

Ba₁₉Li₄₄ Structure:

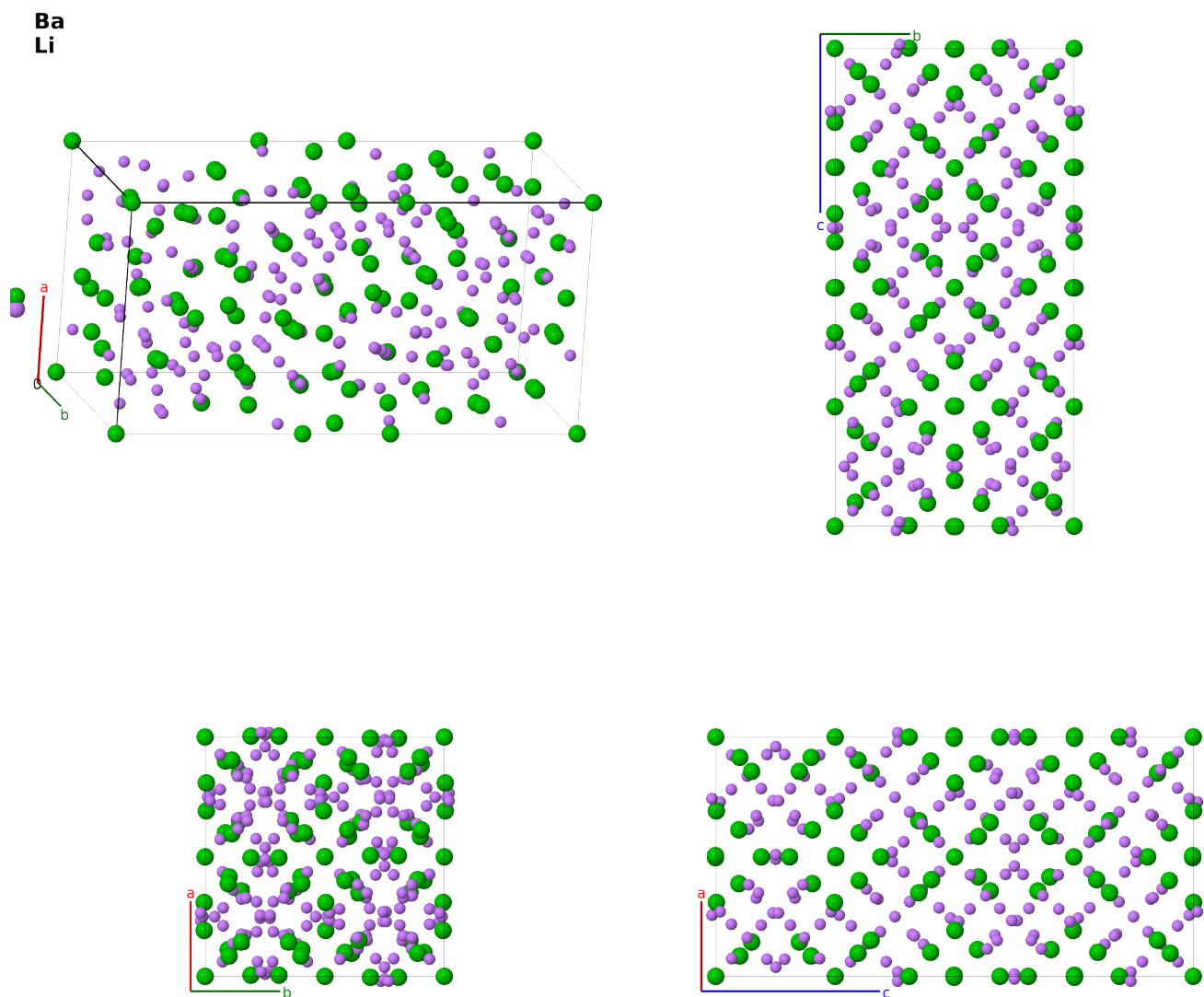
A19B44_tI252_122_ac4e_2d10e-001

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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/HB2V>

https://aflow.org/prototype-encyclopedia/A19B44_tI252_122_ac4e_2d10e-001



Prototype

Ba₁₉Li₄₄

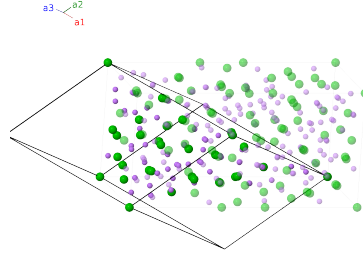
AFLOW prototype label

A19B44_tI252_122_ac4e_2d10e-001

ICSD	249574
CCDC	1779274
Pearson symbol	tI252
Space group number	122
Space group symbol	$I\bar{4}2d$
AFLOW prototype command	aflow --proto=A19B44_tI252_122_ac4e_2d10e-001 --params= $a, c/a, z_2, x_3, x_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}$

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
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Ba I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$cz_2 \hat{\mathbf{z}}$	(8c)	Ba II
$\mathbf{B}_4$	$= -z_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	$=$	$-cz_2 \hat{\mathbf{z}}$	(8c)	Ba II
$\mathbf{B}_5$	$= -\left(z_2 - \frac{3}{4}\right) \mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8c)	Ba II
$\mathbf{B}_6$	$= \left(z_2 + \frac{3}{4}\right) \mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8c)	Ba II
$\mathbf{B}_7$	$= \frac{3}{8} \mathbf{a}_1 + \left(x_3 + \frac{1}{8}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_8$	$= \frac{7}{8} \mathbf{a}_1 - \left(x_3 - \frac{1}{8}\right) \mathbf{a}_2 - \left(x_3 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_9$	$= -\left(x_3 - \frac{7}{8}\right) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_{10}$	$= \left(x_3 + \frac{7}{8}\right) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_{11}$	$= \frac{3}{8} \mathbf{a}_1 + \left(x_4 + \frac{1}{8}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Li II
$\mathbf{B}_{12}$	$= \frac{7}{8} \mathbf{a}_1 - \left(x_4 - \frac{1}{8}\right) \mathbf{a}_2 - \left(x_4 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(8d)	Li II
$\mathbf{B}_{13}$	$= -\left(x_4 - \frac{7}{8}\right) \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 - \left(x_4 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Li II
$\mathbf{B}_{14}$	$= \left(x_4 + \frac{7}{8}\right) \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \left(x_4 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(8d)	Li II
$\mathbf{B}_{15}$	$= (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16e)	Ba III

$$\begin{aligned}
\mathbf{B}_{16} &= \begin{matrix} -(y_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - \\ (x_5 + y_5) \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{17} &= \begin{matrix} -(x_5 + z_5) \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 - \\ (x_5 - y_5) \mathbf{a}_3 \end{matrix} = ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{18} &= \begin{matrix} (x_5 - z_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 + \\ (x_5 - y_5) \mathbf{a}_3 \end{matrix} = -ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{19} &= \begin{matrix} (y_5 - z_5 + \frac{3}{4}) \mathbf{a}_1 - \\ (x_5 + z_5 - \frac{1}{4}) \mathbf{a}_2 + \\ (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{20} &= \begin{matrix} -(y_5 + z_5 - \frac{3}{4}) \mathbf{a}_1 + \\ (x_5 - z_5 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{21} &= \begin{matrix} (-x_5 + z_5 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_5 + z_5 + \frac{1}{4}) \mathbf{a}_2 - \\ (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{22} &= \begin{matrix} (x_5 + z_5 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_5 + z_5 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ay_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba III} \\
\mathbf{B}_{23} &= \begin{matrix} (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6) \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{24} &= \begin{matrix} -(y_6 - z_6) \mathbf{a}_1 - (x_6 - z_6) \mathbf{a}_2 - \\ (x_6 + y_6) \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{25} &= \begin{matrix} -(x_6 + z_6) \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 - \\ (x_6 - y_6) \mathbf{a}_3 \end{matrix} = ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{26} &= \begin{matrix} (x_6 - z_6) \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 + \\ (x_6 - y_6) \mathbf{a}_3 \end{matrix} = -ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{27} &= \begin{matrix} (y_6 - z_6 + \frac{3}{4}) \mathbf{a}_1 - \\ (x_6 + z_6 - \frac{1}{4}) \mathbf{a}_2 + \\ (-x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{28} &= \begin{matrix} -(y_6 + z_6 - \frac{3}{4}) \mathbf{a}_1 + \\ (x_6 - z_6 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_6 - y_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{29} &= \begin{matrix} (-x_6 + z_6 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_6 + z_6 + \frac{1}{4}) \mathbf{a}_2 - \\ (x_6 + y_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{30} &= \begin{matrix} (x_6 + z_6 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_6 + z_6 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ay_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Ba IV} \\
\mathbf{B}_{31} &= \begin{matrix} (y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + \\ (x_7 + y_7) \mathbf{a}_3 \end{matrix} = ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
\mathbf{B}_{32} &= \begin{matrix} -(y_7 - z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 - \\ (x_7 + y_7) \mathbf{a}_3 \end{matrix} = -ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
\mathbf{B}_{33} &= \begin{matrix} -(x_7 + z_7) \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 - \\ (x_7 - y_7) \mathbf{a}_3 \end{matrix} = ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
\mathbf{B}_{34} &= \begin{matrix} (x_7 - z_7) \mathbf{a}_1 - (y_7 + z_7) \mathbf{a}_2 + \\ (x_7 - y_7) \mathbf{a}_3 \end{matrix} = -ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16e) & \text{Ba V}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{35} &= \begin{pmatrix} y_7 - z_7 + \frac{3}{4} \\ x_7 + z_7 - \frac{1}{4} \\ -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= & -ax_7 \hat{\mathbf{x}} + a \left(y_7 + \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
&\begin{pmatrix} x_7 + z_7 - \frac{1}{4} \\ -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} -x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{36} &= - \begin{pmatrix} y_7 + z_7 - \frac{3}{4} \\ x_7 - z_7 + \frac{1}{4} \\ x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ax_7 \hat{\mathbf{x}} - a \left(y_7 - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
&\begin{pmatrix} x_7 - z_7 + \frac{1}{4} \\ x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} x_7 - y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{37} &= \begin{pmatrix} -x_7 + z_7 + \frac{3}{4} \\ -y_7 + z_7 + \frac{1}{4} \\ x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & -ay_7 \hat{\mathbf{x}} - a \left(x_7 - \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
&\begin{pmatrix} -y_7 + z_7 + \frac{1}{4} \\ x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \\
&\begin{pmatrix} x_7 + y_7 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{38} &= \begin{pmatrix} x_7 + z_7 + \frac{3}{4} \\ y_7 + z_7 + \frac{1}{4} \\ x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ay_7 \hat{\mathbf{x}} + a \left(x_7 + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba V} \\
&\begin{pmatrix} y_7 + z_7 + \frac{1}{4} \\ x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} x_7 + y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{39} &= (y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + &= & ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&(x_8 + y_8) \mathbf{a}_3 \\
\mathbf{B}_{40} &= -(y_8 - z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 - &= & -ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&(x_8 + y_8) \mathbf{a}_3 \\
\mathbf{B}_{41} &= -(x_8 + z_8) \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 - &= & ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&(x_8 - y_8) \mathbf{a}_3 \\
\mathbf{B}_{42} &= (x_8 - z_8) \mathbf{a}_1 - (y_8 + z_8) \mathbf{a}_2 + &= & -ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&(x_8 - y_8) \mathbf{a}_3 \\
\mathbf{B}_{43} &= \begin{pmatrix} y_8 - z_8 + \frac{3}{4} \\ x_8 + z_8 - \frac{1}{4} \\ -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= & -ax_8 \hat{\mathbf{x}} + a \left(y_8 + \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&\begin{pmatrix} x_8 + z_8 - \frac{1}{4} \\ -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} -x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{44} &= - \begin{pmatrix} y_8 + z_8 - \frac{3}{4} \\ x_8 - z_8 + \frac{1}{4} \\ x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ax_8 \hat{\mathbf{x}} - a \left(y_8 - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&\begin{pmatrix} x_8 - z_8 + \frac{1}{4} \\ x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} x_8 - y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{45} &= \begin{pmatrix} -x_8 + z_8 + \frac{3}{4} \\ -y_8 + z_8 + \frac{1}{4} \\ x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & -ay_8 \hat{\mathbf{x}} - a \left(x_8 - \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&\begin{pmatrix} -y_8 + z_8 + \frac{1}{4} \\ x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \\
&\begin{pmatrix} x_8 + y_8 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{46} &= \begin{pmatrix} x_8 + z_8 + \frac{3}{4} \\ y_8 + z_8 + \frac{1}{4} \\ x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ay_8 \hat{\mathbf{x}} + a \left(x_8 + \frac{1}{2} \right) \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Ba VI} \\
&\begin{pmatrix} y_8 + z_8 + \frac{1}{4} \\ x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} x_8 + y_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{47} &= (y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + &= & ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&(x_9 + y_9) \mathbf{a}_3 \\
\mathbf{B}_{48} &= -(y_9 - z_9) \mathbf{a}_1 - (x_9 - z_9) \mathbf{a}_2 - &= & -ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&(x_9 + y_9) \mathbf{a}_3 \\
\mathbf{B}_{49} &= -(x_9 + z_9) \mathbf{a}_1 + (y_9 - z_9) \mathbf{a}_2 - &= & ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&(x_9 - y_9) \mathbf{a}_3 \\
\mathbf{B}_{50} &= (x_9 - z_9) \mathbf{a}_1 - (y_9 + z_9) \mathbf{a}_2 + &= & -ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&(x_9 - y_9) \mathbf{a}_3 \\
\mathbf{B}_{51} &= \begin{pmatrix} y_9 - z_9 + \frac{3}{4} \\ x_9 + z_9 - \frac{1}{4} \\ -x_9 + y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= & -ax_9 \hat{\mathbf{x}} + a \left(y_9 + \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&\begin{pmatrix} x_9 + z_9 - \frac{1}{4} \\ -x_9 + y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} -x_9 + y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 \\
\mathbf{B}_{52} &= - \begin{pmatrix} y_9 + z_9 - \frac{3}{4} \\ x_9 - z_9 + \frac{1}{4} \\ x_9 - y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ax_9 \hat{\mathbf{x}} - a \left(y_9 - \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{4} \right) \hat{\mathbf{z}} & (16e) & \text{Li III} \\
&\begin{pmatrix} x_9 - z_9 + \frac{1}{4} \\ x_9 - y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \\
&\begin{pmatrix} x_9 - y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3
\end{aligned}$$

$\mathbf{B}_{53}$	$=$	$\begin{pmatrix} -x_9 + z_9 + \frac{3}{4} \\ -y_9 + z_9 + \frac{1}{4} \\ x_9 + y_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 +$	$=$	$-ay_9 \hat{\mathbf{x}} - a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li III
$\mathbf{B}_{54}$	$=$	$\begin{pmatrix} x_9 + z_9 + \frac{3}{4} \\ y_9 + z_9 + \frac{1}{4} \\ x_9 + y_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 +$	$=$	$ay_9 \hat{\mathbf{x}} + a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li III
$\mathbf{B}_{55}$	$=$	$(y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 +$	$=$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{56}$	$=$	$(x_{10} - z_{10}) \mathbf{a}_2 - (x_{10} + y_{10}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{57}$	$=$	$-(x_{10} + z_{10}) \mathbf{a}_1 +$	$=$	$ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{58}$	$=$	$(y_{10} - z_{10}) \mathbf{a}_2 - (x_{10} - y_{10}) \mathbf{a}_3$	$=$	$-ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{59}$	$=$	$(x_{10} - z_{10}) \mathbf{a}_1 - (y_{10} + z_{10}) \mathbf{a}_2 +$	$=$	$-ax_{10} \hat{\mathbf{x}} + a \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{60}$	$=$	$(x_{10} + z_{10} - \frac{3}{4}) \mathbf{a}_1 -$	$=$	$ax_{10} \hat{\mathbf{x}} - a \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{61}$	$=$	$(x_{10} - z_{10} + \frac{1}{4}) \mathbf{a}_2 +$	$=$	$-ay_{10} \hat{\mathbf{x}} - a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{62}$	$=$	$(x_{10} - y_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_{10} \hat{\mathbf{x}} + a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li IV
$\mathbf{B}_{63}$	$=$	$(x_{10} + z_{10} + \frac{3}{4}) \mathbf{a}_1 +$	$=$	$ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{64}$	$=$	$(y_{11} + z_{11}) \mathbf{a}_1 + (x_{11} + z_{11}) \mathbf{a}_2 +$	$=$	$-ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{65}$	$=$	$(x_{11} - z_{11}) \mathbf{a}_2 - (x_{11} + y_{11}) \mathbf{a}_3$	$=$	$ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{66}$	$=$	$-(x_{11} + z_{11}) \mathbf{a}_1 +$	$=$	$-ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{67}$	$=$	$(y_{11} - z_{11}) \mathbf{a}_2 - (x_{11} - y_{11}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + a \left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{11} - \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{68}$	$=$	$(x_{11} - z_{11} + \frac{3}{4}) \mathbf{a}_1 -$	$=$	$ax_{11} \hat{\mathbf{x}} - a \left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{11} - \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{69}$	$=$	$(x_{11} + z_{11} - \frac{1}{4}) \mathbf{a}_2 +$	$=$	$-ay_{11} \hat{\mathbf{x}} - a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{70}$	$=$	$(x_{11} - y_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_{11} \hat{\mathbf{x}} + a \left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}}$	$(16e)$	Li V
$\mathbf{B}_{71}$	$=$	$(x_{11} + z_{11} + \frac{3}{4}) \mathbf{a}_1 +$	$=$	$ax_{12} \hat{\mathbf{x}} + ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	$(16e)$	Li VI

$$\begin{aligned}
\mathbf{B}_{72} &= \begin{aligned} &-(y_{12} - z_{12}) \mathbf{a}_1 - \\ &(x_{12} - z_{12}) \mathbf{a}_2 - (x_{12} + y_{12}) \mathbf{a}_3 \end{aligned} &= & -ax_{12} \hat{\mathbf{x}} - ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{73} &= \begin{aligned} &-(x_{12} + z_{12}) \mathbf{a}_1 + \\ &(y_{12} - z_{12}) \mathbf{a}_2 - (x_{12} - y_{12}) \mathbf{a}_3 \end{aligned} &= & ay_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{74} &= \begin{aligned} &(x_{12} - z_{12}) \mathbf{a}_1 - (y_{12} + z_{12}) \mathbf{a}_2 + \\ &(x_{12} - y_{12}) \mathbf{a}_3 \end{aligned} &= & -ay_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{75} &= \begin{aligned} &(y_{12} - z_{12} + \frac{3}{4}) \mathbf{a}_1 - \\ &(x_{12} + z_{12} - \frac{1}{4}) \mathbf{a}_2 + \\ &(-x_{12} + y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & -ax_{12} \hat{\mathbf{x}} + a(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{76} &= \begin{aligned} &-(y_{12} + z_{12} - \frac{3}{4}) \mathbf{a}_1 + \\ &(x_{12} - z_{12} + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_{12} - y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & ax_{12} \hat{\mathbf{x}} - a(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{77} &= \begin{aligned} &(-x_{12} + z_{12} + \frac{3}{4}) \mathbf{a}_1 + \\ &(-y_{12} + z_{12} + \frac{1}{4}) \mathbf{a}_2 - \\ &(x_{12} + y_{12} - \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & -ay_{12} \hat{\mathbf{x}} - a(x_{12} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{12} + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{78} &= \begin{aligned} &(x_{12} + z_{12} + \frac{3}{4}) \mathbf{a}_1 + \\ &(y_{12} + z_{12} + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_{12} + y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & ay_{12} \hat{\mathbf{x}} + a(x_{12} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{12} + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VI} \\
\mathbf{B}_{79} &= \begin{aligned} &(y_{13} + z_{13}) \mathbf{a}_1 + (x_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} + y_{13}) \mathbf{a}_3 \end{aligned} &= & ax_{13} \hat{\mathbf{x}} + ay_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{80} &= \begin{aligned} &-(y_{13} - z_{13}) \mathbf{a}_1 - \\ &(x_{13} - z_{13}) \mathbf{a}_2 - (x_{13} + y_{13}) \mathbf{a}_3 \end{aligned} &= & -ax_{13} \hat{\mathbf{x}} - ay_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{81} &= \begin{aligned} &-(x_{13} + z_{13}) \mathbf{a}_1 + \\ &(y_{13} - z_{13}) \mathbf{a}_2 - (x_{13} - y_{13}) \mathbf{a}_3 \end{aligned} &= & ay_{13} \hat{\mathbf{x}} - ax_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{82} &= \begin{aligned} &(x_{13} - z_{13}) \mathbf{a}_1 - (y_{13} + z_{13}) \mathbf{a}_2 + \\ &(x_{13} - y_{13}) \mathbf{a}_3 \end{aligned} &= & -ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{83} &= \begin{aligned} &(y_{13} - z_{13} + \frac{3}{4}) \mathbf{a}_1 - \\ &(x_{13} + z_{13} - \frac{1}{4}) \mathbf{a}_2 + \\ &(-x_{13} + y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & -ax_{13} \hat{\mathbf{x}} + a(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{84} &= \begin{aligned} &-(y_{13} + z_{13} - \frac{3}{4}) \mathbf{a}_1 + \\ &(x_{13} - z_{13} + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_{13} - y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & ax_{13} \hat{\mathbf{x}} - a(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{85} &= \begin{aligned} &(-x_{13} + z_{13} + \frac{3}{4}) \mathbf{a}_1 + \\ &(-y_{13} + z_{13} + \frac{1}{4}) \mathbf{a}_2 - \\ &(x_{13} + y_{13} - \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & -ay_{13} \hat{\mathbf{x}} - a(x_{13} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{86} &= \begin{aligned} &(x_{13} + z_{13} + \frac{3}{4}) \mathbf{a}_1 + \\ &(y_{13} + z_{13} + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_{13} + y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= & ay_{13} \hat{\mathbf{x}} + a(x_{13} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{4}) \hat{\mathbf{z}} & (16e) & \text{Li VII} \\
\mathbf{B}_{87} &= \begin{aligned} &(y_{14} + z_{14}) \mathbf{a}_1 + (x_{14} + z_{14}) \mathbf{a}_2 + \\ &(x_{14} + y_{14}) \mathbf{a}_3 \end{aligned} &= & ax_{14} \hat{\mathbf{x}} + ay_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{Li VIII} \\
\mathbf{B}_{88} &= \begin{aligned} &-(y_{14} - z_{14}) \mathbf{a}_1 - \\ &(x_{14} - z_{14}) \mathbf{a}_2 - (x_{14} + y_{14}) \mathbf{a}_3 \end{aligned} &= & -ax_{14} \hat{\mathbf{x}} - ay_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16e) & \text{Li VIII} \\
\mathbf{B}_{89} &= \begin{aligned} &-(x_{14} + z_{14}) \mathbf{a}_1 + \\ &(y_{14} - z_{14}) \mathbf{a}_2 - (x_{14} - y_{14}) \mathbf{a}_3 \end{aligned} &= & ay_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (16e) & \text{Li VIII} \\
\mathbf{B}_{90} &= \begin{aligned} &(x_{14} - z_{14}) \mathbf{a}_1 - (y_{14} + z_{14}) \mathbf{a}_2 + \\ &(x_{14} - y_{14}) \mathbf{a}_3 \end{aligned} &= & -ay_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (16e) & \text{Li VIII}
\end{aligned}$$

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