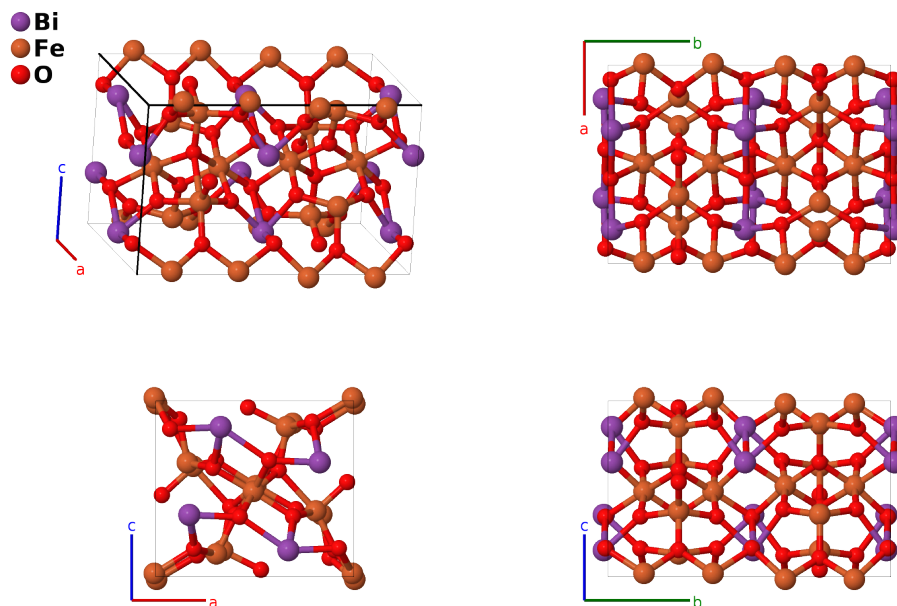


# High pressure $\text{Bi}_2\text{Fe}_4\text{O}_9$ Structure: A2B4C9\_oP60\_62\_d\_2cd\_3c3d-001

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

[https://aflow.org/p/A2B4C9\\_oP60\\_62\\_d\\_2cd\\_3c3d-001](https://aflow.org/p/A2B4C9_oP60_62_d_2cd_3c3d-001)

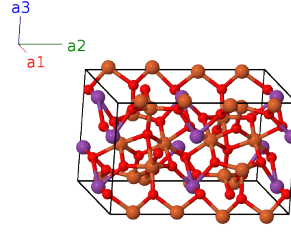


Prototype	$\text{Bi}_2\text{Fe}_4\text{O}_9$
AFLOW prototype label	A2B4C9_oP60_62_d_2cd_3c3d-001
ICSD	186444
Pearson symbol	oP60
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<pre>aflow --proto=A2B4C9_oP60_62_d_2cd_3c3d-001       --params=a, b/a, c/a, x1, z1, x2, z2, x3, z3, x4, z4, x5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8,       x9, y9, z9, x10, y10, z10</pre>

- This is the high pressure phase of  $\text{Bi}_2\text{Fe}_4\text{O}_9$ , using data taken by (Friedrich, 2012) at 9.4GPa. Below 6.89GPa it transforms to the low pressure  $\text{Bi}_2\text{Fe}_4\text{O}_9$  structure.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_2$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_4$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B}_6$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B}_8$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe II
$\mathbf{B}_9$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{10}$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{11}$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{12}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_{13}$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{14}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{15}$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{16}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{17}$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{18}$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{19}$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{20}$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{21}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B}_{22}$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B}_{23}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B}_{24}$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B}_{25}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8d)	Bi I
$\mathbf{B}_{26}$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	Bi I

$$\begin{aligned}
\mathbf{B}_{27} &= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(8d) & \text{Bi I} \\
\mathbf{B}_{28} &= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{Bi I} \\
\mathbf{B}_{29} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{30} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{31} &= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{32} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 &= a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{33} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{34} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 &= a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{35} &= x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{36} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{Fe III} \\
\mathbf{B}_{37} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{38} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{39} &= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{40} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 &= a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{41} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{42} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 &= a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{43} &= x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{44} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O IV} \\
\mathbf{B}_{45} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{46} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{47} &= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{48} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 &= a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{49} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{50} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 &= a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{51} &= x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{52} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O V} \\
\mathbf{B}_{53} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(8d) & \text{O VI} \\
\mathbf{B}_{54} &= -(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3 &= -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O VI} \\
\mathbf{B}_{55} &= -x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8d) & \text{O VI} \\
\mathbf{B}_{56} &= (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3 &= a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}} &(8d) & \text{O VI} \\
\mathbf{B}_{57} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(8d) & \text{O VI}
\end{aligned}$$

$$\mathbf{B}_{58} = \begin{pmatrix} (x_{10} + \frac{1}{2}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - \\ (z_{10} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}} \quad (8d) \quad \text{O VI}$$

$$\mathbf{B}_{59} = x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} \quad (8d) \quad \text{O VI}$$

$$\mathbf{B}_{60} = -\begin{pmatrix} (x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} \quad (8d) \quad \text{O VI}$$

## References

- [1] A. Friedrich, J. Biehler, W. Morgenroth, L. Wiehl, B. Winkler, M. Hanfland, M. Tolkieln, M. Burianek, and M. Mühlberg, *High-pressure phase transition of  $\text{Bi}_2\text{Fe}_4\text{O}_9$* , J. Phys.: Condens. Matter **24**, 145401 (2012), doi:10.1088/0953-8984/24/14/145401.