

Ga₄Ni₃ Structure:

A4B3_cI112_230_af_g-001

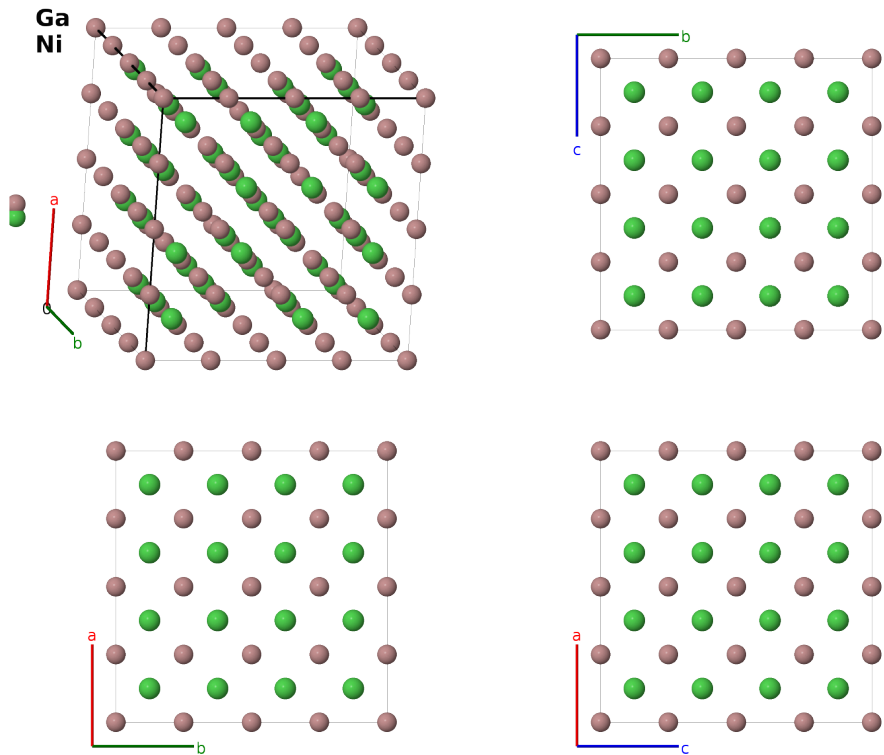
This structure previously used the label(s) **A4B3_cI112_230_af_g**. Calls to these addresses will be redirected here.

Cite this page as:

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/K0Z6>

https://aflow.org/prototype-encyclopedia/A4B3_cI112_230_af_g-001

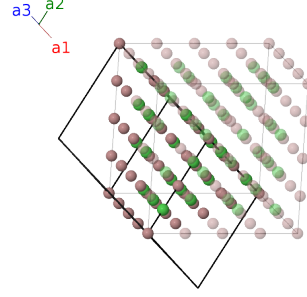


Prototype	Ga ₄ Ni ₃
AFLOW prototype label	A4B3_cI112_230_af_g-001
ICSD	103864
CCDC	1661798
Pearson symbol	cI112
Space group number	230
Space group symbol	$Ia\bar{3}d$
AFLOW prototype command	<code>aflow --proto=A4B3_cI112_230_af_g-001</code> <code>--params=a, x₂, y₃</code>

- 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 $Ia\bar{3}d$ #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

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(16a)	Ga I
$\mathbf{B}_2$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(16a)	Ga I
$\mathbf{B}_3$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(16a)	Ga I
$\mathbf{B}_4$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B}_5$	$\frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B}_6$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B}_7$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B}_8$	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16a)	Ga I
$\mathbf{B}_9$	$\frac{1}{4}\mathbf{a}_1 + (x_2 + \frac{1}{4})\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{10}$	$\frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{1}{4})\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{11}$	$x_2\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_2 + \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B}_{12}$	$-(x_2 - \frac{1}{2})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_2 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{13}$	$(x_2 + \frac{1}{4})\mathbf{a}_1 + x_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{14}$	$-(x_2 - \frac{1}{4})\mathbf{a}_1 - (x_2 - \frac{1}{2})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{15}$	$(x_2 + \frac{1}{4})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{16}$	$-(x_2 - \frac{1}{4})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B}_{17}$	$\frac{3}{4}\mathbf{a}_1 + x_2\mathbf{a}_2 + (x_2 + \frac{1}{4})\mathbf{a}_3$	$=$	$a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{18}$	$\frac{1}{4}\mathbf{a}_1 - (x_2 - \frac{1}{2})\mathbf{a}_2 - (x_2 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{19}$	$-(x_2 - \frac{1}{2})\mathbf{a}_1 - (x_2 - \frac{1}{4})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{20}$	$x_2\mathbf{a}_1 + (x_2 + \frac{1}{4})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{21}$	$\frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{3}{4})\mathbf{a}_2 - x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{22}$	$\frac{1}{4}\mathbf{a}_1 + (x_2 + \frac{3}{4})\mathbf{a}_2 + (x_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga II

$\mathbf{B}_{23} =$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (x_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B}_{24} =$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(48f)	Ga II
$\mathbf{B}_{25} =$	$-(x_2 - \frac{3}{4}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} - a x_2 \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{26} =$	$(x_2 + \frac{3}{4}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{27} =$	$-(x_2 - \frac{3}{4}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-\frac{1}{4} a \hat{\mathbf{x}} - a (x_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{28} =$	$(x_2 + \frac{3}{4}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a (x_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{29} =$	$\frac{1}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{4} a \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{30} =$	$\frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{31} =$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{3}{4}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + a (x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{32} =$	$-x_2 \mathbf{a}_1 - (x_2 - \frac{3}{4}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} - a (x_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48f)	Ga II
$\mathbf{B}_{33} =$	$\frac{1}{4} \mathbf{a}_1 - (y_3 - \frac{3}{8}) \mathbf{a}_2 + (y_3 + \frac{1}{8}) \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{34} =$	$-(2y_3 - \frac{3}{4}) \mathbf{a}_1 - (y_3 - \frac{1}{8}) \mathbf{a}_2 -$ $(y_3 - \frac{3}{8}) \mathbf{a}_3$	$=$	$-\frac{1}{8} a \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{35} =$	$(2y_3 + \frac{3}{4}) \mathbf{a}_1 + (y_3 + \frac{1}{8}) \mathbf{a}_2 +$ $(y_3 + \frac{3}{8}) \mathbf{a}_3$	$=$	$-\frac{1}{8} a \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{36} =$	$\frac{1}{4} \mathbf{a}_1 + (y_3 + \frac{3}{8}) \mathbf{a}_2 - (y_3 - \frac{1}{8}) \mathbf{a}_3$	$=$	$\frac{1}{8} a \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{37} =$	$(y_3 + \frac{1}{8}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (y_3 - \frac{3}{8}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + a y_3 \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{38} =$	$-(y_3 - \frac{3}{8}) \mathbf{a}_1 - (2y_3 - \frac{3}{4}) \mathbf{a}_2 -$ $(y_3 - \frac{1}{8}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{4}) \hat{\mathbf{x}} - \frac{1}{8} a \hat{\mathbf{y}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{39} =$	$(y_3 + \frac{3}{8}) \mathbf{a}_1 + (2y_3 + \frac{3}{4}) \mathbf{a}_2 +$ $(y_3 + \frac{1}{8}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{4}) \hat{\mathbf{x}} - \frac{1}{8} a \hat{\mathbf{y}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{40} =$	$-(y_3 - \frac{1}{8}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 +$ $(y_3 + \frac{3}{8}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} - a y_3 \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{41} =$	$-(y_3 - \frac{3}{8}) \mathbf{a}_1 + (y_3 + \frac{1}{8}) \mathbf{a}_2 +$ $\frac{1}{4} \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{42} =$	$-(y_3 - \frac{1}{8}) \mathbf{a}_1 - (y_3 - \frac{3}{8}) \mathbf{a}_2 -$ $(2y_3 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8} a \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{43} =$	$(y_3 + \frac{1}{8}) \mathbf{a}_1 + (y_3 + \frac{3}{8}) \mathbf{a}_2 +$ $(2y_3 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8} a \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{44} =$	$(y_3 + \frac{3}{8}) \mathbf{a}_1 - (y_3 - \frac{1}{8}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{45} =$	$\frac{3}{4} \mathbf{a}_1 + (y_3 + \frac{5}{8}) \mathbf{a}_2 - (y_3 - \frac{7}{8}) \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{46} =$	$(2y_3 + \frac{1}{4}) \mathbf{a}_1 + (y_3 + \frac{7}{8}) \mathbf{a}_2 +$ $(y_3 + \frac{5}{8}) \mathbf{a}_3$	$=$	$\frac{5}{8} a \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{47} =$	$-(2y_3 - \frac{1}{4}) \mathbf{a}_1 - (y_3 - \frac{7}{8}) \mathbf{a}_2 -$ $(y_3 - \frac{5}{8}) \mathbf{a}_3$	$=$	$\frac{5}{8} a \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{48} =$	$\frac{3}{4} \mathbf{a}_1 - (y_3 - \frac{5}{8}) \mathbf{a}_2 + (y_3 + \frac{7}{8}) \mathbf{a}_3$	$=$	$\frac{3}{8} a \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{49} =$	$-(y_3 - \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $(y_3 + \frac{5}{8}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{50} =$	$(y_3 + \frac{5}{8}) \mathbf{a}_1 + (2y_3 + \frac{1}{4}) \mathbf{a}_2 +$ $(y_3 + \frac{7}{8}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} + a y_3 \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{51} =$	$-(y_3 - \frac{5}{8}) \mathbf{a}_1 - (2y_3 - \frac{1}{4}) \mathbf{a}_2 -$ $(y_3 - \frac{7}{8}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} - a y_3 \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{52} =$	$(y_3 + \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (y_3 - \frac{5}{8}) \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{53} =$	$(y_3 + \frac{5}{8}) \mathbf{a}_1 - (y_3 - \frac{7}{8}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}}$	(48g)	Ni I

$$\begin{aligned}
\mathbf{B}_{54} &= \begin{pmatrix} (y_3 + \frac{7}{8}) \mathbf{a}_1 + (y_3 + \frac{5}{8}) \mathbf{a}_2 + \\ (2y_3 + \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}} & (48g) & \text{Ni I} \\
\mathbf{B}_{55} &= \begin{pmatrix} -(y_3 - \frac{7}{8}) \mathbf{a}_1 - (y_3 - \frac{5}{8}) \mathbf{a}_2 - \\ (2y_3 - \frac{1}{4}) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}} & (48g) & \text{Ni I} \\
\mathbf{B}_{56} &= \begin{pmatrix} -(y_3 - \frac{5}{8}) \mathbf{a}_1 + (y_3 + \frac{7}{8}) \mathbf{a}_2 + \\ \frac{3}{4} \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} & (48g) & \text{Ni I}
\end{aligned}$$

References

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Found in

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