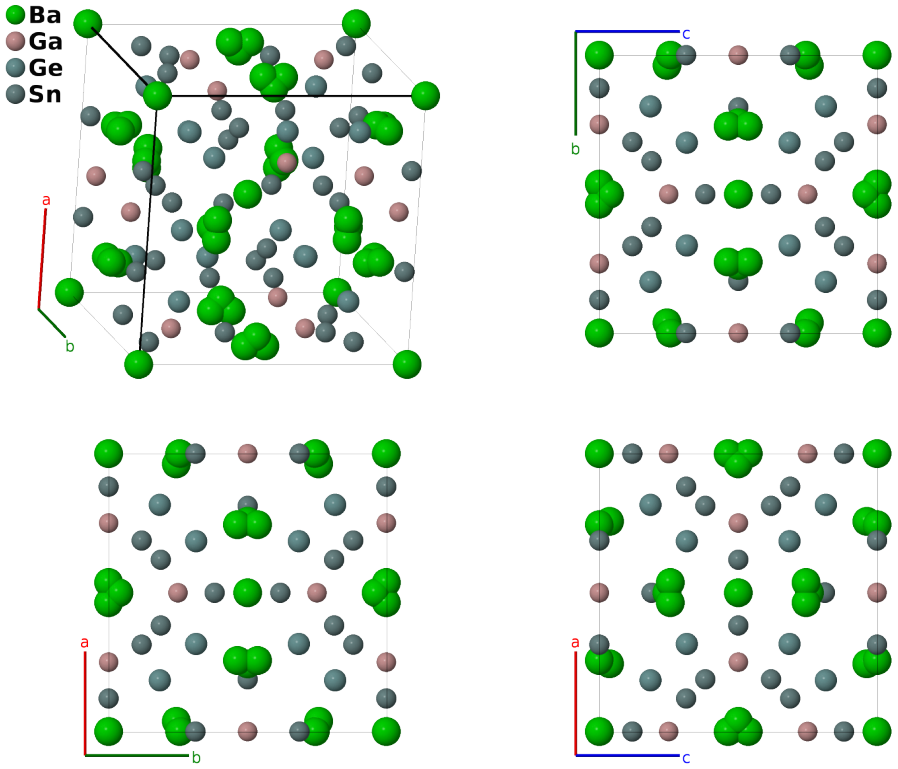
# $\beta$-$Ba_8Ga_{16}Sn_{30}$ Clathrate Structure: A13B3C8D12_cP72_223_ak_c_i_k-001

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/KF6U

https://aflow.org/p/A13B3C8D12_cP72_223_ak_c_i_k-001




| | |
|---|---|
| **Prototype** | $Ba_4Ga_8Sn_{15}$ |
| **AFLOW prototype label** | A13B3C8D12_cP72_223_ak_c_i_k-001 |
| **ICSD** | none |
| **Pearson symbol** | cP72 |
| **Space group number** | 223 |
| **Space group symbol** | $Pm\bar{3}n$ |
| **AFLOW prototype command** | `aflow --proto=A13B3C8D12_cP72_223_ak_c_i_k-001 --params=`$a, x_3, y_4, z_4, y_5, z_5$ |

**Other compounds with this structure**
$Ba_8Ga_{16}Ge_{30}$

- There is a considerable amount of disorder in this system:
  - The (2a) site is pure barium and labeled Ba.

- The (6c) site is pure gallium and labeled Ga.
- The (16i) site is 64.4% tin and 35.6% gallium. We label this as germanium, Ge, as that is another possible component of this compound and to avoid confusion with the other gallium and tin sites.
- The first (24k) site is 25% barium, with the remainder of the sites vacant. This can be seen as four-lobed atom clusters in the figure, when it is expanded beyond one unit cell. We label this site as barium, Ba.
- The final (24k) site is 74.8% tin and 25.2% gallium. We label this as tin, Sn.

- (Aliva, 2006) found another clathrate structure with this stoichiometry, $\alpha$-$Ba_8Ga_{16}Sn_{30}$.

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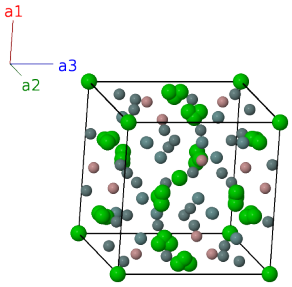
**Simple Cubic primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Ba I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (2a) | Ba I |
| $\mathbf{B_3}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (6c) | Ga I |
| $\mathbf{B_4}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (6c) | Ga I |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$ | (6c) | Ga I |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$ | (6c) | Ga I |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$ | (6c) | Ga I |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$ | (6c) | Ga I |
| $\mathbf{B_9}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{10}}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{11}}$ | = | $-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{12}}$ | = | $x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{13}}$ | = | $\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{14}}$ | = | $-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{15}}$ | = | $\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{16}}$ | = | $-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{17}}$ | = | $-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{18}}$ | = | $x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |
| $\mathbf{B_{19}}$ | = | $x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$ | (16i) | Ge I |

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\begin{array}{lcccll}
\mathbf{B_{20}} & = & -x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 & = & -ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}} & \text{(16i)} \quad \text{Ge I} \\
\mathbf{B_{21}} & = & -\left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(16i)} \quad \text{Ge I} \\
\mathbf{B_{22}} & = & \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(16i)} \quad \text{Ge I} \\
\mathbf{B_{23}} & = & -\left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & -a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(16i)} \quad \text{Ge I} \\
\mathbf{B_{24}} & = & \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(16i)} \quad \text{Ge I} \\
\mathbf{B_{25}} & = & y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{26}} & = & -y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & -ay_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{27}} & = & y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 & = & ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{28}} & = & -y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 & = & -ay_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{29}} & = & z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3 & = & az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{30}} & = & z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3 & = & az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{31}} & = & -z_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3 & = & -az_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{32}} & = & -z_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3 & = & -az_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{33}} & = & y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 & = & ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{34}} & = & -y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 & = & -ay_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{35}} & = & y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 & = & ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{36}} & = & -y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 & = & -ay_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{37}} & = & \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{38}} & = & -\left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & -a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{39}} & = & \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{40}} & = & -\left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & -a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{41}} & = & \tfrac{1}{2}\,\mathbf{a}_1 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & \tfrac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{42}} & = & \tfrac{1}{2}\,\mathbf{a}_1 + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & \tfrac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{43}} & = & \tfrac{1}{2}\,\mathbf{a}_1 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_3 & = & \tfrac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{44}} & = & \tfrac{1}{2}\,\mathbf{a}_1 - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_3 & = & \tfrac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{45}} & = & \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 & = & a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{46}} & = & \left(z_4 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 & = & a\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{47}} & = & -\left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 & = & -a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{48}} & = & -\left(z_4 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3 & = & -a\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Ba II} \\
\mathbf{B_{49}} & = & y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I} \\
\mathbf{B_{50}} & = & -y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & -ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I} \\
\mathbf{B_{51}} & = & y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 & = & ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I} \\
\mathbf{B_{52}} & = & -y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 & = & -ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I} \\
\mathbf{B_{53}} & = & z_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_3 & = & az_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I} \\
\mathbf{B_{54}} & = & z_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_3 & = & az_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{z}} & \text{(24k)} \quad \text{Sn I}
\end{array}
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|---|---|---|---|---|---|---|
| $\mathbf{B_{55}}$ | = | $-z_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_3$ | = | $-az_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{56}}$ | = | $-z_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_3$ | = | $-az_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{57}}$ | = | $y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$ | = | $ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}}$ | (24k) | Sn I |
| $\mathbf{B_{58}}$ | = | $-y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$ | = | $-ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}}$ | (24k) | Sn I |
| $\mathbf{B_{59}}$ | = | $y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$ | = | $ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}}$ | (24k) | Sn I |
| $\mathbf{B_{60}}$ | = | $-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$ | = | $-ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}}$ | (24k) | Sn I |
| $\mathbf{B_{61}}$ | = | $\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{62}}$ | = | $-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{63}}$ | = | $\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{64}}$ | = | $-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{65}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{66}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{67}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{68}}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - \left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{69}}$ | = | $\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{70}}$ | = | $\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{71}}$ | = | $-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (24k) | Sn I |
| $\mathbf{B_{72}}$ | = | $-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$ | (24k) | Sn I |

## References


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