

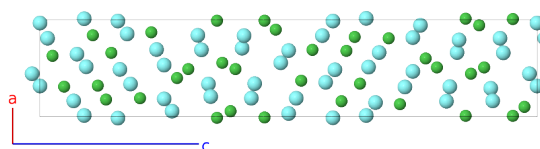
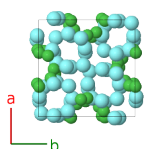
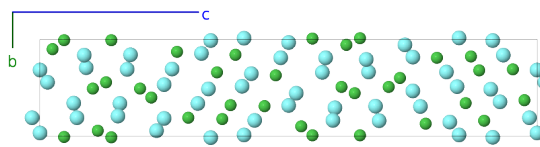
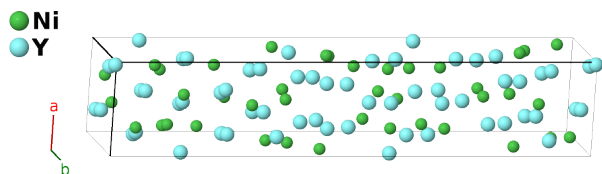
Y₃Ni₂ Structure:

A2B3_tP80_92_4b_2a5b-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://afLOW.org/p/J821>

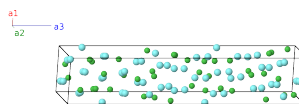
https://afLOW.org/p/A2B3_tP80_92_4b_2a5b-001



Prototype	Ni ₂ Y ₃
AFLOW prototype label	A2B3_tP80_92_4b_2a5b-001
ICSD	1287
Pearson symbol	tP80
Space group number	92
Space group symbol	<i>P</i> 4 ₁ 2 ₁ 2
AFLOW prototype command	<code>afLOW --proto=A2B3_tP80_92_4b_2a5b-001</code> <code>--params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁</code>

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B ₁	=	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	=	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}}$	(4a) Y I
B ₂	=	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a x_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) Y I
B ₃	=	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$-a (x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a) Y I
B ₄	=	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$a (x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a) Y I
B ₅	=	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	=	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}}$	(4a) Y II

$$\begin{aligned}
\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) & \text{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 + \left(z_{10} + \frac{1}{4}\right) \mathbf{a}_3 = -a \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VI} \\
\mathbf{B}_{68} &= \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{3}{4}\right) \mathbf{a}_3 = a \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VI} \\
\mathbf{B}_{69} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{4}\right) \mathbf{a}_3 = -a \left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{10} - \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VI} \\
\mathbf{B}_{70} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{3}{4}\right) \mathbf{a}_3 = a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{10} - \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Y VI} \\
\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) & \text{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) & \text{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) & \text{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) & \text{Y VII} \\
\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.