

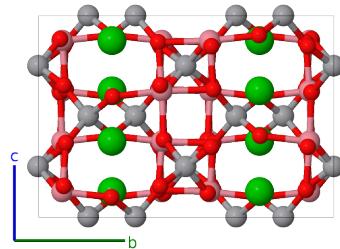
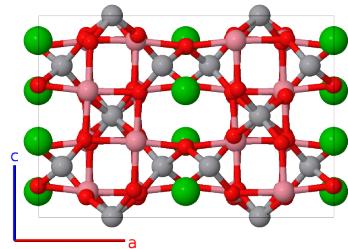
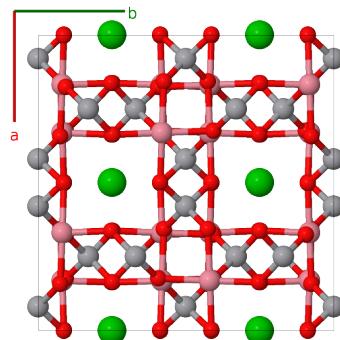
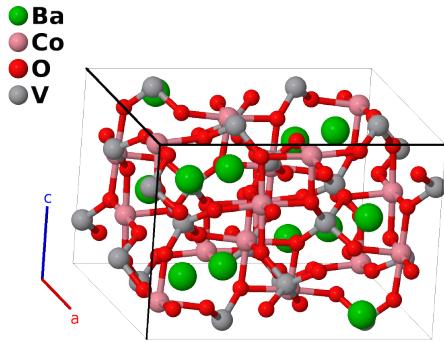
BaCo₂V₂O₈ Structure:

AB₂C₈D₂_tI104_142_a_f_2g_e-001

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

https://aflow.org/p/AB2C8D2_tI104_142_a_f_2g_e-001



Prototype

BaCo₂O₈V₂

AFLOW prototype label

AB₂C₈D₂_tI104_142_a_f_2g_e-001

ICSD

60580

Pearson symbol

tI104

Space group number

142

Space group symbol

*I*4₁/*acd*

AFLOW prototype command

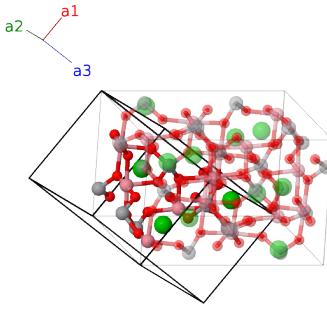
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--params=a,c/a,x2,x3,x4,y4,z4,x5,y5,z5
```

Other compounds with this structure

BaMg₂V₂O₈, BaMn₂V₂O₈, BaMo₂V₂O₈, BaV₂Co₂O₈, PbNi₂V₂O₈

Body-centered Tetragonal primitive vectors

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



Basis vectors

| | Lattice coordinates | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|--|---|------------------|-----------|
| \mathbf{B}_1 | $\frac{5}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$ | $\frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$ | (8a) | Ba I |
| \mathbf{B}_2 | $\frac{3}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$ | $\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$ | (8a) | Ba I |
| \mathbf{B}_3 | $\frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$ | $\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$ | (8a) | Ba I |
| \mathbf{B}_4 | $\frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$ | $\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$ | (8a) | Ba I |
| \mathbf{B}_5 | $\frac{1}{4}\mathbf{a}_1 + (x_2 + \frac{1}{4})\mathbf{a}_2 + x_2\mathbf{a}_3$ | $ax_2\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_6 | $\frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{1}{4})\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$ | $-ax_2\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_7 | $(x_2 + \frac{1}{4})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + x_2\mathbf{a}_3$ | $\frac{1}{4}a\hat{\mathbf{x}} + a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_8 | $-(x_2 - \frac{1}{4})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$ | $\frac{1}{4}a\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}}$ | (16e) | V I |
| \mathbf{B}_9 | $\frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{3}{4})\mathbf{a}_2 - x_2\mathbf{a}_3$ | $-ax_2\hat{\mathbf{x}} + \frac{3}{4}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_{10} | $\frac{1}{4}\mathbf{a}_1 + (x_2 + \frac{3}{4})\mathbf{a}_2 + (x_2 + \frac{1}{2})\mathbf{a}_3$ | $a(x_2 + \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_{11} | $-(x_2 - \frac{3}{4})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - x_2\mathbf{a}_3$ | $-\frac{1}{4}a\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_{12} | $(x_2 + \frac{3}{4})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + (x_2 + \frac{1}{2})\mathbf{a}_3$ | $\frac{1}{4}a\hat{\mathbf{x}} + a(x_2 + \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$ | (16e) | V I |
| \mathbf{B}_{13} | $(x_3 + \frac{3}{8})\mathbf{a}_1 + (x_3 + \frac{1}{8})\mathbf{a}_2 + (2x_3 + \frac{1}{4})\mathbf{a}_3$ | $ax_3\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{14} | $-(x_3 - \frac{3}{8})\mathbf{a}_1 - (x_3 - \frac{1}{8})\mathbf{a}_2 - (2x_3 - \frac{1}{4})\mathbf{a}_3$ | $-ax_3\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{15} | $(x_3 + \frac{1}{8})\mathbf{a}_1 - (x_3 - \frac{3}{8})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$ | $-a(x_3 - \frac{1}{2})\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} - \frac{1}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{16} | $-(x_3 - \frac{1}{8})\mathbf{a}_1 + (x_3 + \frac{3}{8})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$ | $a(x_3 + \frac{1}{2})\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} - \frac{1}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{17} | $-(x_3 - \frac{5}{8})\mathbf{a}_1 - (x_3 - \frac{7}{8})\mathbf{a}_2 - (2x_3 - \frac{3}{4})\mathbf{a}_3$ | $-a(x_3 - \frac{1}{2})\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{18} | $(x_3 + \frac{5}{8})\mathbf{a}_1 + (x_3 + \frac{7}{8})\mathbf{a}_2 + (2x_3 + \frac{3}{4})\mathbf{a}_3$ | $a(x_3 + \frac{1}{2})\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} + \frac{3}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{19} | $-(x_3 - \frac{7}{8})\mathbf{a}_1 + (x_3 + \frac{5}{8})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$ | $ax_3\hat{\mathbf{x}} - a(x_3 - \frac{1}{4})\hat{\mathbf{y}} + \frac{5}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{20} | $(x_3 + \frac{7}{8})\mathbf{a}_1 - (x_3 - \frac{5}{8})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$ | $-ax_3\hat{\mathbf{x}} + a(x_3 + \frac{1}{4})\hat{\mathbf{y}} + \frac{5}{8}c\hat{\mathbf{z}}$ | (16f) | Co I |
| \mathbf{B}_{21} | $(y_4 + z_4)\mathbf{a}_1 + (x_4 + z_4)\mathbf{a}_2 + (x_4 + y_4)\mathbf{a}_3$ | $ay_4\hat{\mathbf{x}} + ay_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{22} | $(-y_4 + z_4 + \frac{1}{2})\mathbf{a}_1 - (x_4 - z_4)\mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2})\mathbf{a}_3$ | $-ax_4\hat{\mathbf{x}} - a(y_4 - \frac{1}{2})\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$ | (32g) | O I |

| | | | | | | |
|-------------------|-----|---|-----|--|-------|------|
| \mathbf{B}_{23} | $=$ | $(x_4 + z_4) \mathbf{a}_1 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$ | $=$ | $-a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{24} | $=$ | $-(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{25} | $=$ | $(y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{26} | $=$ | $-(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$ | $=$ | $ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{27} | $=$ | $(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$ | $=$ | $a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{28} | $=$ | $-(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{29} | $=$ | $-(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{30} | $=$ | $(y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{31} | $=$ | $-(x_4 + z_4) \mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$ | $=$ | $a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{32} | $=$ | $(x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{33} | $=$ | $-(y_4 - z_4) \mathbf{a}_1 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{34} | $=$ | $(y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$ | $=$ | $-ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{35} | $=$ | $(-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$ | $=$ | $-a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{36} | $=$ | $(x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O I |
| \mathbf{B}_{37} | $=$ | $(y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3$ | $=$ | $ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{38} | $=$ | $(-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{39} | $=$ | $(x_5 + z_5) \mathbf{a}_1 + (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3$ | $=$ | $-a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{40} | $=$ | $-(x_5 - z_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{41} | $=$ | $(y_5 - z_5) \mathbf{a}_1 - (x_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{42} | $=$ | $-(y_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3$ | $=$ | $ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{43} | $=$ | $(x_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3$ | $=$ | $a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O II |
| \mathbf{B}_{44} | $=$ | $-(x_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 - (y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 - (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}}$ | (32g) | O II |

$$\begin{aligned}
\mathbf{B}_{45} &= -(y_5 + z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 - (x_5 + y_5) \mathbf{a}_3 & = & -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{46} &= (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 & = & ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{47} &= -(x_5 + z_5) \mathbf{a}_1 + (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3 & = & a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{48} &= (x_5 - z_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 & = & -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{49} &= -(y_5 - z_5) \mathbf{a}_1 + (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 & = & a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{50} &= (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3 & = & -ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{51} &= (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 - (x_5 + y_5) \mathbf{a}_3 & = & -a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (32g) & \text{O II} \\
\mathbf{B}_{52} &= (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 & = & a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (32g) & \text{O II}
\end{aligned}$$

References

- [1] R. Wichmann and H. Müller-Buschbaum, *Neue Verbindungen mit SrNi₂V₂O₈-Struktur: BaCo₂V₂O₈ und BaMg₂V₂O₈*, Z. Anorganische und Allgemeine Chemie **534**, 153–158 (1986), doi:10.1002/zaac.19865340320.

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- [1] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, DGunter, G. D. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.