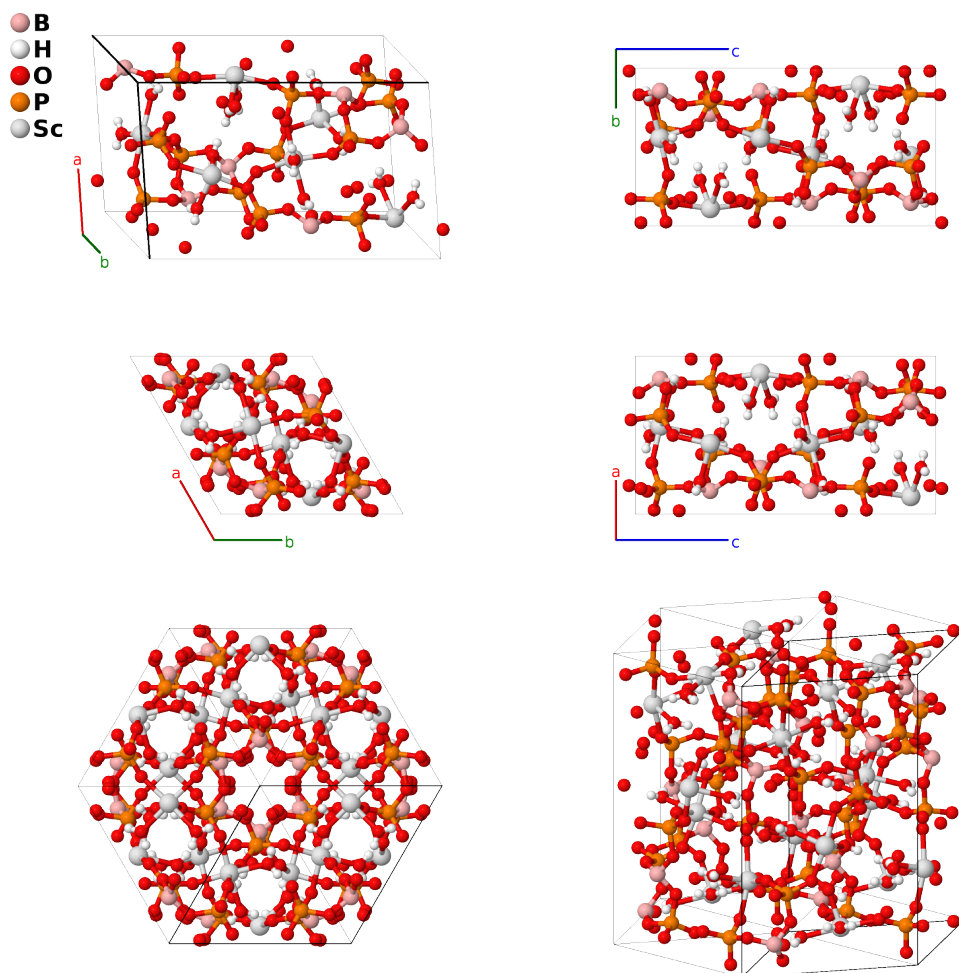


# Sc(H<sub>2</sub>O)<sub>2</sub>[BP<sub>2</sub>O<sub>8</sub>]·H<sub>2</sub>O Structure: AB4C12D2E\_hP120\_179\_b\_2c\_6c\_c\_b-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/1CPH>

[https://aflow.org/p/AB4C12D2E\\_hP120\\_179\\_b\\_2c\\_6c\\_c\\_b-001](https://aflow.org/p/AB4C12D2E_hP120_179_b_2c_6c_c_b-001)

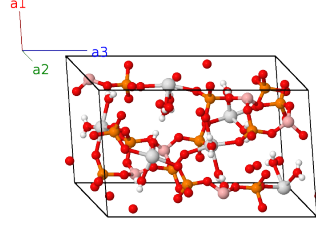


Prototype	BH <sub>4</sub> O <sub>12</sub> P <sub>2</sub> Sc
AFLOW prototype label	AB4C12D2E_hP120_179_b_2c_6c_c_b-001
ICSD	416075
Pearson symbol	hP120
Space group number	179
Space group symbol	<i>P</i> 6 <sub>5</sub> 22
AFLOW prototype command	<pre>aflow --proto=AB4C12D2E_hP120_179_b_2c_6c_c_b-001       --params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>,       y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub></pre>

- The O-VI (12c) site, actually a water molecule with undetermined hydrogen positions, is only occupied 50% of the time.
- There is also a “dehydrated” form,  $\text{Sc}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]$ , where these water molecules are not present.
- This structure can also be found in the enantiomorphic space group  $P6_122$  #178.

### Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_2$	$-2x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{5}{12} \mathbf{a}_3$	=	$-\frac{3}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_3$	$x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{12} \mathbf{a}_3$	=	$-\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{1}{12}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_4$	$-x_1 \mathbf{a}_1 - 2x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-\frac{3}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_5$	$2x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{11}{12} \mathbf{a}_3$	=	$\frac{3}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{11}{12}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_6$	$-x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{7}{12} \mathbf{a}_3$	=	$\sqrt{3}ax_1 \hat{\mathbf{y}} + \frac{7}{12}c \hat{\mathbf{z}}$	(6b)	B I
$\mathbf{B}_7$	$x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_8$	$-2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{5}{12} \mathbf{a}_3$	=	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_9$	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{12} \mathbf{a}_3$	=	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{12}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_{10}$	$-x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_{11}$	$2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{11}{12} \mathbf{a}_3$	=	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{11}{12}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_{12}$	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{7}{12} \mathbf{a}_3$	=	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{7}{12}c \hat{\mathbf{z}}$	(6b)	Sc I
$\mathbf{B}_{13}$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{14}$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{15}$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{16}$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{17}$	$y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{6}) \mathbf{a}_3$	=	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{18}$	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{5}{6}) \mathbf{a}_3$	=	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{6}c(6z_3 + 5) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{19}$	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{20}$	$(x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{21}$	$-x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	H I
$\mathbf{B}_{22}$	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{6}) \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - c(z_3 - \frac{1}{6}) \hat{\mathbf{z}}$	(12c)	H I

$$\begin{aligned}
\mathbf{B}_{23} &= -(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{H I} \\
\mathbf{B}_{24} &= x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - \frac{1}{6}c(6z_3 - 5) \hat{\mathbf{z}} & (12c) & \text{H I} \\
\mathbf{B}_{25} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 = \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{26} &= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{27} &= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{28} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{29} &= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{30} &= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{6}c(6z_4 + 5) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{31} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{32} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{33} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{34} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - c(z_4 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{35} &= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{36} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - \frac{1}{6}c(6z_4 - 5) \hat{\mathbf{z}} & (12c) & \text{H II} \\
\mathbf{B}_{37} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{38} &= -y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{39} &= -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{40} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{41} &= y_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{42} &= (x_5 - y_5) \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{6}c(6z_5 + 5) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{43} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - (z_5 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - \frac{1}{3}c(3z_5 - 2) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{44} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{45} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{46} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - c(z_5 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{47} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{48} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - \frac{1}{6}c(6z_5 - 5) \hat{\mathbf{z}} & (12c) & \text{O I} \\
\mathbf{B}_{49} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{50} &= -y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{51} &= -(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{52} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{53} &= y_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{54} &= (x_6 - y_6) \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{6}c(6z_6 + 5) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{55} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - \frac{1}{3}c(3z_6 - 2) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{56} &= (x_6 - y_6) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = \frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{57} &= -x_6 \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{58} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} - c(z_6 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{59} &= -(x_6 - y_6) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_6 + 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{60} &= x_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} - \frac{1}{6}c(6z_6 - 5) \hat{\mathbf{z}} & (12c) & \text{O II} \\
\mathbf{B}_{61} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 = \frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{62} &= -y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{63} &= -(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{64} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{65} &= y_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{66} &= (x_7 - y_7) \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + \frac{1}{6}c(6z_7 + 5) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{67} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - (z_7 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - \frac{1}{3}c(3z_7 - 2) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{68} &= (x_7 - y_7) \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 = \frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{69} &= -x_7 \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{70} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - (z_7 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} - c(z_7 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{71} &= -(x_7 - y_7) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_7 + 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{72} &= x_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 - (z_7 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} - \frac{1}{6}c(6z_7 - 5) \hat{\mathbf{z}} & (12c) & \text{O III} \\
\mathbf{B}_{73} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = \frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{74} &= -y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + \frac{1}{3}c(3z_8 + 2) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{75} &= -(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{76} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{77} &= y_8 \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_8 + 2y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{78} &= (x_8 - y_8) \mathbf{a}_1 + x_8 \mathbf{a}_2 + (z_8 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + \frac{1}{6}c(6z_8 + 5) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{79} &= y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - (z_8 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} - \frac{1}{3}c(3z_8 - 2) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{80} &= (x_8 - y_8) \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = \frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (12c) & \text{O IV}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{81} &= -x_8 \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - (z_8 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{82} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - (z_8 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} - c(z_8 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{83} &= -(x_8 - y_8) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_8 + 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{84} &= x_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 - (z_8 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} - \frac{1}{6}c(6z_8 - 5) \hat{\mathbf{z}} & (12c) & \text{O IV} \\
\mathbf{B}_{85} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = \frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{86} &= -y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + \frac{1}{3}c(3z_9 + 2) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{87} &= -(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + (z_9 + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{88} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{89} &= y_9 \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_9 + 2y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{90} &= (x_9 - y_9) \mathbf{a}_1 + x_9 \mathbf{a}_2 + (z_9 + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + \frac{1}{6}c(6z_9 + 5) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{91} &= y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - (z_9 - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} - \frac{1}{3}c(3z_9 - 2) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{92} &= (x_9 - y_9) \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = \frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{93} &= -x_9 \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - (z_9 - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{94} &= -y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - (z_9 - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} - c(z_9 - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{95} &= -(x_9 - y_9) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_9 + 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{96} &= x_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 - (z_9 - \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} - \frac{1}{6}c(6z_9 - 5) \hat{\mathbf{z}} & (12c) & \text{O V} \\
\mathbf{B}_{97} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{98} &= -y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + \frac{1}{3}c(3z_{10} + 2) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{99} &= -(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{100} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 = -\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{101} &= y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{6}) \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{102} &= (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + (z_{10} + \frac{5}{6}) \mathbf{a}_3 = \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + \frac{1}{6}c(6z_{10} + 5) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{103} &= y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - (z_{10} - \frac{2}{3}) \mathbf{a}_3 = \frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(3z_{10} - 2) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{104} &= (x_{10} - y_{10}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 = \frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{105} &= -x_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{1}{3}) \mathbf{a}_3 = -\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{3}) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{106} &= -y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{6}) \mathbf{a}_3 = -\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{6}) \hat{\mathbf{z}} & (12c) & \text{O VI} \\
\mathbf{B}_{107} &= -(x_{10} - y_{10}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}} & (12c) & \text{O VI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{108} &= x_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 - (z_{10} - \frac{5}{6}) \mathbf{a}_3 &= \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} - \frac{1}{6}c(6z_{10} - 5) \hat{\mathbf{z}} &(12c) & \text{O VI} \\
\mathbf{B}_{109} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= \frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{110} &= -y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{2}{3}) \mathbf{a}_3 &= \frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + \frac{1}{3}c(3z_{11} + 2) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{111} &= -(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{3}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{112} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3 &= -\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{113} &= y_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{6}) \mathbf{a}_3 &= \frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{6}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{114} &= (x_{11} - y_{11}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + (z_{11} + \frac{5}{6}) \mathbf{a}_3 &= \frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + \frac{1}{6}c(6z_{11} + 5) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{115} &= y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - (z_{11} - \frac{2}{3}) \mathbf{a}_3 &= \frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} - \frac{1}{3}c(3z_{11} - 2) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{116} &= (x_{11} - y_{11}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= \frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{117} &= -x_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - (z_{11} - \frac{1}{3}) \mathbf{a}_3 &= -\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{3}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{118} &= -y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{6}) \mathbf{a}_3 &= -\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{6}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{119} &= -(x_{11} - y_{11}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}} &(12c) & \text{P I} \\
\mathbf{B}_{120} &= x_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 - (z_{11} - \frac{5}{6}) \mathbf{a}_3 &= \frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} - \frac{1}{6}c(6z_{11} - 5) \hat{\mathbf{z}} &(12c) & \text{P I}
\end{aligned}$$

## References

- [1] B. Ewald, Y. Prots, C. Kudla, D. Grüner, R. Cardoso-Gil, and R. Kniep, *Crystal Structure and Thermochemical Properties of a First Scandium Borophosphate,  $Sc(H_2O)_2[BP_2O_8] \cdot H_2O$* , Chem. Mater. **18**, 673–679 (2006), doi:10.1021/cm051577o.