

Nd₂Fe₁₄B Structure:

AB14C2_tP68_136_f_ce2j2k_fg-001

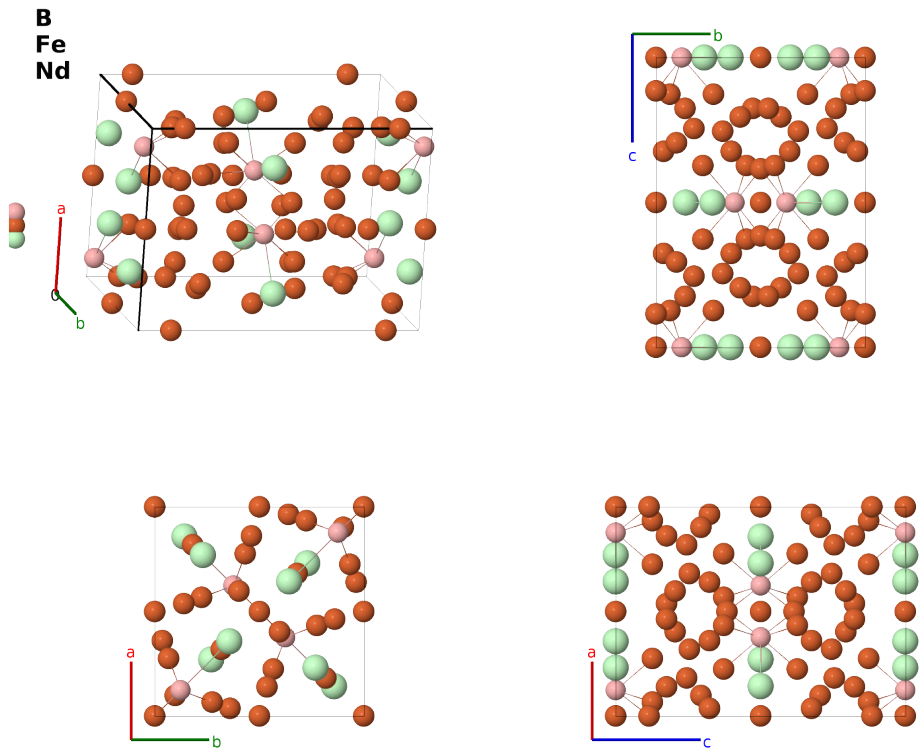
This structure previously used the label(s) **AB14C2_tP68_136_f_ce2j2k_fg**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/FUR0>

https://aflow.org/prototype-encyclopedia/AB14C2_tP68_136_f_ce2j2k_fg-001



Prototype	BFe ₁₄ Nd ₂
AFLOW prototype label	AB14C2_tP68_136_f_ce2j2k_fg-001
ICSD	67224
CCDC	1629242
Pearson symbol	tP68
Space group number	136
Space group symbol	$P4_2/mnm$
AFLOW prototype command	<pre>aflow --proto=AB14C2_tP68_136_f_ce2j2k_fg-001 --params=a,c/a,z2,x3,x4,x5,x6,z6,x7,z7,x8,y8,z8,x9,y9,z9</pre>

Other compounds with this structure

Gd₂Co₁₄B, Gd₂Co₁₄C, Gd₂Fe₁₄B, Gd₂Fe₁₄C, Ho₂Fe₁₄B, Ho₂Fe₁₄C, La₂Fe₁₄B, La₂Fe₁₄C, Lu₂Fe₁₄B, Lu₂Fe₁₄C, Nd₂Co₁₄B, Pr₂Co₁₄B, Pr₂Fe₁₄B, Pr₂Fe₁₄C, Sm₂Co₁₄B, Sm₂Fe₁₄B, Sm₂Fe₁₄C, Tb₂Co₁₄B, Tb₂Fe₁₄B, Tb₂Fe₁₄C, Th₂Fe₁₄B, Tm₂Fe₁₄B, Tm₂Fe₁₄C, Y₂Co₁₄B, Y₂Fe₁₄B, Gd₂(Co₁₀Mn₄)B, Gd₂(Co₇Fe₇)B, La₂(Co₇Fe₇)B, Nd₂(Co₇Fe₇)B, Pr₂(Co₇Fe₇)B, Tm₂(Fe₁₀Mn₄)B, Y₂(Fe₁₀Mn₄)B, (GdNd)Fe₁₄B, (HoNd)Fe₁₄B, (NdPr)Fe₁₄B, (NdTb)Co₁₄B, (NdTb)Fe₁₄B, (NdY)Co₁₄B, (NdY)Fe₁₄B, (ThY)Fe₁₄B

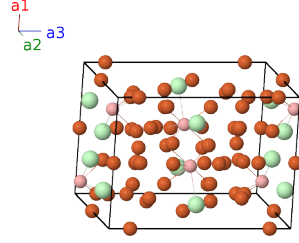
- In many cases the boron site can be partially occupied with boron or carbon, or have a mixture of boron and carbon.

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
$\mathbf{B}_5$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_8$	$= -z_2 \mathbf{a}_3$	$=$	$-c z_2 \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}}$	(4f)	B I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-a x_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}}$	(4f)	B I
$\mathbf{B}_{11}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	B I
$\mathbf{B}_{12}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	B I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}}$	(4f)	Nd I
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-a x_4 \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}}$	(4f)	Nd I
$\mathbf{B}_{15}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Nd I
$\mathbf{B}_{16}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Nd I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$a x_5 \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}}$	(4g)	Nd II
$\mathbf{B}_{18}$	$= -x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2$	$=$	$-a x_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}}$	(4g)	Nd II
$\mathbf{B}_{19}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g)	Nd II

$$\begin{aligned}
\mathbf{B}_{49} &= \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe V} \\
\mathbf{B}_{50} &= -\begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_8 + \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_8 - \frac{1}{2} \\ z_8 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe V} \\
\mathbf{B}_{51} &= -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}} &(16k) & \text{Fe V} \\
\mathbf{B}_{52} &= 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}} &(16k) & \text{Fe V} \\
\mathbf{B}_{53} &= 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}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{54} &= -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}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{55} &= -\begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{56} &= \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{57} &= -\begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{58} &= \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \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}} &(16k) & \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}} &(16k) & \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}} &(16k) & \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}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{63} &= \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{64} &= -\begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_2 - \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} - c \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{65} &= \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= a \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - a \begin{pmatrix} y_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \text{Fe VI} \\
\mathbf{B}_{66} &= -\begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -a \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + a \begin{pmatrix} y_9 + \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_9 - \frac{1}{2} \\ z_9 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} &(16k) & \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}} &(16k) & \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}} &(16k) & \text{Fe VI}
\end{aligned}$$

References

- [1] D. Givord, H. S. Li, and J. M. Moreau, *Magnetic properties and crystal structure of Nd₂Fe₁₄B*, Solid State Commun. **50**, 497–499 (1984), doi:10.1016/0038-1098(84)90315-6.

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