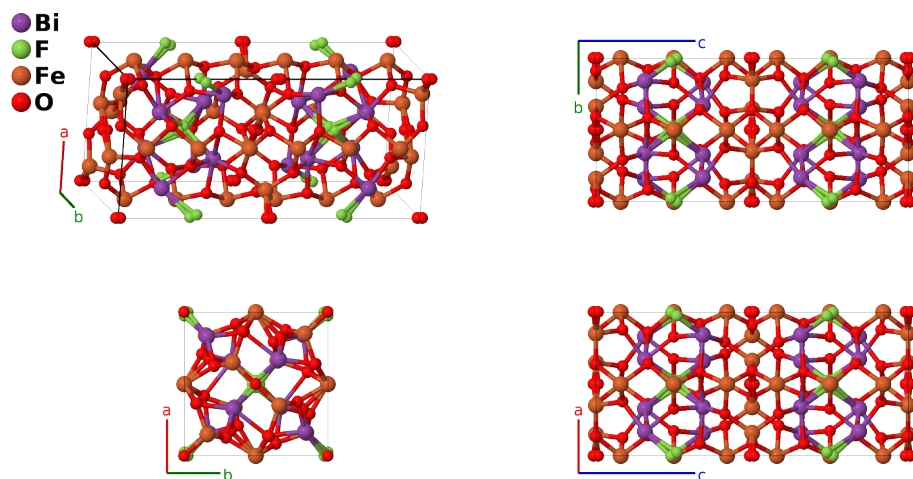


Bi₄Fe₅O₁₃F Structure: A4B4C5D14_tP108_135_i_i_dfh_egh2i-001

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<https://aflow.org/p/55HD>

https://aflow.org/p/A4B4C5D14_tP108_135_i_i_dfh_egh2i-001

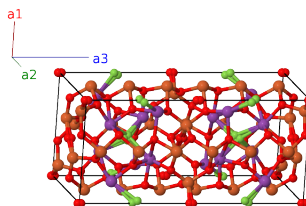


Prototype	Bi ₄ FFe ₅ O ₁₃
AFLOW prototype label	A4B4C5D14_tP108_135_i_i_dfh_egh2i-001
ICSD	236370
Pearson symbol	tP108
Space group number	135
Space group symbol	$P4_2/mbc$
AFLOW prototype command	aflow --proto=A4B4C5D14_tP108_135_i_i_dfh_egh2i-001 --params= $a, c/a, z_2, z_3, x_4, x_5, y_5, x_6, y_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- The O-I (8e) and F-I (16i) sites are only 1/4 occupied.

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Fe I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Fe I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Fe I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Fe I
\mathbf{B}_5	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_6	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_7	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_8	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_9	$= -z_2 \mathbf{a}_3$	$=$	$-c z_2 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{10}	$= -(z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{11}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{12}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O I
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c z_3 \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{17}	$= \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{18}	$= \frac{1}{2} \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{19}	$= \frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_3 \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{20}	$= \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Fe II
\mathbf{B}_{21}	$= x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{22}	$= -x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{23}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{24}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{25}	$= -x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{26}	$= x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{27}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{28}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8g)	O II
\mathbf{B}_{29}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$a x_5 \hat{\mathbf{x}} + a y_5 \hat{\mathbf{y}}$	(8h)	Fe III
\mathbf{B}_{30}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-a x_5 \hat{\mathbf{x}} - a y_5 \hat{\mathbf{y}}$	(8h)	Fe III
\mathbf{B}_{31}	$= -y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a y_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Fe III
\mathbf{B}_{32}	$= y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a y_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Fe III
\mathbf{B}_{33}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_5 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Fe III
\mathbf{B}_{34}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_5 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Fe III
\mathbf{B}_{35}	$= (y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Fe III
\mathbf{B}_{36}	$= -(y_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	Fe III
\mathbf{B}_{37}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}}$	(8h)	O III
\mathbf{B}_{38}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-a x_6 \hat{\mathbf{x}} - a y_6 \hat{\mathbf{y}}$	(8h)	O III
\mathbf{B}_{39}	$= -y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a y_6 \hat{\mathbf{x}} + a x_6 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	O III

$$\mathbf{B}_{105} = \begin{pmatrix} (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + \\ z_{10} \mathbf{a}_3 \end{pmatrix} = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - a(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} \quad (16i) \quad \text{O V}$$

$$\mathbf{B}_{106} = \begin{pmatrix} -(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ z_{10} \mathbf{a}_3 \end{pmatrix} = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} \quad (16i) \quad \text{O V}$$

$$\mathbf{B}_{107} = \begin{pmatrix} -(y_{10} - \frac{1}{2}) \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + \\ (z_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_{10} - \frac{1}{2}) \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} \quad (16i) \quad \text{O V}$$

$$\mathbf{B}_{108} = \begin{pmatrix} (y_{10} + \frac{1}{2}) \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (z_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}} \quad (16i) \quad \text{O V}$$

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