

Gd₂Ni₃Ga₅ Structure:

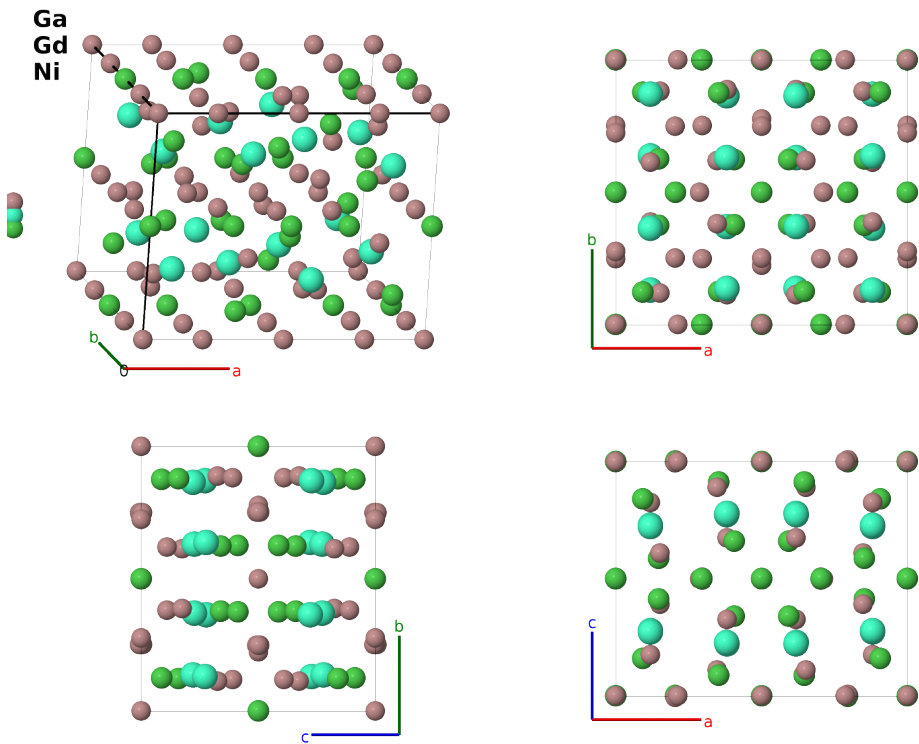
A5B2C3_oP80_48_abgij3m_2m_cdh2m-001

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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/E4GG>

https://aflow.org/prototype-encyclopedia/A5B2C3_oP80_48_abgij3m_2m_cdh2m-001

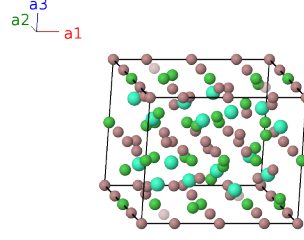


Prototype	Ga ₅ Gd ₂ Ni ₃
AFLOW prototype label	A5B2C3_oP80_48_abgij3m_2m_cdh2m-001
ICSD	281205
CCDC	1721779
Pearson symbol	oP80
Space group number	48
Space group symbol	<i>Pnnn</i>
AFLOW prototype command	<pre>aflow --proto=A5B2C3_oP80_48_abgij3m_2m_cdh2m-001 --params=a, b/a, c/a, x₅, x₆, y₇, y₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅</pre>

- AFLOW rotates the lattice by 90° about the y-axis ($x \ y \ z \rightarrow -z \ y \ x$) and shifts the origin so that the gallium atoms which were originally at the (2b) and (2d) Wyckoff positions are now on the (2a) and (2b) sites.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Ga I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Ga I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Ga II
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Ga II
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2c)	Ni I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2c)	Ni I
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2d)	Ni II
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2d)	Ni II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Ga III
$\mathbf{B}_{10}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4g)	Ga III
$\mathbf{B}_{11}$	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Ga III
$\mathbf{B}_{12}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4g)	Ga III
$\mathbf{B}_{13}$	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4h)	Ni III
$\mathbf{B}_{14}$	$= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4h)	Ni III
$\mathbf{B}_{15}$	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4h)	Ni III
$\mathbf{B}_{16}$	$= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4h)	Ni III
$\mathbf{B}_{17}$	$= \frac{1}{4} \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4i)	Ga IV
$\mathbf{B}_{18}$	$= \frac{1}{4} \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - b \left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4i)	Ga IV
$\mathbf{B}_{19}$	$= \frac{3}{4} \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4i)	Ga IV
$\mathbf{B}_{20}$	$= \frac{3}{4} \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + b \left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4i)	Ga IV
$\mathbf{B}_{21}$	$= \frac{3}{4} \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4j)	Ga V
$\mathbf{B}_{22}$	$= \frac{3}{4} \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - b \left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4j)	Ga V
$\mathbf{B}_{23}$	$= \frac{1}{4} \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4j)	Ga V
$\mathbf{B}_{24}$	$= \frac{1}{4} \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + b \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4j)	Ga V
$\mathbf{B}_{25}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$a x_9 \hat{\mathbf{x}} + b y_9 \hat{\mathbf{y}} + c z_9 \hat{\mathbf{z}}$	(8m)	Ga VI
$\mathbf{B}_{26}$	$= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_9 \hat{\mathbf{z}}$	(8m)	Ga VI

$\mathbf{B}_{27} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 -$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VI
	$(z_9 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VI
$\mathbf{B}_{29} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8m)	Ga VI
$\mathbf{B}_{30} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8m)	Ga VI
$\mathbf{B}_{31} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VI
$\mathbf{B}_{32} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VI
	$(z_9 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{33} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8m)	Ga VII
$\mathbf{B}_{34} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8m)	Ga VII
	$z_{10} \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 -$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VII
	$(z_{10} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$ax_{10} \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VII
	$(z_{10} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{37} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8m)	Ga VII
$\mathbf{B}_{38} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8m)	Ga VII
	$z_{10} \mathbf{a}_3$				
$\mathbf{B}_{39} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 +$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VII
	$(z_{10} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{40} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VII
	$(z_{10} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8m)	Ga VIII
$\mathbf{B}_{42} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8m)	Ga VIII
	$z_{11} \mathbf{a}_3$				
$\mathbf{B}_{43} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 -$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VIII
	$(z_{11} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{44} =$	$x_{11} \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$ax_{11} \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VIII
	$(z_{11} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{45} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8m)	Ga VIII
$\mathbf{B}_{46} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8m)	Ga VIII
	$z_{11} \mathbf{a}_3$				
$\mathbf{B}_{47} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 +$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VIII
	$(z_{11} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{48} =$	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-ax_{11} \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Ga VIII
	$(z_{11} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{49} =$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(8m)	Gd I
$\mathbf{B}_{50} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(8m)	Gd I
	$z_{12} \mathbf{a}_3$				
$\mathbf{B}_{51} =$	$-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + y_{12} \mathbf{a}_2 -$	$=$	$-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Gd I
	$(z_{12} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{52} =$	$x_{12} \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 -$	$=$	$ax_{12} \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$	(8m)	Gd I
	$(z_{12} - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{53} =$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(8m)	Gd I
$\mathbf{B}_{54} =$	$(x_{12} + \frac{1}{2}) \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} + b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$	(8m)	Gd I
	$z_{12} \mathbf{a}_3$				

References

- [1] T. Chen, J. Yao, A. V. Knotko, V. O. Yapaskurt, and A. Morozkin, *The Gd-Ni-Ga system at 870 K as a representative of rare-earth nickel gallides: Crystal structure and magnetic properties*, J. Solid State Chem. **305**, 122692 (2022), doi:10.1016/j.jssc.2021.122692.

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