Ga$_4$Ni$_3$ Structure:
# A4B3_cI112_230_af_g-001

This structure originally had the label `A4B3_cI112_230_af_g`. Calls to that address will be redirected here.

https://aflow.org/p/K0Z6

https://aflow.org/p/A4B3_cI112_230_af_g-001
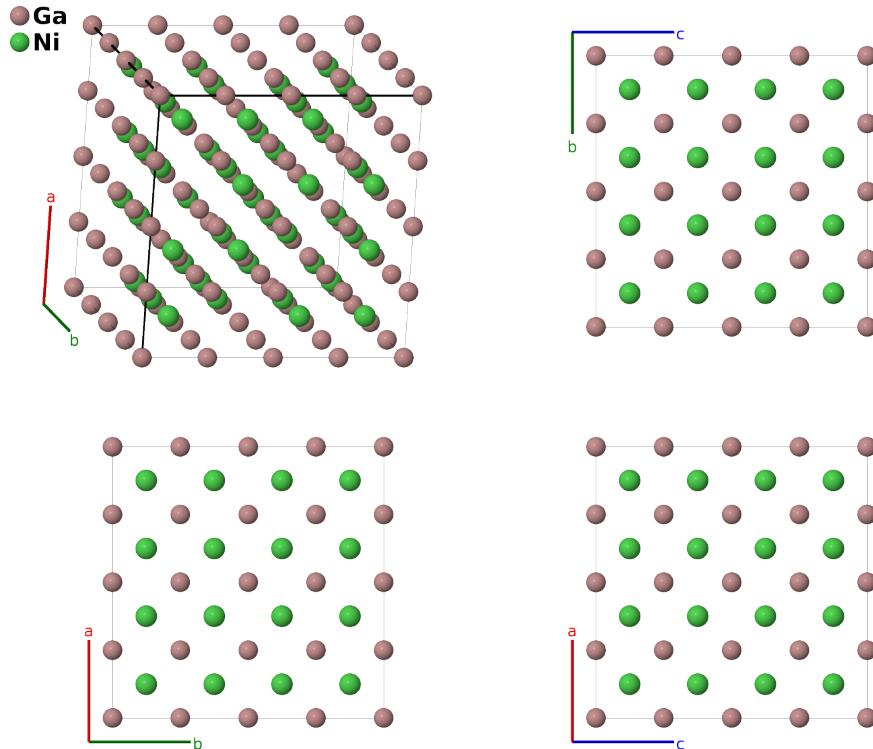
Prototype	Ga$_4$Ni$_3$
AFLOW prototype label	A4B3_cI112_230_af_g-001
ICSD	103864
Pearson symbol	cI112
Space group number	230
Space group symbol	$Ia\overline{3}d$
AFLOW prototype command	aflow --proto=A4B3_cI112_230_af_g-001 --params=a, x_2, y_3

- This is a simple defect superstructure of the CsCl ($B2$) structure. If GaNi $B2$ is expanded into a 128 atom supercell, we can describe it using space group $Ia\overline{3}d$ #230, with Ga atoms on the (16a) and (48f) Wyckoff sites and Ni atoms on the (16b) and (48g) sites. Removing the Ni atoms from the (16b) sites yields this structure.

Body-centered Cubic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}$$
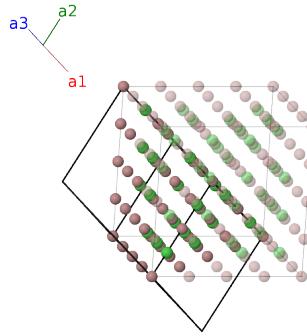
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(16a)	Ga I
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_3$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{y}}$	(16a)	Ga I
$\mathbf{B_3}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}}$	(16a)	Ga I
$\mathbf{B_4}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B_5}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_1$	$=$	$-\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B_6}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_1 + \tfrac{1}{2}\,\mathbf{a}_2 + \tfrac{1}{2}\,\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B_7}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} - \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B_8}$	$=$	$\tfrac{1}{2}\,\mathbf{a}_2$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - \tfrac{1}{4}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B_9}$	$=$	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_2 + x_2\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{10}}$	$=$	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_2 - \left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{11}}$	$=$	$x_2\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B_{12}}$	$=$	$-\left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - \left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{13}}$	$=$	$\left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{14}}$	$=$	$-\left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_1 - \left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{15}}$	$=$	$\left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{16}}$	$=$	$-\left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 - \left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B_{17}}$	$=$	$\tfrac{3}{4}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_3$	$=$	$a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{18}}$	$=$	$\tfrac{1}{4}\,\mathbf{a}_1 - \left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_2 - \left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_3$	$=$	$-a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{19}}$	$=$	$-\left(x_2 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_2 - \tfrac{1}{4}\right)\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{20}}$	$=$	$x_2\,\mathbf{a}_1 + \left(x_2 + \tfrac{1}{4}\right)\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{21}}$	$=$	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_2 - x_2\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + \tfrac{3}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{22}}$	$=$	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_2 + \left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_2 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B_{23}}$	$=$	$-x_2\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - \left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_3$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B_{24}}$	$=$	$\left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_3$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \tfrac{1}{2}\right)\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B_{25}}$	$=$	$-\left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(48f)	Ga II

$$\mathbf{B_{26}} = \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{4}\mathbf{a}_3 = \tfrac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{27}} = -\left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - x_2\,\mathbf{a}_3 = -\tfrac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{28}} = \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_3 = \tfrac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{29}} = \tfrac{1}{4}\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_3 = -a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{4}a\,\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{30}} = \tfrac{3}{4}\mathbf{a}_1 + \left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_2 + \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_3 = a\left(x_2 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{31}} = \left(x_2 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_2 + \tfrac{3}{4}\right)\mathbf{a}_2 + \tfrac{3}{4}\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_2 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{32}} = -x_2\,\mathbf{a}_1 - \left(x_2 - \tfrac{3}{4}\right)\mathbf{a}_2 + \tfrac{1}{4}\mathbf{a}_3 = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_2 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48f)}\quad\text{Ga II}$$

$$\mathbf{B_{33}} = \tfrac{1}{4}\mathbf{a}_1 - \left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_3 = \tfrac{1}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{34}} = -\left(2y_3 - \tfrac{3}{4}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_3 = -\tfrac{1}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{35}} = \left(2y_3 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_3 = -\tfrac{1}{8}a\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{36}} = \tfrac{1}{4}\mathbf{a}_1 + \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_3 = \tfrac{1}{8}a\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{37}} = \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 - \left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{38}} = -\left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_1 - \left(2y_3 - \tfrac{3}{4}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - \tfrac{1}{8}a\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{39}} = \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_1 + \left(2y_3 + \tfrac{3}{4}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - \tfrac{1}{8}a\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{40}} = -\left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_1 + \tfrac{1}{4}\mathbf{a}_2 + \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{1}{8}a\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{41}} = -\left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_2 + \tfrac{1}{4}\mathbf{a}_3 = ay_3\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{42}} = -\left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{3}{8}\right)\mathbf{a}_2 - \left(2y_3 - \tfrac{3}{4}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - \tfrac{1}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{43}} = \left(y_3 + \tfrac{1}{8}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_2 + \left(2y_3 + \tfrac{3}{4}\right)\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - \tfrac{1}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{44}} = \left(y_3 + \tfrac{3}{8}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{1}{8}\right)\mathbf{a}_2 + \tfrac{1}{4}\mathbf{a}_3 = -ay_3\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{1}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{45}} = \tfrac{3}{4}\mathbf{a}_1 + \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{46}} = \left(2y_3 + \tfrac{1}{4}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_3 = \tfrac{5}{8}a\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{47}} = -\left(2y_3 - \tfrac{1}{4}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_3 = \tfrac{5}{8}a\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{48}} = \tfrac{3}{4}\mathbf{a}_1 - \left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_3 = \tfrac{3}{8}a\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{49}} = -\left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 + \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} - a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{50}} = \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_1 + \left(2y_3 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_3 = a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{5}{8}a\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{51}} = -\left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_1 - \left(2y_3 - \tfrac{1}{4}\right)\mathbf{a}_2 - \left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{5}{8}a\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{52}} = \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_1 + \tfrac{3}{4}\mathbf{a}_2 - \left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + \tfrac{3}{8}a\,\hat{\mathbf{y}} + a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{53}} = \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_2 + \tfrac{3}{4}\mathbf{a}_3 = -a\left(y_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{54}} = \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{5}{8}\right)\mathbf{a}_2 + \left(2y_3 + \tfrac{1}{4}\right)\mathbf{a}_3 = ay_3\,\hat{\mathbf{x}} + a\left(y_3 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{5}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{55}} = -\left(y_3 - \tfrac{7}{8}\right)\mathbf{a}_1 - \left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_2 - \left(2y_3 - \tfrac{1}{4}\right)\mathbf{a}_3 = -ay_3\,\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{5}{8}a\,\hat{\mathbf{z}} \quad\text{(48g)}\quad\text{Ni I}$$

$$\mathbf{B_{56}} \quad = \quad -\left(y_3 - \tfrac{5}{8}\right)\mathbf{a}_1 + \left(y_3 + \tfrac{7}{8}\right)\mathbf{a}_2 + \quad = \quad a\left(y_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_3 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + \tfrac{3}{8}a\,\hat{\mathbf{z}} \qquad (48\mathrm{g}) \qquad \mathrm{Ni\ I}$$
$$\tfrac{3}{4}\,\mathbf{a}_3$$

References

[1] M. Ellner, K. Best, H. Jacobi, and K. Schubert, *Struktur von Ni$_3$Ga$_4$*, J. Less-Common Met. **19**, 294–296 (1969), doi:10.1016/0022-5088(69)90109-X.

Found in

[1] P. Villars and K. Cenzual, eds., *Structure Types. Part 1: Space Groups (230) Ia-3d – (219) F43-c* (Springer-Verlag, Berlin Heidelberg, 2004), chap. Ni$_3$Ga$_4$.