Stepanovite (NaMgFe(C_2O_4)$_3$·9H$_2$O) Structure: A6BC18DEF21_hR96_161_2b_a_6b_a_a_7b-001

https://aflow.org/p/KKZD

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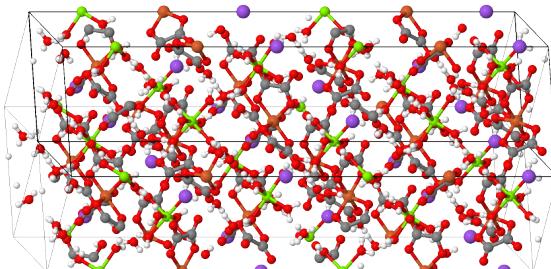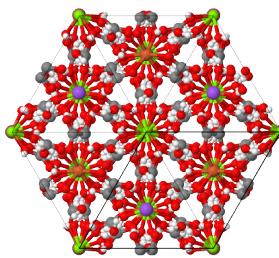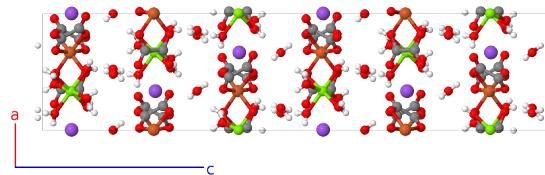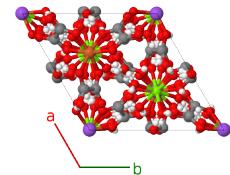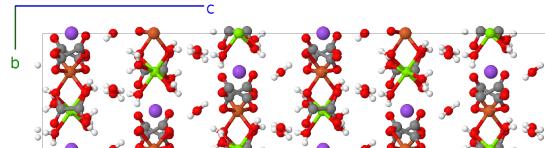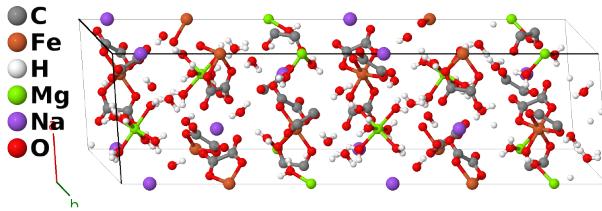
Prototype	$C_2FeH_6MgNaO_7$
AFLOW prototype label	A6BC18DEF21_hR96_161_2b_a_6b_a_a_7b-001
Mineral name	stepanovite
ICSD	252894
Pearson symbol	hR96
Space group number	161
Space group symbol	$R3c$
AFLOW prototype command	aflow --proto=A6BC18DEF21_hR96_161_2b_a_6b_a_a_7b-001

$$\text{--params=}a, c/a, x_1, x_2, x_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9,$$
$$x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17},$$
$$y_{17}, z_{17}, x_{18}, y_{18}, z_{18}$$

Other compounds with this structure

NaMgAl(C_2O_4)$_3$·8H$_2$O (zhemchuzhnikovite)

- We use the data for stoichiometric synthetic stepanovite from (Huskć, 2016). Natural stepanovite, as well as zhemchuzhnikovite, contains between 8 and 9 water molecules per formula unit.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
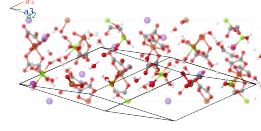
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + x_1\,\mathbf{a_3}$	$=$	$cx_1\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_2}$	$=$	$\left(x_1+\tfrac{1}{2}\right)\mathbf{a_1} + \left(x_1+\tfrac{1}{2}\right)\mathbf{a_2} + \left(x_1+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$c\left(x_1+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_3}$	$=$	$x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	$=$	$cx_2\,\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_4}$	$=$	$\left(x_2+\tfrac{1}{2}\right)\mathbf{a_1} + \left(x_2+\tfrac{1}{2}\right)\mathbf{a_2} + \left(x_2+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$c\left(x_2+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2a)	Mg I
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + x_3\,\mathbf{a_3}$	$=$	$cx_3\,\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_6}$	$=$	$\left(x_3+\tfrac{1}{2}\right)\mathbf{a_1} + \left(x_3+\tfrac{1}{2}\right)\mathbf{a_2} + \left(x_3+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$c\left(x_3+\tfrac{1}{2}\right)\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_7}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_8}$	$=$	$z_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_9}$	$=$	$y_4\,\mathbf{a_1} + z_4\,\mathbf{a_2} + x_4\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_4+y_4+z_4\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_{10}}$	$=$	$\left(z_4+\tfrac{1}{2}\right)\mathbf{a_1} + \left(y_4+\tfrac{1}{2}\right)\mathbf{a_2} + \left(x_4+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_4-z_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4-2y_4+z_4\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_{11}}$	$=$	$\left(y_4+\tfrac{1}{2}\right)\mathbf{a_1} + \left(x_4+\tfrac{1}{2}\right)\mathbf{a_2} + \left(z_4+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_4-z_4\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_4-y_4-z_4\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_{12}}$	$=$	$\left(x_4+\tfrac{1}{2}\right)\mathbf{a_1} + \left(z_4+\tfrac{1}{2}\right)\mathbf{a_2} + \left(y_4+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_4-y_4\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_4+y_4-2z_4\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_4+2y_4+2z_4+3\right)\hat{\mathbf{z}}$	(6b)	C I
$\mathbf{B_{13}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(6b)	C II
$\mathbf{B_{14}}$	$=$	$z_5\,\mathbf{a_1} + x_5\,\mathbf{a_2} + y_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(6b)	C II
$\mathbf{B_{15}}$	$=$	$y_5\,\mathbf{a_1} + z_5\,\mathbf{a_2} + x_5\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_5+y_5+z_5\right)\hat{\mathbf{z}}$	(6b)	C II
$\mathbf{B_{16}}$	$=$	$\left(z_5+\tfrac{1}{2}\right)\mathbf{a_1} + \left(y_5+\tfrac{1}{2}\right)\mathbf{a_2} + \left(x_5+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_5-z_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5-2y_5+z_5\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(6b)	C II
$\mathbf{B_{17}}$	$=$	$\left(y_5+\tfrac{1}{2}\right)\mathbf{a_1} + \left(x_5+\tfrac{1}{2}\right)\mathbf{a_2} + \left(z_5+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(y_5-z_5\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_5-y_5-z_5\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(6b)	C II
$\mathbf{B_{18}}$	$=$	$\left(x_5+\tfrac{1}{2}\right)\mathbf{a_1} + \left(z_5+\tfrac{1}{2}\right)\mathbf{a_2} + \left(y_5+\tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_5-y_5\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_5+y_5-2z_5\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_5+2y_5+2z_5+3\right)\hat{\mathbf{z}}$	(6b)	C II

$$\mathbf{B_{19}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \frac{1}{2}a\left(x_6 - z_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_6 - 2y_6 + z_6\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_6 + y_6 + z_6\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{20}} = z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3 = -\frac{1}{2}a\left(y_6 - z_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_6 - y_6 - z_6\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_6 + y_6 + z_6\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{21}} = y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3 = -\frac{1}{2}a\left(x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_6 + y_6 - 2z_6\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_6 + y_6 + z_6\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{22}} = \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\frac{1}{2}a\left(x_6 - z_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_6 - 2y_6 + z_6\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_6 + 2y_6 + 2z_6 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{23}} = \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(y_6 - z_6\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_6 - y_6 - z_6\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_6 + 2y_6 + 2z_6 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{24}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(x_6 - y_6\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_6 + y_6 - 2z_6\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_6 + 2y_6 + 2z_6 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H I}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \frac{1}{2}a\left(x_7 - z_7\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_7 - 2y_7 + z_7\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{26}} = z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + y_7\,\mathbf{a}_3 = -\frac{1}{2}a\left(y_7 - z_7\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_7 - y_7 - z_7\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{27}} = y_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3 = -\frac{1}{2}a\left(x_7 - y_7\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_7 + y_7 - 2z_7\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_7 + y_7 + z_7\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{28}} = \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\frac{1}{2}a\left(x_7 - z_7\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_7 - 2y_7 + z_7\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_7 + 2y_7 + 2z_7 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{29}} = \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(y_7 - z_7\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_7 - y_7 - z_7\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_7 + 2y_7 + 2z_7 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{30}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(x_7 - y_7\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_7 + y_7 - 2z_7\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_7 + 2y_7 + 2z_7 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H II}$$

$$\mathbf{B_{31}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \frac{1}{2}a\left(x_8 - z_8\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_8 - 2y_8 + z_8\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{32}} = z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = -\frac{1}{2}a\left(y_8 - z_8\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_8 - y_8 - z_8\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{33}} = y_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3 = -\frac{1}{2}a\left(x_8 - y_8\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_8 + y_8 - 2z_8\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_8 + y_8 + z_8\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{34}} = \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\frac{1}{2}a\left(x_8 - z_8\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_8 - 2y_8 + z_8\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_8 + 2y_8 + 2z_8 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{35}} = \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(y_8 - z_8\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_8 - y_8 - z_8\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_8 + 2y_8 + 2z_8 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{36}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(x_8 - y_8\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_8 + y_8 - 2z_8\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_8 + 2y_8 + 2z_8 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H III}$$

$$\mathbf{B_{37}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \frac{1}{2}a\left(x_9 - z_9\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_9 - 2y_9 + z_9\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H IV}$$

$$\mathbf{B_{38}} = z_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = -\frac{1}{2}a\left(y_9 - z_9\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_9 - y_9 - z_9\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H IV}$$

$$\mathbf{B_{39}} = y_9\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + x_9\,\mathbf{a}_3 = -\frac{1}{2}a\left(x_9 - y_9\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_9 + y_9 - 2z_9\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_9 + y_9 + z_9\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H IV}$$

$$\mathbf{B_{40}} = \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = -\frac{1}{2}a\left(x_9 - z_9\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_9 - 2y_9 + z_9\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_9 + 2y_9 + 2z_9 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H IV}$$

$$\mathbf{B_{41}} = \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = \frac{1}{2}a\left(y_9 - z_9\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_9 - y_9 - z_9\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_9 + 2y_9 + 2z_9 + 3\right)\hat{\mathbf{z}} \quad (6b) \qquad \text{H IV}$$

$$\mathbf{B_{42}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_9 - y_9\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_9 + y_9 - 2z_9\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_9 + 2y_9 + 2z_9 + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H IV}$$

$$\mathbf{B_{43}} = x_{10}\mathbf{a}_1 + y_{10}\mathbf{a}_2 + z_{10}\mathbf{a}_3 = \tfrac{1}{2}a\left(x_{10} - z_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} - 2y_{10} + z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{44}} = z_{10}\mathbf{a}_1 + x_{10}\mathbf{a}_2 + y_{10}\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_{10} - z_{10}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{10} - y_{10} - z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{45}} = y_{10}\mathbf{a}_1 + z_{10}\mathbf{a}_2 + x_{10}\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_{10} - y_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} + y_{10} - 2z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{10} + y_{10} + z_{10}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{46}} = \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_{10} - z_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} - 2y_{10} + z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{10} + 2y_{10} + 2z_{10} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{47}} = \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_{10} - z_{10}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{10} - y_{10} - z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{10} + 2y_{10} + 2z_{10} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{48}} = \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_{10} - y_{10}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{10} + y_{10} - 2z_{10}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{10} + 2y_{10} + 2z_{10} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H V}$$

$$\mathbf{B_{49}} = x_{11}\mathbf{a}_1 + y_{11}\mathbf{a}_2 + z_{11}\mathbf{a}_3 = \tfrac{1}{2}a\left(x_{11} - z_{11}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{11} - 2y_{11} + z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{11} + y_{11} + z_{11}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{50}} = z_{11}\mathbf{a}_1 + x_{11}\mathbf{a}_2 + y_{11}\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_{11} - z_{11}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{11} - y_{11} - z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{11} + y_{11} + z_{11}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{51}} = y_{11}\mathbf{a}_1 + z_{11}\mathbf{a}_2 + x_{11}\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_{11} - y_{11}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{11} + y_{11} - 2z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{11} + y_{11} + z_{11}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{52}} = \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{11} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_{11} - z_{11}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{11} - 2y_{11} + z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{11} + 2y_{11} + 2z_{11} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{53}} = \left(y_{11} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(y_{11} - z_{11}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{11} - y_{11} - z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{11} + 2y_{11} + 2z_{11} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{54}} = \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{11} + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{2}a\left(x_{11} - y_{11}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{11} + y_{11} - 2z_{11}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{11} + 2y_{11} + 2z_{11} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{H VI}$$

$$\mathbf{B_{55}} = x_{12}\mathbf{a}_1 + y_{12}\mathbf{a}_2 + z_{12}\mathbf{a}_3 = \tfrac{1}{2}a\left(x_{12} - z_{12}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{12} - 2y_{12} + z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{12} + y_{12} + z_{12}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{56}} = z_{12}\mathbf{a}_1 + x_{12}\mathbf{a}_2 + y_{12}\mathbf{a}_3 = -\tfrac{1}{2}a\left(y_{12} - z_{12}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{12} - y_{12} - z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{12} + y_{12} + z_{12}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{57}} = y_{12}\mathbf{a}_1 + z_{12}\mathbf{a}_2 + x_{12}\mathbf{a}_3 = -\tfrac{1}{2}a\left(x_{12} - y_{12}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{12} + y_{12} - 2z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{12} + y_{12} + z_{12}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{58}} = \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{12} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(x_{12} - z_{12}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{12} - 2y_{12} + z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{12} + 2y_{12} + 2z_{12} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{59}} = \left(y_{12} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(y_{12} - z_{12}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{12} - y_{12} - z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{12} + 2y_{12} + 2z_{12} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{60}} = \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{12} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{12} - y_{12}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{12} + y_{12} - 2z_{12}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{12} + 2y_{12} + 2z_{12} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O I}$$

$$\mathbf{B_{61}} = x_{13}\mathbf{a}_1 + y_{13}\mathbf{a}_2 + z_{13}\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{13} - z_{13}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{13} - 2y_{13} + z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{13} + y_{13} + z_{13}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{62}} = z_{13}\mathbf{a}_1 + x_{13}\mathbf{a}_2 + y_{13}\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(y_{13} - z_{13}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{13} - y_{13} - z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{13} + y_{13} + z_{13}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{63}} = y_{13}\mathbf{a}_1 + z_{13}\mathbf{a}_2 + x_{13}\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(x_{13} - y_{13}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{13} + y_{13} - 2z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{13} + y_{13} + z_{13}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{64}} = \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{13} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(x_{13} - z_{13}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{13} - 2y_{13} + z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{13} + 2y_{13} + 2z_{13} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{65}} = \left(y_{13} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(y_{13} - z_{13}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{13} - y_{13} - z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{13} + 2y_{13} + 2z_{13} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{66}} = \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{13} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{13} - y_{13}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{13} + y_{13} - 2z_{13}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{13} + 2y_{13} + 2z_{13} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O II}$$

$$\mathbf{B_{67}} = x_{14}\mathbf{a}_1 + y_{14}\mathbf{a}_2 + z_{14}\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{14} - z_{14}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{14} - 2y_{14} + z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{14} + y_{14} + z_{14}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{68}} = z_{14}\mathbf{a}_1 + x_{14}\mathbf{a}_2 + y_{14}\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(y_{14} - z_{14}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{14} - y_{14} - z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{14} + y_{14} + z_{14}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{69}} = y_{14}\mathbf{a}_1 + z_{14}\mathbf{a}_2 + x_{14}\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(x_{14} - y_{14}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{14} + y_{14} - 2z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{14} + y_{14} + z_{14}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{70}} = \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{14} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad -\tfrac{1}{2}a\left(x_{14} - z_{14}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{14} - 2y_{14} + z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{14} + 2y_{14} + 2z_{14} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{71}} = \left(y_{14} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(y_{14} - z_{14}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{14} - y_{14} - z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{14} + 2y_{14} + 2z_{14} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{72}} = \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{14} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{14} - y_{14}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{14} + y_{14} - 2z_{14}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{14} + 2y_{14} + 2z_{14} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O III}$$

$$\mathbf{B_{73}} = x_{15}\mathbf{a}_1 + y_{15}\mathbf{a}_2 + z_{15}\mathbf{a}_3 \qquad = \qquad \tfrac{1}{2}a\left(x_{15} - z_{15}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{15} - 2y_{15} + z_{15}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{15} + y_{15} + z_{15}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O IV}$$

$$\mathbf{B_{74}} = z_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + y_{15}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(y_{15} - z_{15})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{15} - y_{15} - z_{15})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{15} + y_{15} + z_{15})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O IV

$$\mathbf{B_{75}} = y_{15}\,\mathbf{a}_1 + z_{15}\,\mathbf{a}_2 + x_{15}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{15} - y_{15})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{15} + y_{15} - 2z_{15})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{15} + y_{15} + z_{15})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O IV

$$\mathbf{B_{76}} = \left(z_{15} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{15} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{15} - z_{15})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{15} - 2y_{15} + z_{15})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{15} + 2y_{15} + 2z_{15} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O IV

$$\mathbf{B_{77}} = \left(y_{15} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{15} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(y_{15} - z_{15})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{15} - y_{15} - z_{15})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{15} + 2y_{15} + 2z_{15} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O IV

$$\mathbf{B_{78}} = \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{15} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{15} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(x_{15} - y_{15})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{15} + y_{15} - 2z_{15})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{15} + 2y_{15} + 2z_{15} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O IV

$$\mathbf{B_{79}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(x_{16} - z_{16})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{16} - 2y_{16} + z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{16} + y_{16} + z_{16})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{80}} = z_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + y_{16}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(y_{16} - z_{16})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{16} - y_{16} - z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{16} + y_{16} + z_{16})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{81}} = y_{16}\,\mathbf{a}_1 + z_{16}\,\mathbf{a}_2 + x_{16}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{16} - y_{16})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{16} + y_{16} - 2z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{16} + y_{16} + z_{16})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{82}} = \left(z_{16} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{16} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{16} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{16} - z_{16})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{16} - 2y_{16} + z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{16} + 2y_{16} + 2z_{16} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{83}} = \left(y_{16} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{16} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{16} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(y_{16} - z_{16})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{16} - y_{16} - z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{16} + 2y_{16} + 2z_{16} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{84}} = \left(x_{16} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{16} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{16} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(x_{16} - y_{16})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{16} + y_{16} - 2z_{16})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{16} + 2y_{16} + 2z_{16} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O V

$$\mathbf{B_{85}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(x_{17} - z_{17})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{17} - 2y_{17} + z_{17})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{17} + y_{17} + z_{17})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O VI

$$\mathbf{B_{86}} = z_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + y_{17}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(y_{17} - z_{17})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{17} - y_{17} - z_{17})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{17} + y_{17} + z_{17})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O VI

$$\mathbf{B_{87}} = y_{17}\,\mathbf{a}_1 + z_{17}\,\mathbf{a}_2 + x_{17}\,\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{17} - y_{17})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{17} + y_{17} - 2z_{17})\,\hat{\mathbf{y}} + \\ \frac{1}{3}c\,(x_{17} + y_{17} + z_{17})\,\hat{\mathbf{z}} \end{array}$$ (6b)   O VI

$$\mathbf{B_{88}} = \left(z_{17} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{17} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{17} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} -\frac{1}{2}a\,(x_{17} - z_{17})\,\hat{\mathbf{x}} - \\ \frac{\sqrt{3}}{6}a\,(x_{17} - 2y_{17} + z_{17})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{17} + 2y_{17} + 2z_{17} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O VI

$$\mathbf{B_{89}} = \left(y_{17} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{17} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{17} + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{array}{l} \frac{1}{2}a\,(y_{17} - z_{17})\,\hat{\mathbf{x}} + \\ \frac{\sqrt{3}}{6}a\,(2x_{17} - y_{17} - z_{17})\,\hat{\mathbf{y}} + \\ \frac{1}{6}c\,(2x_{17} + 2y_{17} + 2z_{17} + 3)\,\hat{\mathbf{z}} \end{array}$$ (6b)   O VI

$$\mathbf{B_{90}} = \left(x_{17} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{17} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{17} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad \tfrac{1}{2}a\left(x_{17} - y_{17}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{17} + y_{17} - 2z_{17}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{17} + 2y_{17} + 2z_{17} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VI}$$

$$\mathbf{B_{91}} = x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 \quad = \quad \tfrac{1}{2}a\left(x_{18} - z_{18}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{18} - 2y_{18} + z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{18} + y_{18} + z_{18}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

$$\mathbf{B_{92}} = z_{18}\,\mathbf{a}_1 + x_{18}\,\mathbf{a}_2 + y_{18}\,\mathbf{a}_3 \quad = \quad -\tfrac{1}{2}a\left(y_{18} - z_{18}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{18} - y_{18} - z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{18} + y_{18} + z_{18}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

$$\mathbf{B_{93}} = y_{18}\,\mathbf{a}_1 + z_{18}\,\mathbf{a}_2 + x_{18}\,\mathbf{a}_3 \quad = \quad -\tfrac{1}{2}a\left(x_{18} - y_{18}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{18} + y_{18} - 2z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{3}c\left(x_{18} + y_{18} + z_{18}\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

$$\mathbf{B_{94}} = \left(z_{18} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{18} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_{18} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad -\tfrac{1}{2}a\left(x_{18} - z_{18}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{18} - 2y_{18} + z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{18} + 2y_{18} + 2z_{18} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

$$\mathbf{B_{95}} = \left(y_{18} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_{18} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_{18} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad \tfrac{1}{2}a\left(y_{18} - z_{18}\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\left(2x_{18} - y_{18} - z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{18} + 2y_{18} + 2z_{18} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

$$\mathbf{B_{96}} = \left(x_{18} + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(z_{18} + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_{18} + \tfrac{1}{2}\right)\mathbf{a}_3 \quad = \quad \tfrac{1}{2}a\left(x_{18} - y_{18}\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\left(x_{18} + y_{18} - 2z_{18}\right)\hat{\mathbf{y}} + \tfrac{1}{6}c\left(2x_{18} + 2y_{18} + 2z_{18} + 3\right)\hat{\mathbf{z}} \qquad \text{(6b)} \qquad \text{O VII}$$

References

[1] I. Huskić, I. V. Pekov, S. V. Krivovichev, and T. Friščić, *Minerals with metal-organic framework structures*, Sci. Adv. **2**, 1600621 (2016), doi:10.1126/sciadv.1600621.