + z_{11})\,\mathbf{a}_2 + (x_{11} + y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{58}} = -(y_{11} - z_{11})\,\mathbf{a}_1 - (x_{11} - z_{11})\,\mathbf{a}_2 - (x_{11} + y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{59}} = (y_{11} - z_{11})\,\mathbf{a}_1 - (x_{11} + z_{11})\,\mathbf{a}_2 - (x_{11} - y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{60}} = -(y_{11} + z_{11})\,\mathbf{a}_1 + (x_{11} - z_{11})\,\mathbf{a}_2 + (x_{11} - y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{61}} = -(y_{11} + z_{11})\,\mathbf{a}_1 - (x_{11} + z_{11})\,\mathbf{a}_2 - (x_{11} + y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{62}} = (y_{11} - z_{11})\,\mathbf{a}_1 + (x_{11} - z_{11})\,\mathbf{a}_2 + (x_{11} + y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{63}} = -(y_{11} - z_{11})\,\mathbf{a}_1 + (x_{11} + z_{11})\,\mathbf{a}_2 + (x_{11} - y_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

$$\mathbf{B_{64}} = (y_{11} + z_{11})\,\mathbf{a}_1 - (x_{11} - z_{11})\,\mathbf{a}_2 - (x_{11} - y_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (16\text{o}) \qquad \text{C IX}$$

References

[1] Y. Yoshida, Y. Kubozono, S. Kashino, and Y. Murakami, *Structure and electronic properties of Cs_3C_{60} under ambient pressure revealed by X-ray diffraction and ESR*, Chem. Phys. Lett. **291**, 31–36 (1998), doi:10.1016/S0009-2614(98)00598-3.