

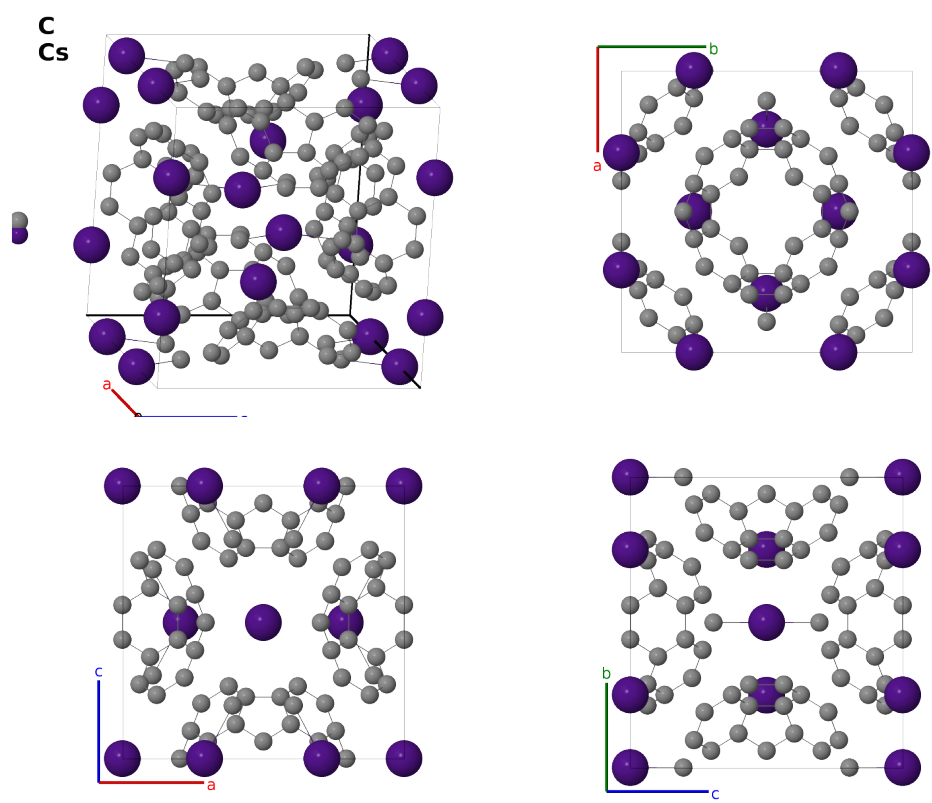
Orthorhombic Fullerene (Cs_3C_{60}) Structure: A15B_oI128_71_lmn6o_eg-001

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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/88NV>

https://aflow.org/prototype-encyclopedia/A15B_oI128_71_lmn6o_eg-001

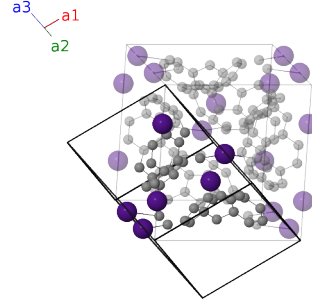


Prototype	C_{60}Cs_3
AFLOW prototype label	A15B_oI128_71_lmn6o_eg-001
Pearson symbol	oI128
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	<pre>aflow --proto=A15B_oI128_71_lmn6o_eg-001 --params=a, b/a, c/a, x1, y2, y3, z3, x4, z4, x5, y5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11</pre>

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

Body-centered Orthorhombic primitive vectors

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



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

$\mathbf{B}_{24}$	$=$	$(y_6 + z_6) \mathbf{a}_1 - (x_6 - z_6) \mathbf{a}_2 -$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	$(16o)$	C IV
		$(x_6 - y_6) \mathbf{a}_3$				
$\mathbf{B}_{25}$	$=$	$(y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 +$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 + y_7) \mathbf{a}_3$				
$\mathbf{B}_{26}$	$=$	$-(y_7 - z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 + y_7) \mathbf{a}_3$				
$\mathbf{B}_{27}$	$=$	$(y_7 - z_7) \mathbf{a}_1 - (x_7 + z_7) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 - y_7) \mathbf{a}_3$				
$\mathbf{B}_{28}$	$=$	$-(y_7 + z_7) \mathbf{a}_1 + (x_7 - z_7) \mathbf{a}_2 +$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 - y_7) \mathbf{a}_3$				
$\mathbf{B}_{29}$	$=$	$-(y_7 + z_7) \mathbf{a}_1 - (x_7 + z_7) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 + y_7) \mathbf{a}_3$				
$\mathbf{B}_{30}$	$=$	$(y_7 - z_7) \mathbf{a}_1 + (x_7 - z_7) \mathbf{a}_2 +$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 + y_7) \mathbf{a}_3$				
$\mathbf{B}_{31}$	$=$	$-(y_7 - z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 +$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 - y_7) \mathbf{a}_3$				
$\mathbf{B}_{32}$	$=$	$(y_7 + z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	$(16o)$	C V
		$(x_7 - y_7) \mathbf{a}_3$				
$\mathbf{B}_{33}$	$=$	$(y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 +$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 + y_8) \mathbf{a}_3$				
$\mathbf{B}_{34}$	$=$	$-(y_8 - z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 + y_8) \mathbf{a}_3$				
$\mathbf{B}_{35}$	$=$	$(y_8 - z_8) \mathbf{a}_1 - (x_8 + z_8) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 - y_8) \mathbf{a}_3$				
$\mathbf{B}_{36}$	$=$	$-(y_8 + z_8) \mathbf{a}_1 + (x_8 - z_8) \mathbf{a}_2 +$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 - y_8) \mathbf{a}_3$				
$\mathbf{B}_{37}$	$=$	$-(y_8 + z_8) \mathbf{a}_1 - (x_8 + z_8) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 + y_8) \mathbf{a}_3$				
$\mathbf{B}_{38}$	$=$	$(y_8 - z_8) \mathbf{a}_1 + (x_8 - z_8) \mathbf{a}_2 +$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 + y_8) \mathbf{a}_3$				
$\mathbf{B}_{39}$	$=$	$-(y_8 - z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 +$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 - y_8) \mathbf{a}_3$				
$\mathbf{B}_{40}$	$=$	$(y_8 + z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	$(16o)$	C VI
		$(x_8 - y_8) \mathbf{a}_3$				
$\mathbf{B}_{41}$	$=$	$(y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 +$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	$(16o)$	C VII
		$(x_9 + y_9) \mathbf{a}_3$				
$\mathbf{B}_{42}$	$=$	$-(y_9 - z_9) \mathbf{a}_1 - (x_9 - z_9) \mathbf{a}_2 -$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	$(16o)$	C VII
		$(x_9 + y_9) \mathbf{a}_3$				
$\mathbf{B}_{43}$	$=$	$(y_9 - z_9) \mathbf{a}_1 - (x_9 + z_9) \mathbf{a}_2 -$	$=$	$-ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	$(16o)$	C VII
		$(x_9 - y_9) \mathbf{a}_3$				
$\mathbf{B}_{44}$	$=$	$-(y_9 + z_9) \mathbf{a}_1 + (x_9 - z_9) \mathbf{a}_2 +$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	$(16o)$	C VII
		$(x_9$				

$$\begin{aligned}
\mathbf{B}_{48} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 - (x_9 - z_9) \mathbf{a}_2 - \\ (x_9 - y_9) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16o) & \text{C VII} \\
\mathbf{B}_{49} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 + \\ (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 - \\ (x_{10} - z_{10}) \mathbf{a}_2 - (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{51} &= \begin{pmatrix} (y_{10} - z_{10}) \mathbf{a}_1 - (x_{10} + z_{10}) \mathbf{a}_2 - \\ (x_{10} - y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{52} &= \begin{pmatrix} -(y_{10} + z_{10}) \mathbf{a}_1 + \\ (x_{10} - z_{10}) \mathbf{a}_2 + (x_{10} - y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{53} &= \begin{pmatrix} -(y_{10} + z_{10}) \mathbf{a}_1 - \\ (x_{10} + z_{10}) \mathbf{a}_2 - (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{54} &= \begin{pmatrix} (y_{10} - z_{10}) \mathbf{a}_1 + (x_{10} - z_{10}) \mathbf{a}_2 + \\ (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{55} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 + \\ (x_{10} + z_{10}) \mathbf{a}_2 + (x_{10} - y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{56} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 - (x_{10} - z_{10}) \mathbf{a}_2 - \\ (x_{10} - y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (16o) & \text{C VIII} \\
\mathbf{B}_{57} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 + (x_{11} + z_{11}) \mathbf{a}_2 + \\ (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{58} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 - \\ (x_{11} - z_{11}) \mathbf{a}_2 - (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{59} &= \begin{pmatrix} (y_{11} - z_{11}) \mathbf{a}_1 - (x_{11} + z_{11}) \mathbf{a}_2 - \\ (x_{11} - y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{60} &= \begin{pmatrix} -(y_{11} + z_{11}) \mathbf{a}_1 + \\ (x_{11} - z_{11}) \mathbf{a}_2 + (x_{11} - y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{61} &= \begin{pmatrix} -(y_{11} + z_{11}) \mathbf{a}_1 - \\ (x_{11} + z_{11}) \mathbf{a}_2 - (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{62} &= \begin{pmatrix} (y_{11} - z_{11}) \mathbf{a}_1 + (x_{11} - z_{11}) \mathbf{a}_2 + \\ (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{63} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 + \\ (x_{11} + z_{11}) \mathbf{a}_2 + (x_{11} - y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX} \\
\mathbf{B}_{64} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 - (x_{11} - z_{11}) \mathbf{a}_2 - \\ (x_{11} - y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (16o) & \text{C IX}
\end{aligned}$$

References

- [1] Y. Yoshida, Y. Kubozono, S. Kashino, and Y. Murakami, *Structure and electronic properties of Cs₃C₆₀ 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.

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