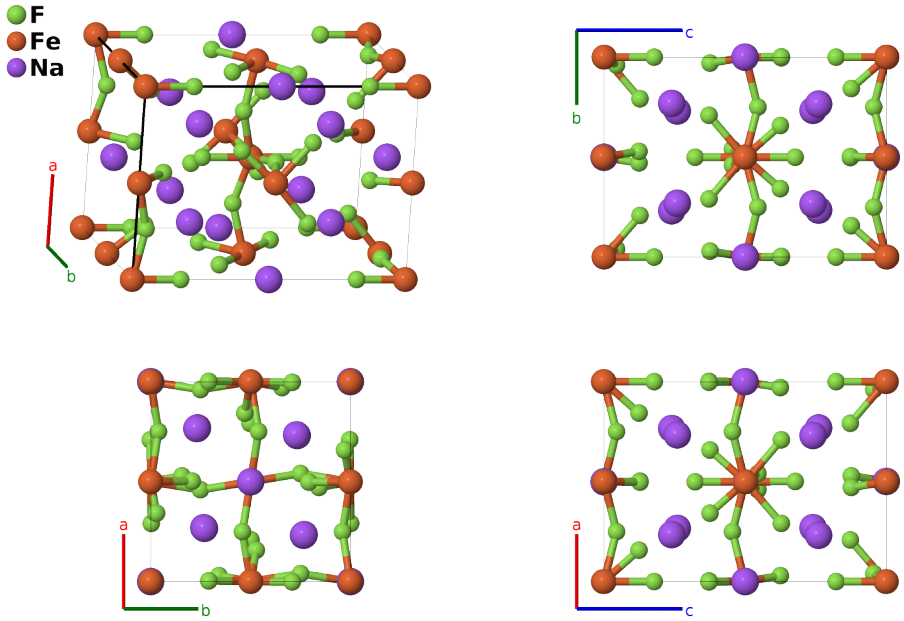
$Na_5Fe_3F_{14}$ Structure: A14B3C5_tP44_94_c3g_ad_bg-001

This structure originally had the label `A14B3C5_tP44_94_c3g_ad_bg`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/CH2B

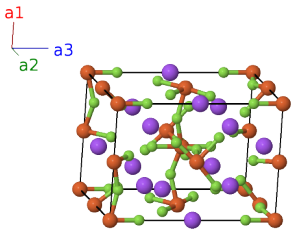
https://aflow.org/p/A14B3C5_tP44_94_c3g_ad_bg-001



Prototype	$F_{14}Fe_3Na_5$
AFLOW prototype label	A14B3C5_tP44_94_c3g_ad_bg-001
ICSD	15928
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
$\mathbf{B_{24}}$	=	$\left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{25}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{26}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{27}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{28}}$	=	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B_{29}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{30}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{31}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F IV

$\mathbf{B_{32}}$	$=$	$\left(y_7+\frac{1}{2}\right)\mathbf{a}_1-\left(x_7-\frac{1}{2}\right)\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_7+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{33}}$	$=$	$-\left(x_7-\frac{1}{2}\right)\mathbf{a}_1+\left(y_7+\frac{1}{2}\right)\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_7-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_7+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{34}}$	$=$	$\left(x_7+\frac{1}{2}\right)\mathbf{a}_1-\left(y_7-\frac{1}{2}\right)\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_7+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_7-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{35}}$	$=$	$y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	$=$	$ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{36}}$	$=$	$-y_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	$=$	$-ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(8g)	F IV
$\mathbf{B_{37}}$	$=$	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{38}}$	$=$	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$-ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{39}}$	$=$	$-\left(y_8-\frac{1}{2}\right)\mathbf{a}_1+\left(x_8+\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_8-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{40}}$	$=$	$\left(y_8+\frac{1}{2}\right)\mathbf{a}_1-\left(x_8-\frac{1}{2}\right)\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_8+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{41}}$	$=$	$-\left(x_8-\frac{1}{2}\right)\mathbf{a}_1+\left(y_8+\frac{1}{2}\right)\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_8-\frac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_8+\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{42}}$	$=$	$\left(x_8+\frac{1}{2}\right)\mathbf{a}_1-\left(y_8-\frac{1}{2}\right)\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_8+\frac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_8-\frac{1}{2}\right)\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{43}}$	$=$	$y_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$ay_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	Na II
$\mathbf{B_{44}}$	$=$	$-y_8\,\mathbf{a}_1-x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$-ay_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(8g)	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.