$Na_5Fe_3F_{14}$ Structure: A14B3C5_tP44_94_c3g_ad_bg-001

This structure previously used the label(s) `A14B3C5_tP44_94_c3g_ad_bg`. Calls to these addresses will be redirected here.

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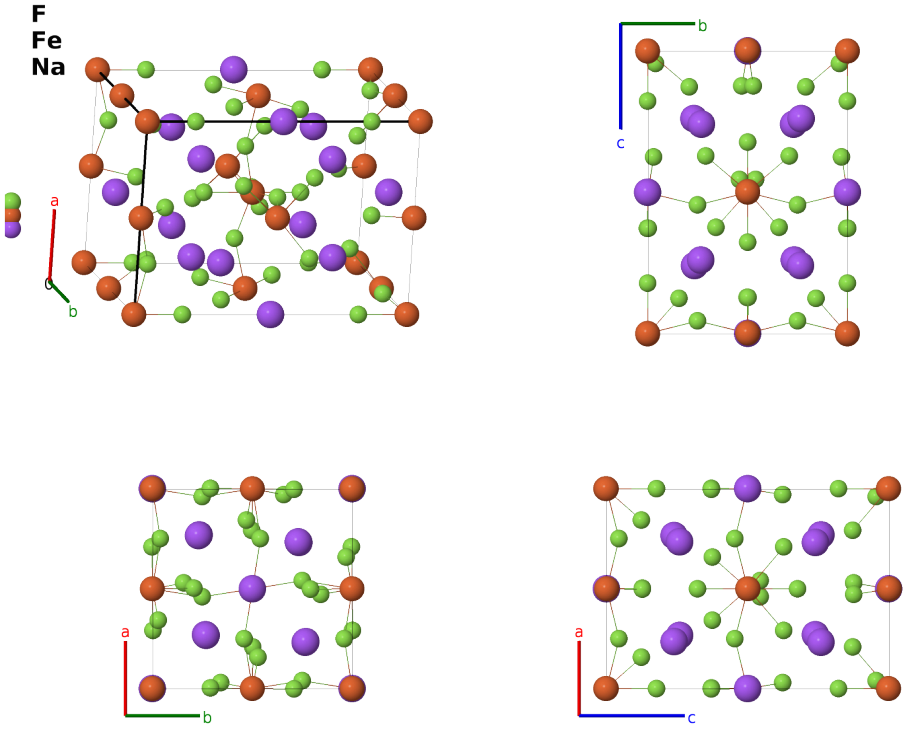
https://aflow.org/prototype-encyclopedia/CH2B

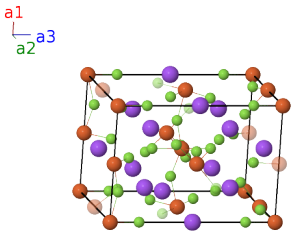
https://aflow.org/prototype-encyclopedia/A14B3C5_tP44_94_c3g_ad_bg-001



Prototype	$F_{14}Fe_3Na_5$
AFLOW prototype label	A14B3C5_tP44_94_c3g_ad_bg-001
ICSD	15928
CCDC	1596594
Pearson symbol	tP44
Space group number	94
Space group symbol	$P4_22_12$
AFLOW prototype command	`aflow --proto=A14B3C5_tP44_94_c3g_ad_bg-001 --params=`$a, c/a, z_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2b)	Na I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_8}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4d)	Fe II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Fe II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	Fe II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(4d)	Fe II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{15}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{16}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{17}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{18}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{19}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{20}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{23}}$	=	$-\left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F III

$$\mathbf{B_{24}} = \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_6-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

$$\mathbf{B_{25}} = -\left(x_6-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_6+\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

$$\mathbf{B_{26}} = \left(x_6+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

$$\mathbf{B_{27}} = y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

$$\mathbf{B_{28}} = -y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

$$\mathbf{B_{29}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{30}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{31}} = -\left(y_7-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{32}} = \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_7-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{33}} = -\left(x_7-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_7-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{34}} = \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_7-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_7-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{35}} = y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{36}} = -y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (8g) \quad \text{F IV}$$

$$\mathbf{B_{37}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{38}} = -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{39}} = -\left(y_8-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_8+\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_8-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_8+\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{40}} = \left(y_8+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_8-\tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_8+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_8-\tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{41}} = -\left(x_8-\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8+\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_8-\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_8+\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{42}} = \left(x_8+\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8-\tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_8+\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_8-\tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8-\tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{43}} = y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

$$\mathbf{B_{44}} = -y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (8g) \quad \text{Na II}$$

References

[1] M. Vlasse, F. Menil, C. Moriliere, J. M. Dance, A. Tressaud, and J. Portier, *Etude cristallographique et par effet Mössbauer du fluorure ferrimagnétique $Na_5Fe_3F_{14}\gamma$*, J. Solid State Chem. **17**, 291–298 (1976), doi:10.1016/0022-4596(76)90134-1.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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