

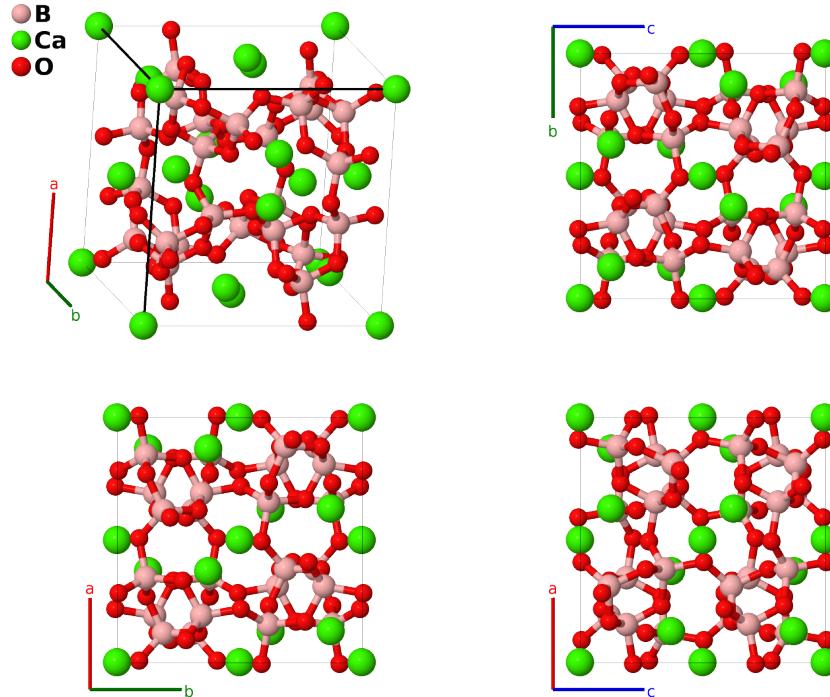
# CaB<sub>2</sub>O<sub>4</sub> (IV) Structure: A2BC4\_cP84\_205\_d\_ac\_2d-001

This structure originally had the label A2BC4\_cP84\_205\_d\_ac\_2d. Calls to that address will be redirected here.

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<https://aflow.org/p/TZRB>

[https://aflow.org/p/A2BC4\\_cP84\\_205\\_d\\_ac\\_2d-001](https://aflow.org/p/A2BC4_cP84_205_d_ac_2d-001)



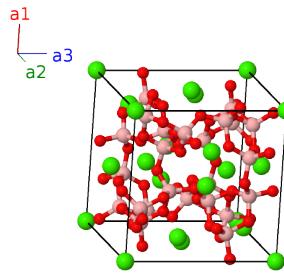
|                                |  |
|--------------------------------|--|
| <b>Prototype</b>               | B <sub>2</sub> CaO <sub>4</sub>  |
| <b>AFLOW prototype label</b>   | A2BC4_cP84_205_d_ac_2d-001   |
| <b>ICSD</b>                    | 23241  |
| <b>Pearson symbol</b>          | cP84   |
| <b>Space group number</b>      | 205  |
| <b>Space group symbol</b>      | $Pa\bar{3}$  |
| <b>AFLOW prototype command</b> | <code>aflow --proto=A2BC4_cP84_205_d_ac_2d-001<br/>--params=a, 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></code> |

- CaB<sub>2</sub>O<sub>4</sub> exists in at least four phase (Marezio, 1969):
  - The ground state, stable below 1.2 GPa, *Strukturbericht E3<sub>2</sub>*
  - 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

- Cubic high pressure structure, stable between 2.5 and 4.0 GPa (this structure)

### Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



### Basis vectors

|                   | Lattice coordinates   | = | Cartesian coordinates  | Wyckoff position | Atom type |
|-------------------|---|---|--|------------------|-----------|
| $\mathbf{B}_1$    | 0   | = | 0  | (4a)             | Ca I      |
| $\mathbf{B}_2$    | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$                                     | = | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$  | (4a)             | Ca I      |
| $\mathbf{B}_3$    | $\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$                                     | = | $\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$  | (4a)             | Ca I      |
| $\mathbf{B}_4$    | $\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$                                     | = | $\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$  | (4a)             | Ca I      |
| $\mathbf{B}_5$    | $x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$                                  | = | $ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$                                  | (8c)             | Ca II     |
| $\mathbf{B}_6$    | $-(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Ca II     |
| $\mathbf{B}_7$    | $-x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$ | = | $-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Ca II     |
| $\mathbf{B}_8$    | $(x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$  | = | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$  | (8c)             | Ca II     |
| $\mathbf{B}_9$    | $-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$                                 | = | $-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$                                 | (8c)             | Ca II     |
| $\mathbf{B}_{10}$ | $(x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$  | = | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Ca II     |
| $\mathbf{B}_{11}$ | $x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$  | = | $ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Ca II     |
| $\mathbf{B}_{12}$ | $-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$ | = | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$ | (8c)             | Ca II     |
| $\mathbf{B}_{13}$ | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                                  | = | $ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$                                  | (24d)            | B I       |
| $\mathbf{B}_{14}$ | $-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d)            | B I       |
| $\mathbf{B}_{15}$ | $-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | = | $-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d)            | B I       |
| $\mathbf{B}_{16}$ | $(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$  | = | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$  | (24d)            | B I       |
| $\mathbf{B}_{17}$ | $z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$                                  | = | $az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$                                  | (24d)            | B I       |
| $\mathbf{B}_{18}$ | $(z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$  | = | $a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$  | (24d)            | B I       |
| $\mathbf{B}_{19}$ | $-(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d)            | B I       |
| $\mathbf{B}_{20}$ | $-z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$ | = | $-az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d)            | B I       |
| $\mathbf{B}_{21}$ | $y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$                                  | = | $ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$                                  | (24d)            | B I       |

|                   |   |     |  |       |     |
|-------------------|---|-----|--|-------|-----|
| $\mathbf{B}_{22}$ | $-y_3 \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ay_3 \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | B I |
| $\mathbf{B}_{23}$ | $(y_3 + \frac{1}{2}) \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3$  | $=$ | $a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{24}$ | $-(y_3 - \frac{1}{2}) \mathbf{a}_1 - z_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | B I |
| $\mathbf{B}_{25}$ | $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$                                 | $=$ | $-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{26}$ | $(x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{27}$ | $x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{28}$ | $-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$ | (24d) | B I |
| $\mathbf{B}_{29}$ | $-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$                                 | $=$ | $-az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{30}$ | $-(z_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + y_3 \mathbf{a}_3$ | $=$ | $-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$ | (24d) | B I |
| $\mathbf{B}_{31}$ | $(z_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{32}$ | $z_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $az_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{33}$ | $-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$                                 | $=$ | $-ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$                                 | (24d) | B I |
| $\mathbf{B}_{34}$ | $y_3 \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ay_3 \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{35}$ | $-(y_3 - \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + x_3 \mathbf{a}_3$ | $=$ | $-a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$ | (24d) | B I |
| $\mathbf{B}_{36}$ | $(y_3 + \frac{1}{2}) \mathbf{a}_1 + z_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | B I |
| $\mathbf{B}_{37}$ | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                                  | $=$ | $ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$                                  | (24d) | O I |
| $\mathbf{B}_{38}$ | $-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{39}$ | $-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{40}$ | $(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$  | (24d) | O I |
| $\mathbf{B}_{41}$ | $z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$                                  | $=$ | $az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$                                  | (24d) | O I |
| $\mathbf{B}_{42}$ | $(z_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - y_4 \mathbf{a}_3$  | $=$ | $a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$  | (24d) | O I |
| $\mathbf{B}_{43}$ | $-(z_4 - \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{44}$ | $-z_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-az_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{45}$ | $y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$                                  | $=$ | $ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$                                  | (24d) | O I |
| $\mathbf{B}_{46}$ | $-y_4 \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ay_4 \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{47}$ | $(y_4 + \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - x_4 \mathbf{a}_3$  | $=$ | $a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$  | (24d) | O I |
| $\mathbf{B}_{48}$ | $-(y_4 - \frac{1}{2}) \mathbf{a}_1 - z_4 \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{49}$ | $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$                                 | $=$ | $-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$                                 | (24d) | O I |
| $\mathbf{B}_{50}$ | $(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I |
| $\mathbf{B}_{51}$ | $x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I |
| $\mathbf{B}_{52}$ | $-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$ | (24d) | O I |
| $\mathbf{B}_{53}$ | $-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$                                 | $=$ | $-az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$                                 | (24d) | O I |

|                   |     |   |     |  |       |      |
|-------------------|-----|---|-----|--|-------|------|
| $\mathbf{B}_{54}$ | $=$ | $-(z_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + y_4 \mathbf{a}_3$ | $=$ | $-a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$ | (24d) | O I  |
| $\mathbf{B}_{55}$ | $=$ | $(z_4 + \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 - (y_4 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I  |
| $\mathbf{B}_{56}$ | $=$ | $z_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (y_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I  |
| $\mathbf{B}_{57}$ | $=$ | $-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$                                 | $=$ | $-ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$                                 | (24d) | O I  |
| $\mathbf{B}_{58}$ | $=$ | $y_4 \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I  |
| $\mathbf{B}_{59}$ | $=$ | $-(y_4 - \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + x_4 \mathbf{a}_3$ | $=$ | $-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$ | (24d) | O I  |
| $\mathbf{B}_{60}$ | $=$ | $(y_4 + \frac{1}{2}) \mathbf{a}_1 + z_4 \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O I  |
| $\mathbf{B}_{61}$ | $=$ | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$                                  | $=$ | $ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$                                  | (24d) | O II |
| $\mathbf{B}_{62}$ | $=$ | $-(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{63}$ | $=$ | $-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{64}$ | $=$ | $(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$  | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{65}$ | $=$ | $z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$                                  | $=$ | $az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$                                  | (24d) | O II |
| $\mathbf{B}_{66}$ | $=$ | $(z_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 - y_5 \mathbf{a}_3$  | $=$ | $a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{67}$ | $=$ | $-(z_5 - \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(z_5 - \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{68}$ | $=$ | $-z_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - (y_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-az_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{69}$ | $=$ | $y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$                                  | $=$ | $ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$                                  | (24d) | O II |
| $\mathbf{B}_{70}$ | $=$ | $-y_5 \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ay_5 \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{71}$ | $=$ | $(y_5 + \frac{1}{2}) \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3$  | $=$ | $a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{72}$ | $=$ | $-(y_5 - \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{73}$ | $=$ | $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$                                 | $=$ | $-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$                                 | (24d) | O II |
| $\mathbf{B}_{74}$ | $=$ | $(x_5 + \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{75}$ | $=$ | $x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{76}$ | $=$ | $-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{77}$ | $=$ | $-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$                                 | $=$ | $-az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$                                 | (24d) | O II |
| $\mathbf{B}_{78}$ | $=$ | $-(z_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + y_5 \mathbf{a}_3$ | $=$ | $-a(z_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{79}$ | $=$ | $(z_5 + \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 - (y_5 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{80}$ | $=$ | $z_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $az_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{81}$ | $=$ | $-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$                                 | $=$ | $-ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$                                 | (24d) | O II |
| $\mathbf{B}_{82}$ | $=$ | $y_5 \mathbf{a}_1 - (z_5 - \frac{1}{2}) \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ay_5 \hat{\mathbf{x}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |
| $\mathbf{B}_{83}$ | $=$ | $-(y_5 - \frac{1}{2}) \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 + x_5 \mathbf{a}_3$ | $=$ | $-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$ | (24d) | O II |
| $\mathbf{B}_{84}$ | $=$ | $(y_5 + \frac{1}{2}) \mathbf{a}_1 + z_5 \mathbf{a}_2 - (x_5 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}}$  | (24d) | O II |

## References

- [1] M. Marezio, J. P. Remeika, and P. D. Dernier, *The crystal structure of the high-pressure phase CaB<sub>2</sub>O<sub>4</sub>(IV), and polymorphism in CaB<sub>2</sub>O<sub>4</sub>*, Acta Crystallogr. Sect. B **25**, 965–970 (1969), doi:10.1107/S0567740869003256.