

RhBi₄ Structure:

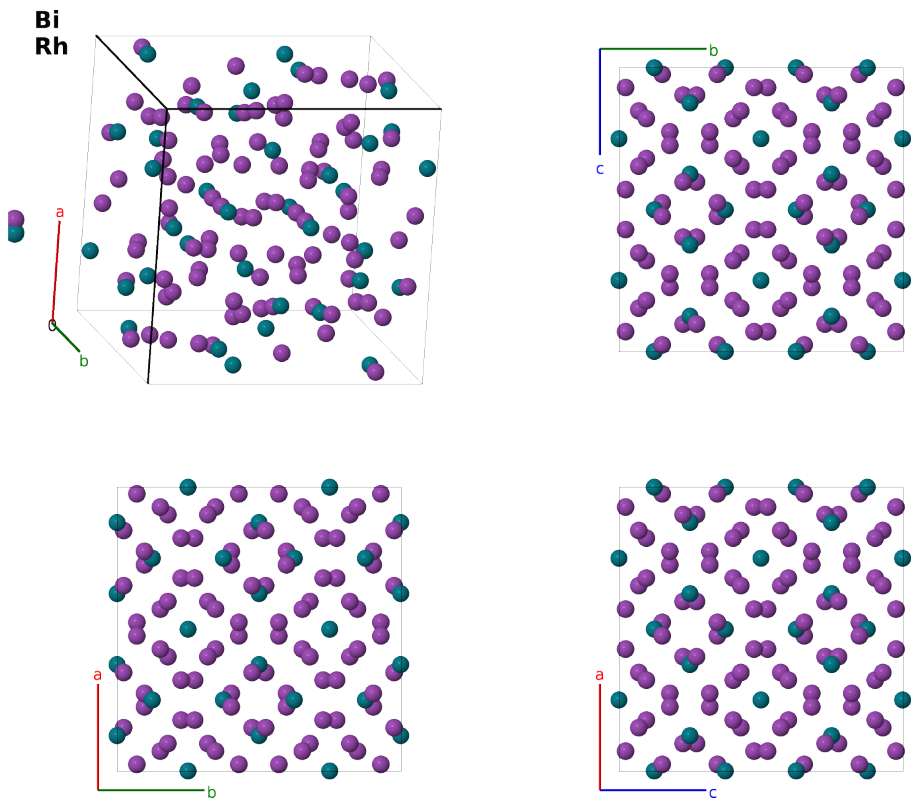
A4B_cI120_230_h_c-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/V61M>

https://aflow.org/prototype-encyclopedia/A4B_cI120_230_h_c-001

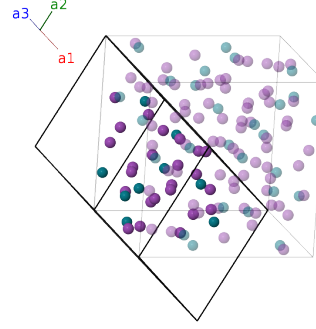


Prototype	Bi ₄ Rh
AFLOW prototype label	A4B_cI120_230_h_c-001
ICSD	58854
CCDC	1622850
Pearson symbol	cI120
Space group number	230
Space group symbol	$Ia\bar{3}d$
AFLOW prototype command	<code>aflow --proto=A4B_cI120_230_h_c-001</code> <code>--params=a, x₂, y₂, z₂</code>

- (Glagoleva, 1956) give three slightly different values for the location of the bismuth atoms. We choose their final set of coordinates. The ICSD entry is from the earlier publication (Zhdanov, 1954).

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
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_3$	$= \frac{1}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}}$	(24c)	Rh I
$\mathbf{B}_4$	$= \frac{3}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_5$	$= \frac{3}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_6$	$= \frac{1}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{8}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_7$	$= \frac{3}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_8$	$= \frac{1}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_9$	$= \frac{7}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_{10}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}}$	(24c)	Rh I
$\mathbf{B}_{11}$	$= \frac{5}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_{12}$	$= \frac{7}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}}$	(24c)	Rh I
$\mathbf{B}_{13}$	$= (y_2 + z_2)\mathbf{a}_1 + (x_2 + z_2)\mathbf{a}_2 + (x_2 + y_2)\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + ay_2\hat{\mathbf{y}} + az_2\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{14}$	$= (-y_2 + z_2 + \frac{1}{2})\mathbf{a}_1 - (x_2 - z_2)\mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - a(y_2 - \frac{1}{2})\hat{\mathbf{y}} + az_2\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{15}$	$= (y_2 - z_2)\mathbf{a}_1 - (x_2 + z_2 - \frac{1}{2})\mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2})\hat{\mathbf{x}} + ay_2\hat{\mathbf{y}} - az_2\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{16}$	$= -(y_2 + z_2 - \frac{1}{2})\mathbf{a}_1 + (x_2 - z_2 + \frac{1}{2})\mathbf{a}_2 + (x_2 - y_2)\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} - ay_2\hat{\mathbf{y}} - a(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{17}$	$= (x_2 + y_2)\mathbf{a}_1 + (y_2 + z_2)\mathbf{a}_2 + (x_2 + z_2)\mathbf{a}_3$	$=$	$az_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + ay_2\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{18}$	$= -(x_2 + y_2 - \frac{1}{2})\mathbf{a}_1 + (-y_2 + z_2 + \frac{1}{2})\mathbf{a}_2 - (x_2 - z_2)\mathbf{a}_3$	$=$	$az_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - a(y_2 - \frac{1}{2})\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{19}$	$= (-x_2 + y_2 + \frac{1}{2})\mathbf{a}_1 + (y_2 - z_2)\mathbf{a}_2 - (x_2 + z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-az_2\hat{\mathbf{x}} - a(x_2 - \frac{1}{2})\hat{\mathbf{y}} + ay_2\hat{\mathbf{z}}$	(96h)	Bi I
$\mathbf{B}_{20}$	$= (x_2 - y_2)\mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2})\mathbf{a}_2 + (x_2 - z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$-a(z_2 - \frac{1}{2})\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} - ay_2\hat{\mathbf{z}}$	(96h)	Bi I

$$\begin{aligned}
\mathbf{B}_{21} &= \begin{pmatrix} (x_2 + z_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + \\ (y_2 + z_2) \mathbf{a}_3 \end{pmatrix} = ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{22} &= \begin{pmatrix} -(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 \end{pmatrix} = -a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(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 \end{pmatrix} = ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{24} &= \begin{pmatrix} (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 \end{pmatrix} = -ay_2 \hat{\mathbf{x}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{25} &= \begin{pmatrix} (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_2 - z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3 \end{pmatrix} = 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{Bi I} \\
\mathbf{B}_{26} &= \begin{pmatrix} -(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 \end{pmatrix} = -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{Bi I} \\
\mathbf{B}_{27} &= \begin{pmatrix} -(x_2 - z_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + \\ (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = 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{Bi I} \\
\mathbf{B}_{28} &= \begin{pmatrix} (x_2 + z_2) \mathbf{a}_1 + \\ (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3 \end{pmatrix} = -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{Bi I} \\
\mathbf{B}_{29} &= \begin{pmatrix} (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_2 - y_2) \mathbf{a}_2 + (x_2 + z_2) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{30} &= \begin{pmatrix} (y_2 + z_2) \mathbf{a}_1 + \\ (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - z_2) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{31} &= \begin{pmatrix} -(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 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{32} &= \begin{pmatrix} (y_2 - z_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + \\ (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{33} &= \begin{pmatrix} (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{34} &= \begin{pmatrix} (x_2 - y_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + \\ (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{35} &= \begin{pmatrix} (x_2 + y_2) \mathbf{a}_1 + \\ (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 - z_2) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{36} &= \begin{pmatrix} -(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 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{37} &= \begin{pmatrix} -(y_2 + z_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 - \\ (x_2 + y_2) \mathbf{a}_3 \end{pmatrix} = -ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{38} &= \begin{pmatrix} (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 \end{pmatrix} = ax_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{39} &= \begin{pmatrix} -(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 \end{pmatrix} = a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{40} &= \begin{pmatrix} (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 \end{pmatrix} = -ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{41} &= \begin{pmatrix} -(x_2 + y_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 - \\ (x_2 + z_2) \mathbf{a}_3 \end{pmatrix} = -az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}} & (96h) & \text{Bi I}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{42} &= \begin{pmatrix} (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 \end{pmatrix} = -az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{43} &= \begin{pmatrix} (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 \end{pmatrix} = az_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(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 \end{pmatrix} = a(z_2 + \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{45} &= \begin{pmatrix} -(x_2 + z_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - \\ (y_2 + z_2) \mathbf{a}_3 \end{pmatrix} = -ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{46} &= \begin{pmatrix} (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 \end{pmatrix} = a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{47} &= \begin{pmatrix} (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 \end{pmatrix} = -ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{48} &= \begin{pmatrix} (-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 \end{pmatrix} = ay_2 \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}} & (96h) & \text{Bi I} \\
\mathbf{B}_{49} &= \begin{pmatrix} (-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_2 - z_2) \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3 \end{pmatrix} = -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{Bi I} \\
\mathbf{B}_{50} &= \begin{pmatrix} (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 \end{pmatrix} = 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{Bi I} \\
\mathbf{B}_{51} &= \begin{pmatrix} (x_2 - z_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 + \\ (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -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{Bi I} \\
\mathbf{B}_{52} &= \begin{pmatrix} -(x_2 + z_2) \mathbf{a}_1 + \\ (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3 \end{pmatrix} = 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{Bi I} \\
\mathbf{B}_{53} &= \begin{pmatrix} (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_2 - y_2) \mathbf{a}_2 - (x_2 + z_2) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{54} &= \begin{pmatrix} -(y_2 + z_2) \mathbf{a}_1 + \\ (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - z_2) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{55} &= \begin{pmatrix} (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 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{56} &= \begin{pmatrix} -(y_2 - z_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 + \\ (-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{57} &= \begin{pmatrix} (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_2 - z_2) \mathbf{a}_2 - (y_2 + z_2) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{58} &= \begin{pmatrix} -(x_2 - y_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 + \\ (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -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) & \text{Bi I} \\
\mathbf{B}_{59} &= \begin{pmatrix} -(x_2 + y_2) \mathbf{a}_1 + \\ (-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3 \end{pmatrix} = 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) & \text{Bi I} \\
\mathbf{B}_{60} &= \begin{pmatrix} (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 \end{pmatrix} = 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) & \text{Bi I}
\end{aligned}$$

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