Nd$_2$Fe$_{14}$B Structure:
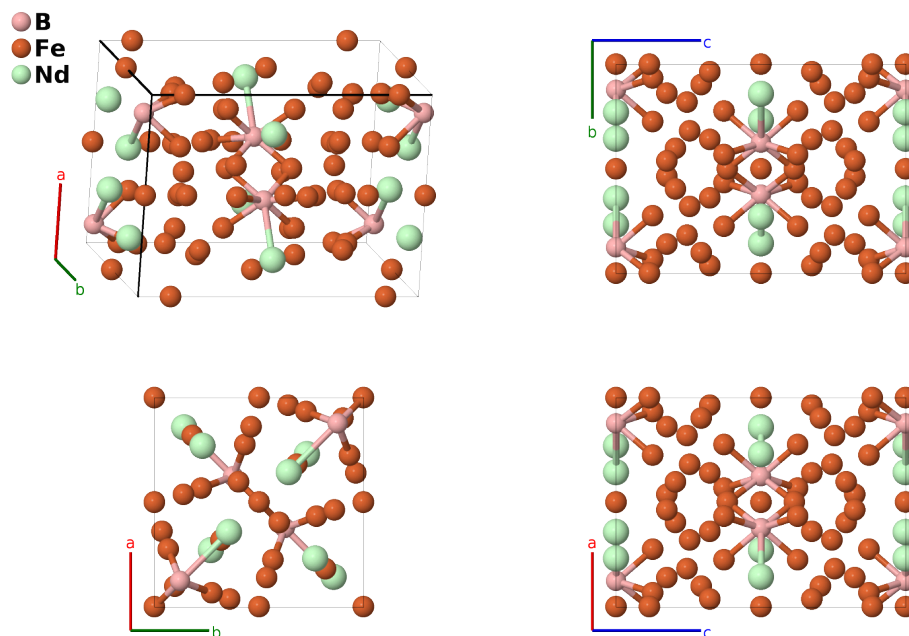# AB14C2_tP68_136_f_ce2j2k_fg-001

This structure originally had the label `AB14C2_tP68_136_f_ce2j2k_fg`. Calls to that address will be redirected here.

https://aflow.org/p/FUR0

https://aflow.org/p/AB14C2_tP68_136_f_ce2j2k_fg-001

Prototype	BFe$_{14}$Nd$_2$
AFLOW prototype label	AB14C2_tP68_136_f_ce2j2k_fg-001
ICSD	67224
Pearson symbol	tP68
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	aflow --proto=AB14C2_tP68_136_f_ce2j2k_fg-001 --params=$a, c/a, z_2, x_3, x_4, x_5, x_6, z_6, x_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure

Gd$_2$Co$_{14}$B, Gd$_2$Co$_{14}$C, Gd$_2$Fe$_{14}$B, Gd$_2$Fe$_{14}$C, Ho$_2$Fe$_{14}$B, Ho$_2$Fe$_{14}$C, La$_2$Fe$_{14}$B, La$_2$Fe$_{14}$C, Lu$_2$Fe$_{14}$B, Lu$_2$Fe$_{14}$C, Nd$_2$Co$_{14}$B, Pr$_2$Co$_{14}$B, Pr$_2$Fe$_{14}$B, Pr$_2$Fe$_{14}$C, Sm$_2$Co$_{14}$B, Sm$_2$Fe$_{14}$B, Sm$_2$Fe$_{14}$C, Tb$_2$Co$_{14}$B, Tb$_2$Fe$_{14}$B, Tb$_2$Fe$_{14}$C, Th$_2$Fe$_{14}$B, Tm$_2$Fe$_{14}$B, Tm$_2$Fe$_{14}$C, Y$_2$Co$_{14}$B, Y$_2$Fe$_{14}$B, Gd$_2$(Co$_{10}$Mn$_4$)B, Gd$_2$(Co$_7$Fe$_7$)B, La$_2$(Co$_7$Fe$_7$)B, Nd$_2$(Co$_7$Fe$_7$)B, Pr$_2$(Co$_7$Fe$_7$)B, Tm$_2$(Fe$_{10}$Mn$_4$)B, Y$_2$(Fe$_{10}$Mn$_4$)B, (GdNd)Fe$_{14}$B, (HoNd)Fe$_{14}$B, (NdPr)Fe$_{14}$B, (NdTb)Co$_{14}$B, (NdTb)Fe$_{14}$B, (NdY)Co$_{14}$B, (NdY)Fe$_{14}$B, (ThY)Fe$_{14}$B

- In many cases the boron site can be partially occupied with boron or carbon, or have a mixture of boron and carbon.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
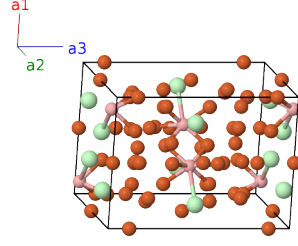
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\frac{1}{2}\,\mathbf{a_2}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Fe I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_3}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B_4}$	$=$	$\frac{1}{2}\,\mathbf{a_1}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Fe I
$\mathbf{B_5}$	$=$	$z_2\,\mathbf{a_3}$	$=$	$cz_2\,\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_6}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_7}$	$=$	$\frac{1}{2}\,\mathbf{a_1} + \frac{1}{2}\,\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_8}$	$=$	$-z_2\,\mathbf{a_3}$	$=$	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2}$	$=$	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4f)	B I
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2}$	$=$	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4f)	B I
$\mathbf{B_{11}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \left(x_3 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	B I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} - \left(x_3 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	B I
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2}$	$=$	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(4f)	Nd I
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2}$	$=$	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(4f)	Nd I
$\mathbf{B_{15}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\mathbf{a_1} + \left(x_4 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Nd I
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\mathbf{a_1} - \left(x_4 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Nd I
$\mathbf{B_{17}}$	$=$	$x_5\,\mathbf{a_1} - x_5\,\mathbf{a_2}$	$=$	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(4g)	Nd II
$\mathbf{B_{18}}$	$=$	$-x_5\,\mathbf{a_1} + x_5\,\mathbf{a_2}$	$=$	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(4g)	Nd II
$\mathbf{B_{19}}$	$=$	$\left(x_5 + \frac{1}{2}\right)\mathbf{a_1} + \left(x_5 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Nd II
$\mathbf{B_{20}}$	$=$	$-\left(x_5 - \frac{1}{2}\right)\mathbf{a_1} - \left(x_5 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	$=$	$-a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4g)	Nd II
$\mathbf{B_{21}}$	$=$	$x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8j)	Fe III
$\mathbf{B_{22}}$	$=$	$-x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	$=$	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8j)	Fe III
$\mathbf{B_{23}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \left(x_6 + \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8j)	Fe III
$\mathbf{B_{24}}$	$=$	$\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} - \left(x_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8j)	Fe III
$\mathbf{B_{25}}$	$=$	$-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} + \left(x_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8j)	Fe III

$$\mathbf{B_{26}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(x_6 - \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe III}$$

$$\mathbf{B_{27}} = x_6\,\mathbf{a_1} + x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} \quad = \quad ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe III}$$

$$\mathbf{B_{28}} = -x_6\,\mathbf{a_1} - x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3} \quad = \quad -ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe III}$$

$$\mathbf{B_{29}} = x_7\,\mathbf{a_1} + x_7\,\mathbf{a_2} + z_7\,\mathbf{a_3} \quad = \quad ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{30}} = -x_7\,\mathbf{a_1} - x_7\,\mathbf{a_2} + z_7\,\mathbf{a_3} \quad = \quad -ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{31}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(x_7 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{32}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(x_7 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{33}} = -\left(x_7 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(x_7 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{34}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(x_7 - \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{35}} = x_7\,\mathbf{a_1} + x_7\,\mathbf{a_2} - z_7\,\mathbf{a_3} \quad = \quad ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{36}} = -x_7\,\mathbf{a_1} - x_7\,\mathbf{a_2} - z_7\,\mathbf{a_3} \quad = \quad -ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(8j)} \quad \text{Fe IV}$$

$$\mathbf{B_{37}} = x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} \quad = \quad ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{38}} = -x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} \quad = \quad -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{39}} = -\left(y_8 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(x_8 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{40}} = \left(y_8 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(x_8 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{41}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{42}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{43}} = y_8\,\mathbf{a_1} + x_8\,\mathbf{a_2} - z_8\,\mathbf{a_3} \quad = \quad ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{44}} = -y_8\,\mathbf{a_1} - x_8\,\mathbf{a_2} - z_8\,\mathbf{a_3} \quad = \quad -ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{45}} = -x_8\,\mathbf{a_1} - y_8\,\mathbf{a_2} - z_8\,\mathbf{a_3} \quad = \quad -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{46}} = x_8\,\mathbf{a_1} + y_8\,\mathbf{a_2} - z_8\,\mathbf{a_3} \quad = \quad ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{47}} = \left(y_8 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(x_8 - \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{48}} = -\left(y_8 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(x_8 + \tfrac{1}{2}\right)\mathbf{a_2} - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{49}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a_1} - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{50}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{51}} = -y_8\,\mathbf{a_1} - x_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} \quad = \quad -ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{52}} = y_8\,\mathbf{a_1} + x_8\,\mathbf{a_2} + z_8\,\mathbf{a_3} \quad = \quad ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe V}$$

$$\mathbf{B_{53}} = x_9\,\mathbf{a_1} + y_9\,\mathbf{a_2} + z_9\,\mathbf{a_3} \quad = \quad ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe VI}$$

$$\mathbf{B_{54}} = -x_9\,\mathbf{a_1} - y_9\,\mathbf{a_2} + z_9\,\mathbf{a_3} \quad = \quad -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe VI}$$

$$\mathbf{B_{55}} = -\left(y_9 - \tfrac{1}{2}\right)\mathbf{a_1} + \left(x_9 + \tfrac{1}{2}\right)\mathbf{a_2} + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a_3} \quad = \quad -a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad \text{(16k)} \quad \text{Fe VI}$$

$$\mathbf{B_{56}} = \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{57}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{58}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{59}} = y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{60}} = -y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{61}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{62}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{63}} = \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{64}} = -\left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{65}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{66}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{67}} = -y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

$$\mathbf{B_{68}} = y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16\text{k}) \quad \text{Fe VI}$$

References

[1] D. Givord, H. S. Li, and J. M. Moreau, *Magnetic properties and crystal structure of $Nd_2Fe_{14}B$*, Solid State Commun. **50**, 497–499 (1984), doi:10.1016/0038-1098(84)90315-6.