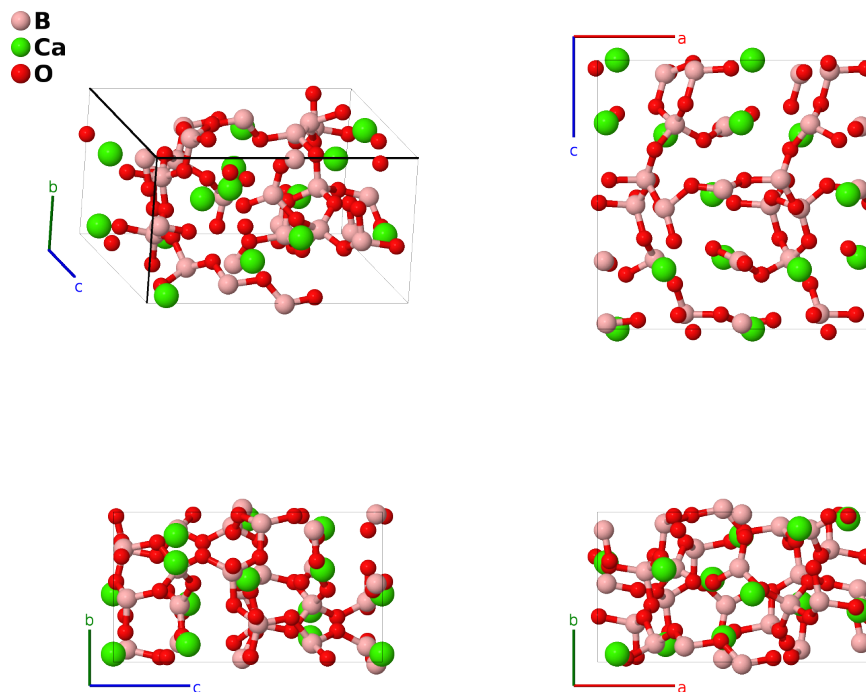# CaB$_2$O$_4$ (III) Structure: A2BC4_oP84_33_6a_3a_12a-001

This structure originally had the label `A2BC4_oP84_33_6a_3a_12a`. Calls to that address will be redirected here.

https://aflow.org/p/S26L

https://aflow.org/p/A2BC4_oP84_33_6a_3a_12a-001

|	
Prototype	B$_2$CaO$_4$
AFLOW prototype label	A2BC4_oP84_33_6a_3a_12a-001
ICSD	23240
Pearson symbol	oP84
Space group number	33
Space group symbol	$Pna2_1$
AFLOW prototype command	aflow --proto=A2BC4_oP84_33_6a_3a_12a-001
	--params=$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7,$ $y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15},$ $y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}$

- CaB$_2$O$_4$ exists in at least four phases (Marezio, 1969):

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- The ground state, stable below 1.2 GPa, *Strukturbericht* $E3_2$
- Orthorhombic high pressure structure, stable between 1.2 and 1.5 GPa, presumably Calciborite
- Orthorhombic high pressure structure, stable between 1.5 and 2.5 GPa (this structure)
- Cubic high pressure structure, stable between 2.5 and 4.0 GPa

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Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
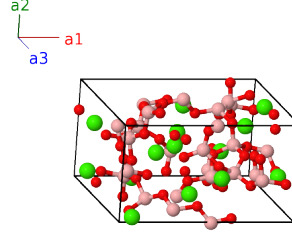
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_3}$	$=$	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$a\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_4}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_6}$	$=$	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_7}$	$=$	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_8}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{11}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{12}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B III
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{15}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{16}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B IV
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	B V
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B V
$\mathbf{B_{19}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + z_5\,\mathbf{a_3}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	B V
$\mathbf{B_{20}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	B V
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	B VI

$$\mathbf{B_{22}} = -x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{B VI}$$

$$\mathbf{B_{23}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a_2} + z_6\,\mathbf{a_3} = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{B VI}$$

$$\mathbf{B_{24}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{B VI}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + z_7\,\mathbf{a_3} = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca I}$$

$$\mathbf{B_{26}} = -x_7\,\mathbf{a_1} - y_7\,\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca I}$$

$$\mathbf{B_{27}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a_2} + z_7\,\mathbf{a_3} = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca I}$$

$$\mathbf{B_{28}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca I}$$

$$\mathbf{B_{29}} = x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} = ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca II}$$

$$\mathbf{B_{30}} = -x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca II}$$

$$\mathbf{B_{31}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a_2} + z_8\,\mathbf{a_3} = a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca II}$$

$$\mathbf{B_{32}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca II}$$

$$\mathbf{B_{33}} = x_9\,\mathbf{a_1} + y_9\,\mathbf{a_2} + z_9\,\mathbf{a_3} = ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca III}$$

$$\mathbf{B_{34}} = -x_9\,\mathbf{a_1} - y_9\,\mathbf{a_2} + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca III}$$

$$\mathbf{B_{35}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a_2} + z_9\,\mathbf{a_3} = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca III}$$

$$\mathbf{B_{36}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{Ca III}$$

$$\mathbf{B_{37}} = x_{10}\,\mathbf{a_1} + y_{10}\,\mathbf{a_2} + z_{10}\,\mathbf{a_3} = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O I}$$

$$\mathbf{B_{38}} = -x_{10}\,\mathbf{a_1} - y_{10}\,\mathbf{a_2} + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O I}$$

$$\mathbf{B_{39}} = \left(x_{10} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{10} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{10}\,\mathbf{a_3} = a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{10} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O I}$$

$$\mathbf{B_{40}} = -\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{10} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{10} + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{10} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O I}$$

$$\mathbf{B_{41}} = x_{11}\,\mathbf{a_1} + y_{11}\,\mathbf{a_2} + z_{11}\,\mathbf{a_3} = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O II}$$

$$\mathbf{B_{42}} = -x_{11}\,\mathbf{a_1} - y_{11}\,\mathbf{a_2} + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O II}$$

$$\mathbf{B_{43}} = \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{11} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{11}\,\mathbf{a_3} = a\left(x_{11} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{11} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O II}$$

$$\mathbf{B_{44}} = -\left(x_{11} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{11} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{11} + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_{11} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{11} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O II}$$

$$\mathbf{B_{45}} = x_{12}\,\mathbf{a_1} + y_{12}\,\mathbf{a_2} + z_{12}\,\mathbf{a_3} = ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O III}$$

$$\mathbf{B_{46}} = -x_{12}\,\mathbf{a_1} - y_{12}\,\mathbf{a_2} + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O III}$$

$$\mathbf{B_{47}} = \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{12} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{12}\,\mathbf{a_3} = a\left(x_{12} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{12} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O III}$$

$$\mathbf{B_{48}} = -\left(x_{12} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{12} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{12} + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_{12} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{12} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O III}$$

$$\mathbf{B_{49}} = x_{13}\,\mathbf{a_1} + y_{13}\,\mathbf{a_2} + z_{13}\,\mathbf{a_3} = ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O IV}$$

$$\mathbf{B_{50}} = -x_{13}\,\mathbf{a_1} - y_{13}\,\mathbf{a_2} + \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a_3} = -ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O IV}$$

$$\mathbf{B_{51}} = \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{13} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{13}\,\mathbf{a_3} = a\left(x_{13} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{13} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O IV}$$

$$\mathbf{B_{52}} = -\left(x_{13} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{13} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{13} + \tfrac{1}{2}\right)\mathbf{a_3} = -a\left(x_{13} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{13} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{13} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (4a) \qquad \text{O IV}$$

$$\mathbf{B_{53}} = x_{14}\,\mathbf{a_1} + y_{14}\,\mathbf{a_2} + z_{14}\,\mathbf{a_3} = ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad (4a) \qquad \text{O V}$$

$$\mathbf{B_{54}} = -x_{14}\,\mathbf{a_1} - y_{14}\,\mathbf{a_2} + \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O V}$$

$$\mathbf{B_{55}} = \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{14} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{14}\,\mathbf{a_3} \qquad = \qquad a\left(x_{14} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{14} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O V}$$

$$\mathbf{B_{56}} = -\left(x_{14} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{14} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{14} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{14} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{14} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{14} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O V}$$

$$\mathbf{B_{57}} = x_{15}\,\mathbf{a_1} + y_{15}\,\mathbf{a_2} + z_{15}\,\mathbf{a_3} \qquad = \qquad ax_{15}\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VI}$$

$$\mathbf{B_{58}} = -x_{15}\,\mathbf{a_1} - y_{15}\,\mathbf{a_2} + \left(z_{15} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{15}\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + c\left(z_{15} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VI}$$

$$\mathbf{B_{59}} = \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{15} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{15}\,\mathbf{a_3} \qquad = \qquad a\left(x_{15} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{15} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VI}$$

$$\mathbf{B_{60}} = -\left(x_{15} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{15} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{15} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{15} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{15} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{15} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VI}$$

$$\mathbf{B_{61}} = x_{16}\,\mathbf{a_1} + y_{16}\,\mathbf{a_2} + z_{16}\,\mathbf{a_3} \qquad = \qquad ax_{16}\,\hat{\mathbf{x}} + by_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VII}$$

$$\mathbf{B_{62}} = -x_{16}\,\mathbf{a_1} - y_{16}\,\mathbf{a_2} + \left(z_{16} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{16}\,\hat{\mathbf{x}} - by_{16}\,\hat{\mathbf{y}} + c\left(z_{16} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VII}$$

$$\mathbf{B_{63}} = \left(x_{16} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{16} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{16}\,\mathbf{a_3} \qquad = \qquad a\left(x_{16} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{16} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VII}$$

$$\mathbf{B_{64}} = -\left(x_{16} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{16} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{16} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{16} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{16} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{16} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VII}$$

$$\mathbf{B_{65}} = x_{17}\,\mathbf{a_1} + y_{17}\,\mathbf{a_2} + z_{17}\,\mathbf{a_3} \qquad = \qquad ax_{17}\,\hat{\mathbf{x}} + by_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VIII}$$

$$\mathbf{B_{66}} = -x_{17}\,\mathbf{a_1} - y_{17}\,\mathbf{a_2} + \left(z_{17} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{17}\,\hat{\mathbf{x}} - by_{17}\,\hat{\mathbf{y}} + c\left(z_{17} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VIII}$$

$$\mathbf{B_{67}} = \left(x_{17} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{17} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{17}\,\mathbf{a_3} \qquad = \qquad a\left(x_{17} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{17} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VIII}$$

$$\mathbf{B_{68}} = -\left(x_{17} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{17} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{17} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{17} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{17} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{17} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O VIII}$$

$$\mathbf{B_{69}} = x_{18}\,\mathbf{a_1} + y_{18}\,\mathbf{a_2} + z_{18}\,\mathbf{a_3} \qquad = \qquad ax_{18}\,\hat{\mathbf{x}} + by_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O IX}$$

$$\mathbf{B_{70}} = -x_{18}\,\mathbf{a_1} - y_{18}\,\mathbf{a_2} + \left(z_{18} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{18}\,\hat{\mathbf{x}} - by_{18}\,\hat{\mathbf{y}} + c\left(z_{18} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O IX}$$

$$\mathbf{B_{71}} = \left(x_{18} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{18} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{18}\,\mathbf{a_3} \qquad = \qquad a\left(x_{18} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{18} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O IX}$$

$$\mathbf{B_{72}} = -\left(x_{18} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{18} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{18} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{18} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{18} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{18} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O IX}$$

$$\mathbf{B_{73}} = x_{19}\,\mathbf{a_1} + y_{19}\,\mathbf{a_2} + z_{19}\,\mathbf{a_3} \qquad = \qquad ax_{19}\,\hat{\mathbf{x}} + by_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O X}$$

$$\mathbf{B_{74}} = -x_{19}\,\mathbf{a_1} - y_{19}\,\mathbf{a_2} + \left(z_{19} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{19}\,\hat{\mathbf{x}} - by_{19}\,\hat{\mathbf{y}} + c\left(z_{19} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O X}$$

$$\mathbf{B_{75}} = \left(x_{19} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{19} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{19}\,\mathbf{a_3} \qquad = \qquad a\left(x_{19} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{19} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O X}$$

$$\mathbf{B_{76}} = -\left(x_{19} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{19} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{19} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{19} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{19} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{19} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O X}$$

$$\mathbf{B_{77}} = x_{20}\,\mathbf{a_1} + y_{20}\,\mathbf{a_2} + z_{20}\,\mathbf{a_3} \qquad = \qquad ax_{20}\,\hat{\mathbf{x}} + by_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XI}$$

$$\mathbf{B_{78}} = -x_{20}\,\mathbf{a_1} - y_{20}\,\mathbf{a_2} + \left(z_{20} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{20}\,\hat{\mathbf{x}} - by_{20}\,\hat{\mathbf{y}} + c\left(z_{20} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XI}$$

$$\mathbf{B_{79}} = \left(x_{20} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{20} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{20}\,\mathbf{a_3} \qquad = \qquad a\left(x_{20} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{20} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XI}$$

$$\mathbf{B_{80}} = -\left(x_{20} - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_{20} + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_{20} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -a\left(x_{20} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{20} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_{20} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XI}$$

$$\mathbf{B_{81}} = x_{21}\,\mathbf{a_1} + y_{21}\,\mathbf{a_2} + z_{21}\,\mathbf{a_3} \qquad = \qquad ax_{21}\,\hat{\mathbf{x}} + by_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XII}$$

$$\mathbf{B_{82}} = -x_{21}\,\mathbf{a_1} - y_{21}\,\mathbf{a_2} + \left(z_{21} + \tfrac{1}{2}\right)\mathbf{a_3} \qquad = \qquad -ax_{21}\,\hat{\mathbf{x}} - by_{21}\,\hat{\mathbf{y}} + c\left(z_{21} + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XII}$$

$$\mathbf{B_{83}} = \left(x_{21} + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_{21} - \tfrac{1}{2}\right)\mathbf{a_2} + z_{21}\,\mathbf{a_3} \qquad = \qquad a\left(x_{21} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - b\left(y_{21} - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}} \qquad\qquad \text{(4a)} \qquad \text{O XII}$$

$$\mathbf{B_{84}} \quad = \quad -\left(x_{21} - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{21} + \tfrac{1}{2}\right)\mathbf{a}_2 + \quad = \quad -a\left(x_{21} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + b\left(y_{21} + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \qquad \text{(4a)} \qquad \text{O XII}$$
$$\left(z_{21} + \tfrac{1}{2}\right)\mathbf{a}_3 \qquad\qquad c\left(z_{21} + \tfrac{1}{2}\right)\hat{\mathbf{z}}$$

References

[1] M. Marezio, J. P. Remeika, and P. D. Dernier, *The crystal structure of the high-pressure phase CaB_2O_4 (III)*, Acta Crystallogr. Sect. B **25**, 955–964 (1969), doi:10.1107/S0567740869003244.