

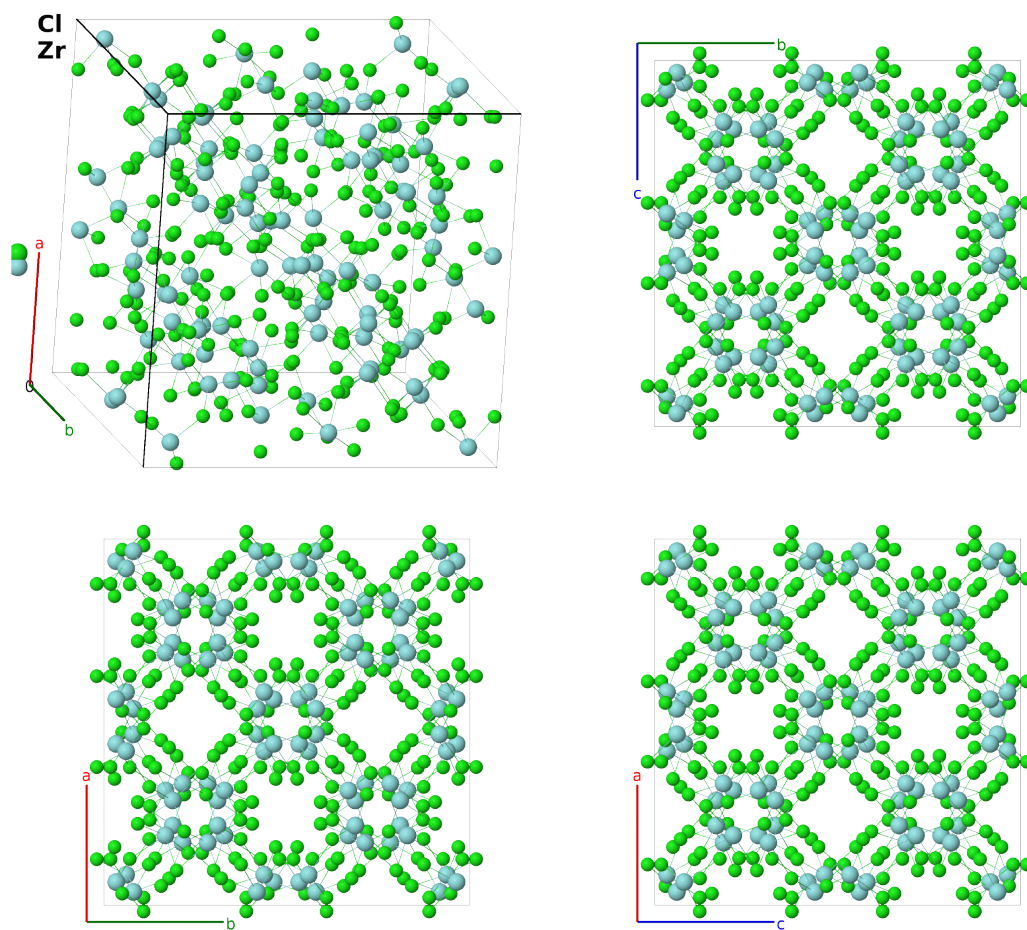
Zr₆Cl₁₅ (Zr₂Cl₅) Structure: A5B2_cI336_230_g2h_h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/8VJC>

https://aflow.org/prototype-encyclopedia/A5B2_cI336_230_g2h_h-001



Prototype	Cl ₅ Zr ₂
AFLOW prototype label	A5B2_cI336_230_g2h_h-001
ICSD	36425
CCDC	1608156
Pearson symbol	cI336
Space group number	230
Space group symbol	$Ia\bar{3}d$

AFLOW prototype command `aflow --proto=A5B2_cI336_230_g2h_h-001`
 `--params=a, y1, x2, y2, z2, x3, y3, z3, x4, y4, z4`

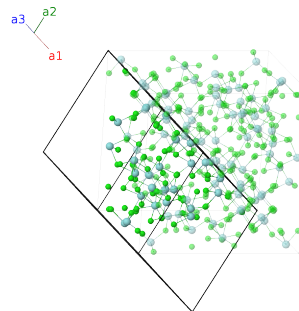
Other compounds with this structure

Ta₆Br₁₅, Ta₆Cl₁₅, Ta₆Zr₁₅

- This is a body-centered cubic ordering of Zr₆Cl₁₅ molecules.
- This structure was first determined by (Corbett, 1978) and reprinted in (Corbett, 1982). The ICSD entry lists the earlier paper as the reference.
- The ICSD using Ta₆Cl₁₅ as the prototype.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 - (y_1 - \frac{3}{8}) \mathbf{a}_2 + (y_1 + \frac{1}{8}) \mathbf{a}_3$	$= \frac{1}{8}a \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} - a(y_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_2$	$= -(2y_1 - \frac{3}{4}) \mathbf{a}_1 - (y_1 - \frac{1}{8}) \mathbf{a}_2 - (y_1 - \frac{3}{8}) \mathbf{a}_3$	$= -\frac{1}{8}a \hat{\mathbf{x}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_3$	$= (2y_1 + \frac{3}{4}) \mathbf{a}_1 + (y_1 + \frac{1}{8}) \mathbf{a}_2 + (y_1 + \frac{3}{8}) \mathbf{a}_3$	$= -\frac{1}{8}a \hat{\mathbf{x}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + (y_1 + \frac{3}{8}) \mathbf{a}_2 - (y_1 - \frac{1}{8}) \mathbf{a}_3$	$= \frac{1}{8}a \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + a(y_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_5$	$= (y_1 + \frac{1}{8}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (y_1 - \frac{3}{8}) \mathbf{a}_3$	$= -a(y_1 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_6$	$= -(y_1 - \frac{3}{8}) \mathbf{a}_1 - (2y_1 - \frac{3}{4}) \mathbf{a}_2 - (y_1 - \frac{1}{8}) \mathbf{a}_3$	$= -a(y_1 - \frac{1}{4}) \hat{\mathbf{x}} - \frac{1}{8}a \hat{\mathbf{y}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_7$	$= (y_1 + \frac{3}{8}) \mathbf{a}_1 + (2y_1 + \frac{3}{4}) \mathbf{a}_2 + (y_1 + \frac{1}{8}) \mathbf{a}_3$	$= a(y_1 + \frac{1}{4}) \hat{\mathbf{x}} - \frac{1}{8}a \hat{\mathbf{y}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_8$	$= -(y_1 - \frac{1}{8}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (y_1 + \frac{3}{8}) \mathbf{a}_3$	$= a(y_1 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_9$	$= -(y_1 - \frac{3}{8}) \mathbf{a}_1 + (y_1 + \frac{1}{8}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= ay_1 \hat{\mathbf{x}} - a(y_1 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_{10}$	$= -(y_1 - \frac{1}{8}) \mathbf{a}_1 - (y_1 - \frac{3}{8}) \mathbf{a}_2 - (2y_1 - \frac{3}{4}) \mathbf{a}_3$	$= -a(y_1 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_1 - \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_{11}$	$= (y_1 + \frac{1}{8}) \mathbf{a}_1 + (y_1 + \frac{3}{8}) \mathbf{a}_2 + (2y_1 + \frac{3}{4}) \mathbf{a}_3$	$= a(y_1 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_1 + \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Cl I
$\mathbf{B}_{12}$	$= (y_1 + \frac{3}{8}) \mathbf{a}_1 - (y_1 - \frac{1}{8}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$= -ay_1 \hat{\mathbf{x}} + a(y_1 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Cl I

$$\begin{aligned}
\mathbf{B}_{13} &= \frac{3}{4} \mathbf{a}_1 + (y_1 + \frac{5}{8}) \mathbf{a}_2 - (y_1 - \frac{7}{8}) \mathbf{a}_3 = \frac{3}{8} a \hat{\mathbf{x}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_1 + \frac{1}{4}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{14} &= (2y_1 + \frac{1}{4}) \mathbf{a}_1 + (y_1 + \frac{7}{8}) \mathbf{a}_2 + (y_1 + \frac{5}{8}) \mathbf{a}_3 = \frac{5}{8} a \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + a (y_1 + \frac{1}{4}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{15} &= -(2y_1 - \frac{1}{4}) \mathbf{a}_1 - (y_1 - \frac{7}{8}) \mathbf{a}_2 - (y_1 - \frac{5}{8}) \mathbf{a}_3 = \frac{5}{8} a \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - a (y_1 - \frac{1}{4}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{16} &= \frac{3}{4} \mathbf{a}_1 - (y_1 - \frac{5}{8}) \mathbf{a}_2 + (y_1 + \frac{7}{8}) \mathbf{a}_3 = \frac{3}{8} a \hat{\mathbf{x}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_1 - \frac{1}{4}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{17} &= -(y_1 - \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (y_1 + \frac{5}{8}) \mathbf{a}_3 = a (y_1 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{18} &= (y_1 + \frac{5}{8}) \mathbf{a}_1 + (2y_1 + \frac{1}{4}) \mathbf{a}_2 + (y_1 + \frac{7}{8}) \mathbf{a}_3 = a (y_1 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{19} &= -(y_1 - \frac{5}{8}) \mathbf{a}_1 - (2y_1 - \frac{1}{4}) \mathbf{a}_2 - (y_1 - \frac{7}{8}) \mathbf{a}_3 = -a (y_1 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{20} &= (y_1 + \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (y_1 - \frac{5}{8}) \mathbf{a}_3 = -a (y_1 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{21} &= (y_1 + \frac{5}{8}) \mathbf{a}_1 - (y_1 - \frac{7}{8}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = -a (y_1 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_1 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{22} &= (y_1 + \frac{7}{8}) \mathbf{a}_1 + (y_1 + \frac{5}{8}) \mathbf{a}_2 + (2y_1 + \frac{1}{4}) \mathbf{a}_3 = ay_1 \hat{\mathbf{x}} + a (y_1 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{23} &= -(y_1 - \frac{7}{8}) \mathbf{a}_1 - (y_1 - \frac{5}{8}) \mathbf{a}_2 - (2y_1 - \frac{1}{4}) \mathbf{a}_3 = -ay_1 \hat{\mathbf{x}} - a (y_1 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{24} &= -(y_1 - \frac{5}{8}) \mathbf{a}_1 + (y_1 + \frac{7}{8}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = a (y_1 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_1 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (48g) & \text{Cl I} \\
\mathbf{B}_{25} &= (y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3 = ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{26} &= (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_3 = -ax_2 \hat{\mathbf{x}} - a (y_2 - \frac{1}{2}) \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{27} &= (y_2 - z_2) \mathbf{a}_1 - (x_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3 = -a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{28} &= -(y_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3 = ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - a (z_2 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{29} &= (x_2 + y_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + (x_2 + z_2) \mathbf{a}_3 = az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{30} &= -(x_2 + y_2 - \frac{1}{2}) \mathbf{a}_1 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - z_2) \mathbf{a}_3 = az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - a (y_2 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{31} &= (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 - (x_2 + z_2 - \frac{1}{2}) \mathbf{a}_3 = -az_2 \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{32} &= (x_2 - y_2) \mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_3 = -a (z_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{33} &= (x_2 + z_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3 = ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{34} &= -(x_2 - z_2) \mathbf{a}_1 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_2 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 = -a (y_2 - \frac{1}{2}) \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{35} &= -(x_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3 = ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{36} &= (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_3 = -ay_2 \hat{\mathbf{x}} - a (z_2 - \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{37} &= (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3 = a (y_2 - \frac{1}{4}) \hat{\mathbf{x}} + a (x_2 + \frac{1}{4}) \hat{\mathbf{y}} - a (z_2 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl II}
\end{aligned}$$

$\mathbf{B}_{38} =$	$-\left(x_2 + z_2 - \frac{1}{2}\right) \mathbf{a}_1 -$ $\left(y_2 + z_2 - \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_2 + y_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{39} =$	$-(x_2 - z_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 +$ $(-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(y_2 + \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{40} =$	$(x_2 + z_2) \mathbf{a}_1 +$ $(-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$=$	$-a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{41} =$	$(-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 - y_2) \mathbf{a}_2 + (x_2 + z_2) \mathbf{a}_3$	$=$	$a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{42} =$	$(y_2 + z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - z_2) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(y_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{43} =$	$-(y_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 -$ $(x_2 + y_2 - \frac{1}{2}) \mathbf{a}_2 -$ $(x_2 + z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{44} =$	$(y_2 - z_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 +$ $(x_2 - z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{45} =$	$(-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{46} =$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 +$ $(-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{47} =$	$(x_2 + y_2) \mathbf{a}_1 +$ $(x_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3$	$=$	$-a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{48} =$	$-(x_2 + y_2 - \frac{1}{2}) \mathbf{a}_1 -$ $(x_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 -$ $(y_2 + z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{49} =$	$-(y_2 + z_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 -$ $(x_2 + y_2) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{50} =$	$(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 - z_2) \mathbf{a}_2 + (x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{51} =$	$-(y_2 - z_2) \mathbf{a}_1 +$ $(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{52} =$	$(y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{53} =$	$-(x_2 + y_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 -$ $(x_2 + z_2) \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{54} =$	$(x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - z_2) \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{55} =$	$(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_1 -$ $(y_2 - z_2) \mathbf{a}_2 + (x_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{56} =$	$-(x_2 - y_2) \mathbf{a}_1 +$ $(y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{57} =$	$-(x_2 + z_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 -$ $(y_2 + z_2) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{58} =$	$(x_2 - z_2) \mathbf{a}_1 + (x_2 + y_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(96h)	Cl II

$\mathbf{B}_{59} =$	$(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{60} =$	$(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_2 - y_2) \mathbf{a}_2 + (y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{61} =$	$(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 -$ $(y_2 - z_2) \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3$	$=$	$-a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{62} =$	$(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{63} =$	$(x_2 - z_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{64} =$	$-(x_2 + z_2) \mathbf{a}_1 +$ $(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{65} =$	$(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_2 - y_2) \mathbf{a}_2 - (x_2 + z_2) \mathbf{a}_3$	$=$	$-a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_2 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{66} =$	$-(y_2 + z_2) \mathbf{a}_1 +$ $(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - z_2) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{67} =$	$(y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 + y_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_2 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{68} =$	$-(y_2 - z_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 +$ $(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{69} =$	$(x_2 - y_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 - z_2) \mathbf{a}_2 - (y_2 + z_2) \mathbf{a}_3$	$=$	$-a(z_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{70} =$	$-(x_2 - y_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 +$ $(y_2 - z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{71} =$	$-(x_2 + y_2) \mathbf{a}_1 +$ $(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3$	$=$	$a(z_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{72} =$	$(x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 +$ $(y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(z_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B}_{73} =$	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 +$ $(x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{74} =$	$(-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{75} =$	$(y_3 - z_3) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 +$ $(-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{76} =$	$-(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 +$ $(x_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{77} =$	$(x_3 + y_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 +$ $(x_3 + z_3) \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{78} =$	$-(x_3 + y_3 - \frac{1}{2}) \mathbf{a}_1 +$ $(-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - z_3) \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{79} =$	$(-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_3 - z_3) \mathbf{a}_2 - (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(96h)	Cl III
$\mathbf{B}_{80} =$	$(x_3 - y_3) \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 +$ $(x_3 - z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(96h)	Cl III

$$\begin{aligned}
\mathbf{B}_{81} &= \begin{pmatrix} (x_3 + z_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + \\ (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{82} &= \begin{pmatrix} -(x_3 - z_3) \mathbf{a}_1 - \\ (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{83} &= \begin{pmatrix} -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{84} &= \begin{pmatrix} (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - y_3) \mathbf{a}_2 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{85} &= \begin{pmatrix} (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3 \end{pmatrix} = a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{86} &= \begin{pmatrix} -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{87} &= \begin{pmatrix} -(x_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{88} &= \begin{pmatrix} (x_3 + z_3) \mathbf{a}_1 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{89} &= \begin{pmatrix} (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - y_3) \mathbf{a}_2 + (x_3 + z_3) \mathbf{a}_3 \end{pmatrix} = a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{90} &= \begin{pmatrix} (y_3 + z_3) \mathbf{a}_1 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{91} &= \begin{pmatrix} -(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{92} &= \begin{pmatrix} (y_3 - z_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + \\ (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{93} &= \begin{pmatrix} (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = a(z_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{94} &= \begin{pmatrix} (x_3 - y_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{95} &= \begin{pmatrix} (x_3 + y_3) \mathbf{a}_1 + \\ (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -a(z_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{96} &= \begin{pmatrix} -(x_3 + y_3 - \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{97} &= \begin{pmatrix} -(y_3 + z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{98} &= \begin{pmatrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{99} &= \begin{pmatrix} -(y_3 - z_3) \mathbf{a}_1 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{100} &= \begin{pmatrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{pmatrix} = -ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{101} &= \begin{pmatrix} -(x_3 + y_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - \\ (x_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (96h) & \text{Cl III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{102} &= \begin{pmatrix} (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{103} &= \begin{pmatrix} (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 - z_3) \mathbf{a}_2 + (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{104} &= \begin{pmatrix} -(x_3 - y_3) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{105} &= \begin{pmatrix} -(x_3 + z_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - \\ (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{106} &= \begin{pmatrix} (x_3 - z_3) \mathbf{a}_1 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{107} &= \begin{pmatrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{108} &= \begin{pmatrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - y_3) \mathbf{a}_2 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{109} &= \begin{pmatrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3 \end{pmatrix} = -a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{110} &= \begin{pmatrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{111} &= \begin{pmatrix} (x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{112} &= \begin{pmatrix} -(x_3 + z_3) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{113} &= \begin{pmatrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - y_3) \mathbf{a}_2 - (x_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{114} &= \begin{pmatrix} -(y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{115} &= \begin{pmatrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{116} &= \begin{pmatrix} -(y_3 - z_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{117} &= \begin{pmatrix} (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{118} &= \begin{pmatrix} -(x_3 - y_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{119} &= \begin{pmatrix} -(x_3 + y_3) \mathbf{a}_1 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{120} &= \begin{pmatrix} (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Cl III} \\
\mathbf{B}_{121} &= \begin{pmatrix} (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{122} &= \begin{pmatrix} (-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 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{123} &= \begin{pmatrix} (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 \end{pmatrix} = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{124} &= \begin{pmatrix} -(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 \end{pmatrix} = ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{125} &= \begin{pmatrix} (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{126} &= \begin{pmatrix} -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{127} &= \begin{pmatrix} (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 - z_4) \mathbf{a}_2 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{128} &= \begin{pmatrix} (x_4 - y_4) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{129} &= \begin{pmatrix} (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \\ (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{130} &= \begin{pmatrix} -(x_4 - z_4) \mathbf{a}_1 - \\ (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{131} &= \begin{pmatrix} -(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{132} &= \begin{pmatrix} (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - y_4) \mathbf{a}_2 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{133} &= \begin{pmatrix} (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{134} &= \begin{pmatrix} -(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 \end{pmatrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{135} &= \begin{pmatrix} -(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{136} &= \begin{pmatrix} (x_4 + z_4) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{137} &= \begin{pmatrix} (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - y_4) \mathbf{a}_2 + (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{138} &= \begin{pmatrix} (y_4 + z_4) \mathbf{a}_1 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{139} &= \begin{pmatrix} -(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{140} &= \begin{pmatrix} (y_4 - z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \\ (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{141} &= \begin{pmatrix} (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{142} &= \begin{pmatrix} (x_4 - y_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{143} &= \begin{pmatrix} (x_4 + y_4) \mathbf{a}_1 + \\ (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{144} &= \begin{pmatrix} -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{145} &= \begin{pmatrix} -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{146} &= \begin{pmatrix} (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 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{147} &= \begin{pmatrix} -(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 \end{pmatrix} = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{148} &= \begin{pmatrix} (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 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{149} &= \begin{pmatrix} -(x_4 + y_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - \\ (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{150} &= \begin{pmatrix} (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{151} &= \begin{pmatrix} (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 - z_4) \mathbf{a}_2 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = az_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{152} &= \begin{pmatrix} -(x_4 - y_4) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{153} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - \\ (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{154} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{155} &= \begin{pmatrix} (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{156} &= \begin{pmatrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - y_4) \mathbf{a}_2 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{157} &= \begin{pmatrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{158} &= \begin{pmatrix} (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 \end{pmatrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{159} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{160} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{161} &= \begin{pmatrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - y_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{162} &= \begin{pmatrix} -(y_4 + z_4) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{163} &= \begin{pmatrix} (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{164} &= \begin{pmatrix} -(y_4 - z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{165} &= \begin{pmatrix} (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{166} &= \begin{pmatrix} -(x_4 - y_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I} \\
\mathbf{B}_{167} &= \begin{pmatrix} -(x_4 + y_4) \mathbf{a}_1 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} & (96h) & \text{Zr I}
\end{aligned}$$

$$\mathbf{B}_{168} = \begin{pmatrix} x_4 + y_4 + \frac{1}{2} \\ x_4 + z_4 + \frac{1}{2} \\ y_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_4 + y_4 + \frac{1}{2} \\ x_4 + z_4 + \frac{1}{2} \\ y_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_4 + y_4 + \frac{1}{2} \\ x_4 + z_4 + \frac{1}{2} \\ y_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} \quad (96h) \quad \text{Zr I}$$

References

- [1] J. D. Corbett, K. R. Poeppelmeier, and R. L. Daake, *Synthesis and structures of $\text{Sc}_7\text{Cl}_{12}$ and $\text{Zr}_6\text{Cl}_{15}$* , Z. Anorganische und Allgemeine Chemie **491**, 51–59 (1982), doi:10.1002/zaac.19824910108.
- [2] J. D. Corbett, R. L. Daake, K. R. Poeppelmeier, and D. H. Guthrie, *Metal-metal bonded clusters in transition metal Groups 3 and 4. Synthesis and structure of three M_6X_{12} -type clusters for scandium and zirconium*, J. Am. Chem. Soc. **100**, 652–654 (1978), doi:10.1021/ja00470a062.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).