

Ga₃Ni₃Zn Structure:

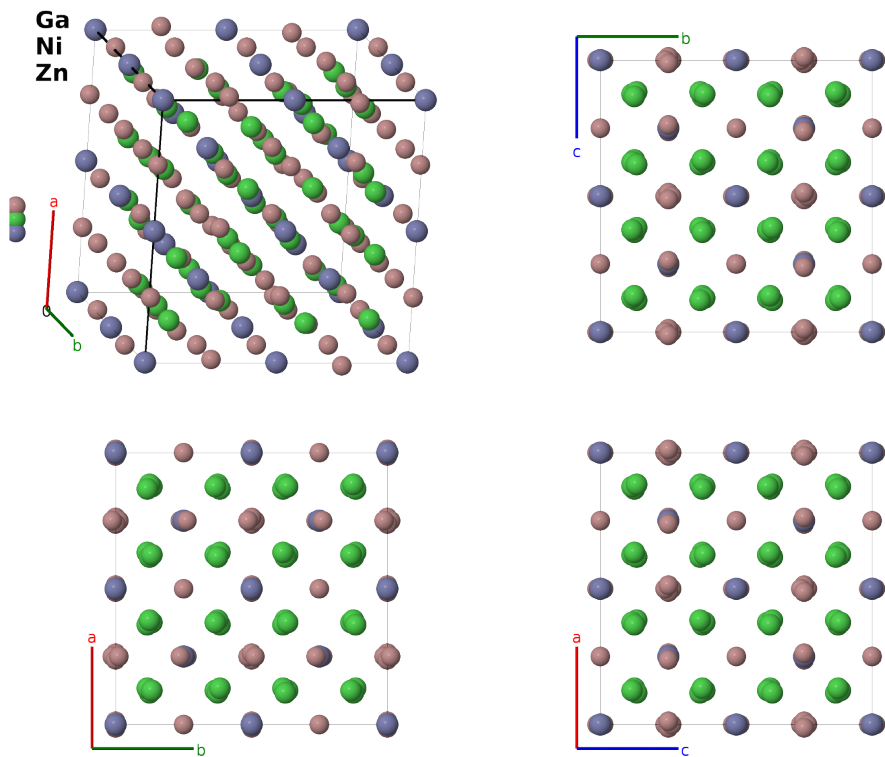
A3B3C_cI112_230_f_g_a-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/B0YQ>

https://aflow.org/prototype-encyclopedia/A3B3C_cI112_230_f_g_a-001

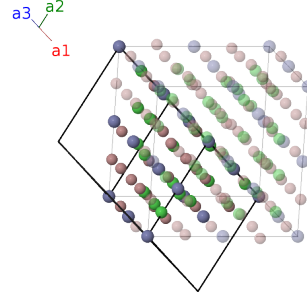


Prototype	Ga ₃ Ni ₃ Zn
AFLOW prototype label	A3B3C_cI112_230_f_g_a-001
ICSD	103898
CCDC	1661829
Pearson symbol	cI112
Space group number	230
Space group symbol	$Ia\bar{3}d$
AFLOW prototype command	<code>aflow --proto=A3B3C_cI112_230_f_g_a-001</code> <code>--params=a, x_2, y_3</code>

- This is the tenary form of Ga₄Ni₃.

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)	Zn I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(16a)	Zn I
$\mathbf{B}_3$	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(16a)	Zn I
$\mathbf{B}_4$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(16a)	Zn 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)	Zn 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)	Zn 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)	Zn 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)	Zn 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 I
$\mathbf{B}_{10}$	$= \frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{1}{4})\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{11}$	$= x_2\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_2 + \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}}$	(48f)	Ga I
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_2 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{13}$	$= (x_2 + \frac{1}{4})\mathbf{a}_1 + x_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{14}$	$= -(x_2 - \frac{1}{4})\mathbf{a}_1 - (x_2 - \frac{1}{2})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{15}$	$= (x_2 + \frac{1}{4})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + x_2\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_2 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{16}$	$= -(x_2 - \frac{1}{4})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - (x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - a(x_2 - \frac{1}{4})\hat{\mathbf{y}}$	(48f)	Ga I
$\mathbf{B}_{17}$	$= \frac{3}{4}\mathbf{a}_1 + x_2\mathbf{a}_2 + (x_2 + \frac{1}{4})\mathbf{a}_3$	$=$	$a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{18}$	$= \frac{1}{4}\mathbf{a}_1 - (x_2 - \frac{1}{2})\mathbf{a}_2 - (x_2 - \frac{1}{4})\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{19}$	$= -(x_2 - \frac{1}{2})\mathbf{a}_1 - (x_2 - \frac{1}{4})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} - a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{20}$	$= x_2\mathbf{a}_1 + (x_2 + \frac{1}{4})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + a(x_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{21}$	$= \frac{3}{4}\mathbf{a}_1 - (x_2 - \frac{3}{4})\mathbf{a}_2 - x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{22}$	$= \frac{1}{4}\mathbf{a}_1 + (x_2 + \frac{3}{4})\mathbf{a}_2 + (x_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{23}$	$= -x_2\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_2 - \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}}$	(48f)	Ga I
$\mathbf{B}_{24}$	$= (x_2 + \frac{1}{2})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_2 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_2 + \frac{1}{2})\hat{\mathbf{y}}$	(48f)	Ga I
$\mathbf{B}_{25}$	$= -(x_2 - \frac{3}{4})\mathbf{a}_1 - x_2\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(48f)	Ga I

$\mathbf{B}_{26} = (x_2 + \frac{3}{4}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$	$\frac{1}{4} a \hat{\mathbf{y}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{27} = -(x_2 - \frac{3}{4}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3 =$	$-\frac{1}{4} a \hat{\mathbf{x}} - a (x_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{28} = (x_2 + \frac{3}{4}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3 =$	$\frac{1}{4} a \hat{\mathbf{x}} + a (x_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{29} = \frac{1}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 - \frac{3}{4}) \mathbf{a}_3 =$	$-a (x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{4} a \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{30} = \frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3 =$	$a (x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{31} = (x_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{3}{4}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 =$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + a (x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{32} = -x_2 \mathbf{a}_1 - (x_2 - \frac{3}{4}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 =$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} - a (x_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48f)	Ga I
$\mathbf{B}_{33} = \frac{1}{4} \mathbf{a}_1 - (y_3 - \frac{3}{8}) \mathbf{a}_2 + (y_3 + \frac{1}{8}) \mathbf{a}_3 =$	$\frac{1}{8} a \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{54} = (y_3 + \frac{7}{8}) \mathbf{a}_1 + (y_3 + \frac{5}{8}) \mathbf{a}_2 + (2y_3 + \frac{1}{4}) \mathbf{a}_3 =$	$a y_3 \hat{\mathbf{x}} + a (y_3 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}}$	(48g)	Ni I
$\mathbf{B}_{55} = -(y_3 - \frac{7}{8}) \mathbf{a}_1 - (y_3 - \frac{5}{8}) \mathbf{a}_2 - (2y_3 - \frac{1}{4}) \mathbf{a}_3 =$	$-a y_3 \hat{\mathbf{x}} - a (y_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}}$	(48g)	Ni I

$$\mathbf{B}_{56} = -\left(y_3 - \frac{5}{8}\right) \mathbf{a}_1 + \left(y_3 + \frac{7}{8}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 = a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}} \quad (48g) \quad \text{Ni I}$$

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First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).