

Y₃Ni₂ Structure:

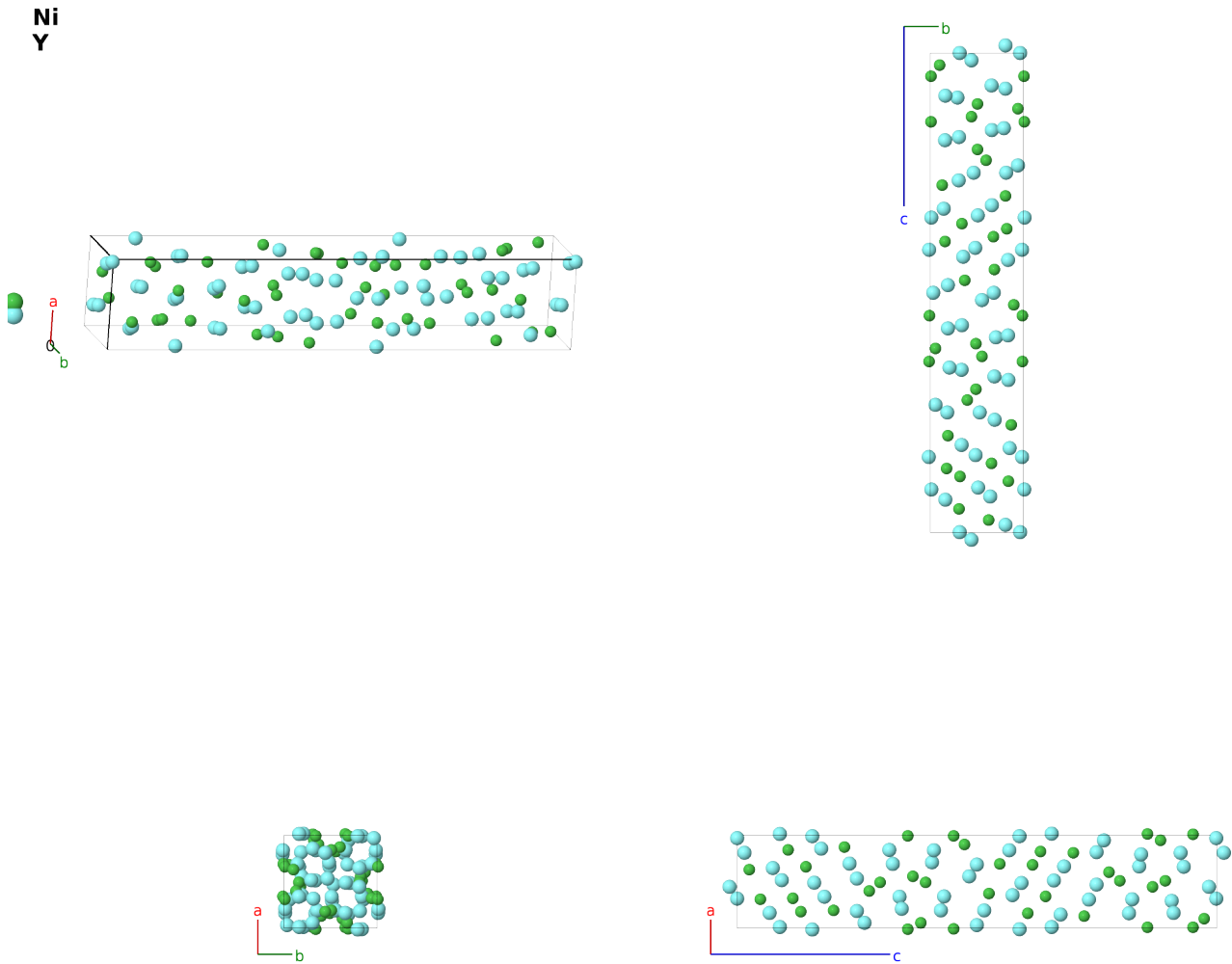
A2B3_tP80_92_4b_2a5b-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/J821>

https://aflow.org/prototype-encyclopedia/A2B3_tP80_92_4b_2a5b-001



Prototype

Ni₂Y₃

AFLOW prototype label

A2B3_tP80_92_4b_2a5b-001

ICSD	1287
CCDC	1591438
Pearson symbol	tP80
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	aflow --proto=A2B3_tP80_92_4b_2a5b-001 --params= $a, c/a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

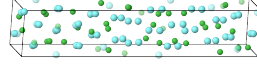
Simple Tetragonal primitive vectors



$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}}$	(4a)	Y I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Y I
$\mathbf{B}_3$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Y I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Y I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(4a)	Y II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Y II
$\mathbf{B}_7$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Y II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Y II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{11}$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{12}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{13}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{14}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Ni I

$\mathbf{B}_{15} =$	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{16} =$	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni I
$\mathbf{B}_{17} =$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{18} =$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{19} =$	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{20} =$	$(y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{21} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{22} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{23} =$	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{24} =$	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni II
$\mathbf{B}_{25} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{26} =$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{27} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{28} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{29} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{30} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{31} =$	$y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{32} =$	$-y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni III
$\mathbf{B}_{33} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{34} =$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{35} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{36} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{37} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{38} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{39} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{40} =$	$-y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Ni IV
$\mathbf{B}_{41} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8b)	Y III
$\mathbf{B}_{42} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8b)	Y III
$\mathbf{B}_{43} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{4}) \mathbf{a}_3$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{4}) \hat{\mathbf{z}}$	(8b)	Y III
$\mathbf{B}_{44} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{3}{4}) \hat{\mathbf{z}}$	(8b)	Y III

$\mathbf{B}_{45} =$	$-\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Y III
	$\left(z_7 - \frac{1}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{46} =$	$\left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Y III
	$\left(z_7 - \frac{3}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{47} =$	$y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8b)	Y III
$\mathbf{B}_{48} =$	$-y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y III
$\mathbf{B}_{49} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8b)	Y IV
$\mathbf{B}_{50} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y IV
$\mathbf{B}_{51} =$	$-\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Y IV
	$\left(z_8 + \frac{1}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{52} =$	$\left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Y IV
	$\left(z_8 + \frac{3}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{53} =$	$-\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Y IV
	$\left(z_8 - \frac{1}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{54} =$	$\left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Y IV
	$\left(z_8 - \frac{3}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{55} =$	$y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8b)	Y IV
$\mathbf{B}_{56} =$	$-y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y IV
$\mathbf{B}_{57} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8b)	Y V
$\mathbf{B}_{58} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y V
$\mathbf{B}_{59} =$	$-\left(y_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_9 + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Y V
	$\left(z_9 + \frac{1}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{60} =$	$\left(y_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_9 - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Y V
	$\left(z_9 + \frac{3}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{61} =$	$-\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Y V
	$\left(z_9 - \frac{1}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{62} =$	$\left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_9 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Y V
	$\left(z_9 - \frac{3}{4}\right) \mathbf{a}_3$				
$\mathbf{B}_{63} =$	$y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8b)	Y V
$\mathbf{B}_{64} =$	$-y_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y V
$\mathbf{B}_{65} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8b)	Y VI
$\mathbf{B}_{66} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ay_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y VI
$\mathbf{B}_{67} =$	$-\left(y_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$-a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} +$	(8b)	Y VI
	$\left(z_{10} + \frac{1}{4}\right) \mathbf{a}_3$		$c\left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$		
$\mathbf{B}_{68} =$	$\left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 +$	$=$	$a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} +$	(8b)	Y VI
	$\left(z_{10} + \frac{3}{4}\right) \mathbf{a}_3$		$c\left(z_{10} + \frac{3}{4}\right) \hat{\mathbf{z}}$		
$\mathbf{B}_{69} =$	$-\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$-a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} -$	(8b)	Y VI
	$\left(z_{10} - \frac{1}{4}\right) \mathbf{a}_3$		$c\left(z_{10} - \frac{1}{4}\right) \hat{\mathbf{z}}$		
$\mathbf{B}_{70} =$	$\left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 -$	$=$	$a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} -$	(8b)	Y VI
	$\left(z_{10} - \frac{3}{4}\right) \mathbf{a}_3$		$c\left(z_{10} - \frac{3}{4}\right) \hat{\mathbf{z}}$		
$\mathbf{B}_{71} =$	$y_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$ay_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8b)	Y VI
$\mathbf{B}_{72} =$	$-y_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y VI
$\mathbf{B}_{73} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8b)	Y VII
$\mathbf{B}_{74} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Y VII

$$\begin{aligned}
\mathbf{B}_{75} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{4}\right) \mathbf{a}_3 = -a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VII} \\
\mathbf{B}_{76} &= \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{3}{4}\right) \mathbf{a}_3 = a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{11} + \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VII} \\
\mathbf{B}_{77} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{1}{4}\right) \mathbf{a}_3 = -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VII} \\
\mathbf{B}_{78} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{11} - \frac{3}{4}\right) \mathbf{a}_3 = a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{11} - \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VII} \\
\mathbf{B}_{79} &= y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 = ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} & (8b) & \text{Y VII} \\
\mathbf{B}_{80} &= -y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 = -ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Y VII}
\end{aligned}$$

References

- [1] J. L. Roy, J.-M. Moreau, and D. Paccard, *Y₃Ni₂: a new tetragonal phase with Ni-centred trigonal prisms*, Acta Crystallogr. Sect. B **33**, 3406–3409 (1977), doi:10.1107/S0567740877011091.

Found in

- [1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Nickel-Yttrium Binary Phase Diagram (1990 Nash P.). Copyright ©2006-2018 ASM International.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.