

CaB₂O₄ (IV) Structure: A2BC4_cP84_205_d_ac_2d-001

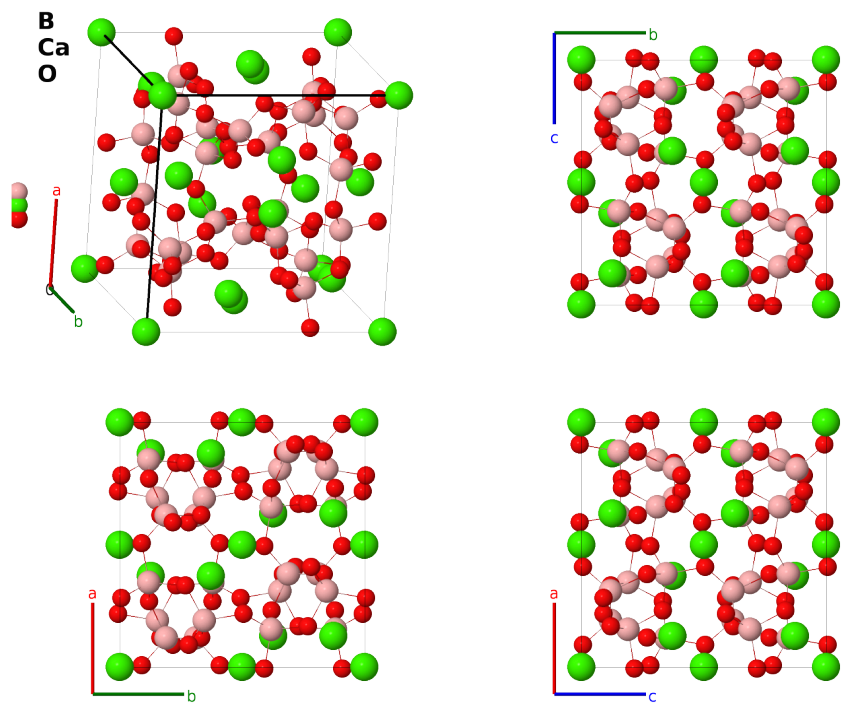
This structure previously used the label(s) **A2BC4_cP84_205_d_ac_2d**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/TZRB>

https://aflow.org/prototype-encyclopedia/A2BC4_cP84_205_d_ac_2d-001



Prototype	B ₂ CaO ₄
AFLOW prototype label	A2BC4_cP84_205_d_ac_2d-001
ICSD	23241
CCDC	1599373
Pearson symbol	cP84
Space group number	205
Space group symbol	$Pa\bar{3}$
AFLOW prototype command	<pre>aflow --proto=A2BC4_cP84_205_d_ac_2d-001 --params=a, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</pre>

- CaB_2O_4 exists in at least four phase (Marezio, 1969):

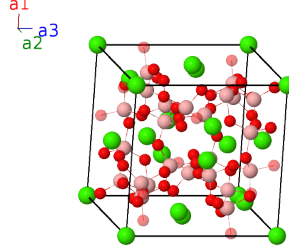
- The ground state, stable below 1.2 GPa, *Strukturbericht E3₂*
- Orthorhombic high pressure structure, stable between 1.2 and 1.5 GPa, presumably Calciborite
- Orthorhombic high pressure structure, stable between 1.5 and 2.5 GPa
- Cubic high pressure structure, stable between 2.5 and 4.0 GPa (this structure)

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



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
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + x_2 \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Ca II
$\mathbf{B}_{12}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{16}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d)	B I

$\mathbf{B}_{19} =$	$-\left(z_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 +$	$=$	$-a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
	$\left(y_3 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$-z_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-az_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
	$\left(y_3 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{21} =$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{22} =$	$-y_3 \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-ay_3 \hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
	$\left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$\left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{24} =$	$-\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 - z_3 \mathbf{a}_2 +$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{25} =$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{26} =$	$\left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{27} =$	$x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{28} =$	$-\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(24d)	B I
	$z_3 \mathbf{a}_3$				
$\mathbf{B}_{29} =$	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{30} =$	$-\left(z_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24d)	B I
	$y_3 \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$\left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 + x_3 \mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{32} =$	$z_3 \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{34} =$	$y_3 \mathbf{a}_1 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	B I
$\mathbf{B}_{35} =$	$-\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(24d)	B I
	$x_3 \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$\left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + z_3 \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{38} =$	$-\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 +$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	O I
	$\left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{39} =$	$-x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-ax_4 \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24d)	O I
	$\left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$				
$\mathbf{B}_{40} =$	$\left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \$				

$$\begin{aligned}
\mathbf{B}_{50} &= (x_4 + \tfrac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \tfrac{1}{2}) \mathbf{a}_3 = a(x_4 + \tfrac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - a(z_4 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{51} &= x_4 \mathbf{a}_1 - (y_4 - \tfrac{1}{2}) \mathbf{a}_2 + (z_4 + \tfrac{1}{2}) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - a(y_4 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(z_4 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{52} &= -(x_4 - \tfrac{1}{2}) \mathbf{a}_1 + (y_4 + \tfrac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3 = -a(x_4 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \tfrac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (24d) & \text{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) & \text{O I} \\
\mathbf{B}_{54} &= -(z_4 - \tfrac{1}{2}) \mathbf{a}_1 + (x_4 + \tfrac{1}{2}) \mathbf{a}_2 + y_4 \mathbf{a}_3 = -a(z_4 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \tfrac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{55} &= (z_4 + \tfrac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 - (y_4 - \tfrac{1}{2}) \mathbf{a}_3 = a(z_4 + \tfrac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - a(y_4 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{56} &= z_4 \mathbf{a}_1 - (x_4 - \tfrac{1}{2}) \mathbf{a}_2 + (y_4 + \tfrac{1}{2}) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} - a(x_4 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(y_4 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{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) & \text{O I} \\
\mathbf{B}_{58} &= y_4 \mathbf{a}_1 - (z_4 - \tfrac{1}{2}) \mathbf{a}_2 + (x_4 + \tfrac{1}{2}) \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} - a(z_4 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{59} &= -(y_4 - \tfrac{1}{2}) \mathbf{a}_1 + (z_4 + \tfrac{1}{2}) \mathbf{a}_2 + x_4 \mathbf{a}_3 = -a(y_4 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(z_4 + \tfrac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (24d) & \text{O I} \\
\mathbf{B}_{60} &= (y_4 + \tfrac{1}{2}) \mathbf{a}_1 + z_4 \mathbf{a}_2 - (x_4 - \tfrac{1}{2}) \mathbf{a}_3 = a(y_4 + \tfrac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - a(x_4 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{62} &= -(x_5 - \tfrac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \tfrac{1}{2}) \mathbf{a}_3 = -a(x_5 - \tfrac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a(z_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{63} &= -x_5 \mathbf{a}_1 + (y_5 + \tfrac{1}{2}) \mathbf{a}_2 - (z_5 - \tfrac{1}{2}) \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} + a(y_5 + \tfrac{1}{2}) \hat{\mathbf{y}} - a(z_5 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{64} &= (x_5 + \tfrac{1}{2}) \mathbf{a}_1 - (y_5 - \tfrac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3 = a(x_5 + \tfrac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \tfrac{1}{2}) \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{66} &= (z_5 + \tfrac{1}{2}) \mathbf{a}_1 - (x_5 - \tfrac{1}{2}) \mathbf{a}_2 - y_5 \mathbf{a}_3 = a(z_5 + \tfrac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \tfrac{1}{2}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{67} &= -(z_5 - \tfrac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (y_5 + \tfrac{1}{2}) \mathbf{a}_3 = -a(z_5 - \tfrac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a(y_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{68} &= -z_5 \mathbf{a}_1 + (x_5 + \tfrac{1}{2}) \mathbf{a}_2 - (y_5 - \tfrac{1}{2}) \mathbf{a}_3 = -az_5 \hat{\mathbf{x}} + a(x_5 + \tfrac{1}{2}) \hat{\mathbf{y}} - a(y_5 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{70} &= -y_5 \mathbf{a}_1 + (z_5 + \tfrac{1}{2}) \mathbf{a}_2 - (x_5 - \tfrac{1}{2}) \mathbf{a}_3 = -ay_5 \hat{\mathbf{x}} + a(z_5 + \tfrac{1}{2}) \hat{\mathbf{y}} - a(x_5 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{71} &= (y_5 + \tfrac{1}{2}) \mathbf{a}_1 - (z_5 - \tfrac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3 = a(y_5 + \tfrac{1}{2}) \hat{\mathbf{x}} - a(z_5 - \tfrac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{72} &= -(y_5 - \tfrac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 + (x_5 + \tfrac{1}{2}) \mathbf{a}_3 = -a(y_5 - \tfrac{1}{2}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a(x_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{74} &= (x_5 + \tfrac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \tfrac{1}{2}) \mathbf{a}_3 = a(x_5 + \tfrac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - a(z_5 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{75} &= x_5 \mathbf{a}_1 - (y_5 - \tfrac{1}{2}) \mathbf{a}_2 + (z_5 + \tfrac{1}{2}) \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} - a(y_5 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(z_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{76} &= -(x_5 - \tfrac{1}{2}) \mathbf{a}_1 + (y_5 + \tfrac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3 = -a(x_5 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \tfrac{1}{2}) \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{78} &= -(z_5 - \tfrac{1}{2}) \mathbf{a}_1 + (x_5 + \tfrac{1}{2}) \mathbf{a}_2 + y_5 \mathbf{a}_3 = -a(z_5 - \tfrac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \tfrac{1}{2}) \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{79} &= (z_5 + \tfrac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 - (y_5 - \tfrac{1}{2}) \mathbf{a}_3 = a(z_5 + \tfrac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - a(y_5 - \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II} \\
\mathbf{B}_{80} &= z_5 \mathbf{a}_1 - (x_5 - \tfrac{1}{2}) \mathbf{a}_2 + (y_5 + \tfrac{1}{2}) \mathbf{a}_3 = az_5 \hat{\mathbf{x}} - a(x_5 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(y_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{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) & \text{O II} \\
\mathbf{B}_{82} &= y_5 \mathbf{a}_1 - (z_5 - \tfrac{1}{2}) \mathbf{a}_2 + (x_5 + \tfrac{1}{2}) \mathbf{a}_3 = ay_5 \hat{\mathbf{x}} - a(z_5 - \tfrac{1}{2}) \hat{\mathbf{y}} + a(x_5 + \tfrac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{O II}
\end{aligned}$$

$$\mathbf{B}_{83} = -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_2 + x_5 \mathbf{a}_3 = -a\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} \quad (24d) \quad \text{O II}$$

$$\mathbf{B}_{84} = \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 + z_5 \mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_3 = a\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (24d) \quad \text{O II}$$

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