

Ambient pressure $\text{Bi}_2\text{Fe}_4\text{O}_9$ Structure:

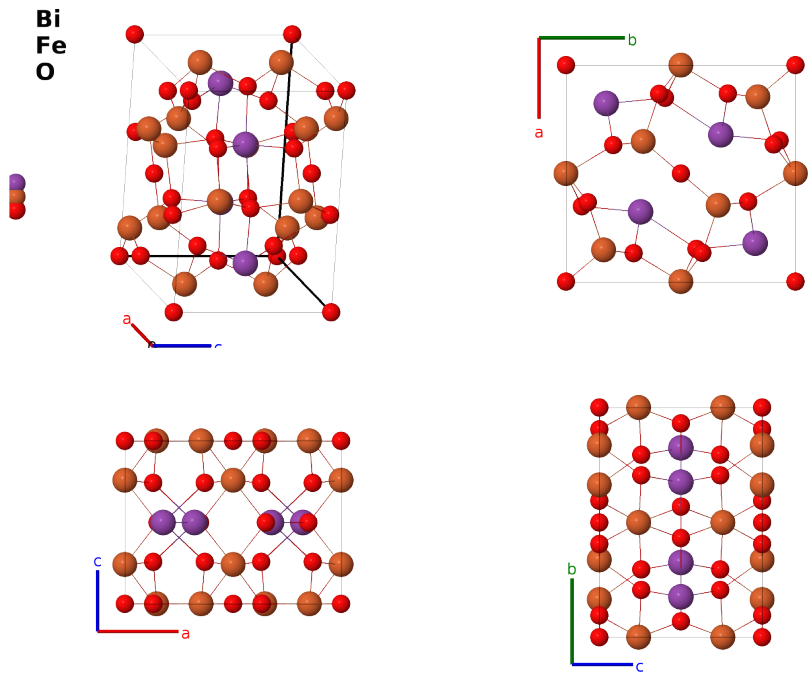
A2B4C9_oP30_55_h_fg_aghi-001

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<https://aflow.org/prototype-encyclopedia/7EHM>

https://aflow.org/prototype-encyclopedia/A2B4C9_oP30_55_h_fg_aghi-001



Prototype	$\text{Bi}_2\text{Fe}_4\text{O}_9$
AFLOW prototype label	A2B4C9_oP30_55_h_fg_aghi-001
ICSD	186440
CCDC	1695605
Pearson symbol	oP30
Space group number	55
Space group symbol	$Pb\bar{a}m$
AFLOW prototype command	<code>aflow --proto=A2B4C9_oP30_55_h_fg_aghi-001</code> <code>--params=a,b/a,c/a,z₂,x₃,y₃,x₄,y₄,x₅,y₅,x₆,y₆,x₇,y₇,z₇</code>

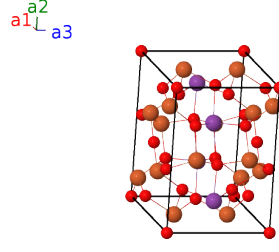
- This is the low pressure phase of $\text{Bi}_2\text{Fe}_4\text{O}_9$, using data take by (Friedrich, 2012) at ambient pressure. Above 6.89 GPa it transforms to the high pressure $\text{Bi}_2\text{Fe}_4\text{O}_9$ structure.

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	O I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a) O I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f) Fe I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(4f) Fe I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f) Fe I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(4f) Fe I
$\mathbf{B}_7$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g) Fe II
$\mathbf{B}_8$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g) Fe II
$\mathbf{B}_9$	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Fe II
$\mathbf{B}_{10}$	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) Fe II
$\mathbf{B}_{11}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g) O II
$\mathbf{B}_{12}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g) O II
$\mathbf{B}_{13}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g) O II
$\mathbf{B}_{14}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g) O II
$\mathbf{B}_{15}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Bi I
$\mathbf{B}_{16}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Bi I
$\mathbf{B}_{17}$	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Bi I
$\mathbf{B}_{18}$	$=$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) Bi I
$\mathbf{B}_{19}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O III
$\mathbf{B}_{20}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O III
$\mathbf{B}_{21}$	$=$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O III
$\mathbf{B}_{22}$	$=$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h) O III
$\mathbf{B}_{23}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8i) O IV
$\mathbf{B}_{24}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8i) O IV
$\mathbf{B}_{25}$	$=$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8i) O IV
$\mathbf{B}_{26}$	$=$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8i) O IV

$$\begin{aligned}
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8i) & \text{O IV} \\
\mathbf{B}_{28} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8i) & \text{O IV} \\
\mathbf{B}_{29} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8i) & \text{O IV} \\
\mathbf{B}_{30} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8i) & \text{O IV}
\end{aligned}$$

References

- [1] A. Friedrich, J. Biehler, W. Morgenroth, L. Wiehl, B. Winkler, M. Hanfland, M. Tolkiehn, 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.

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