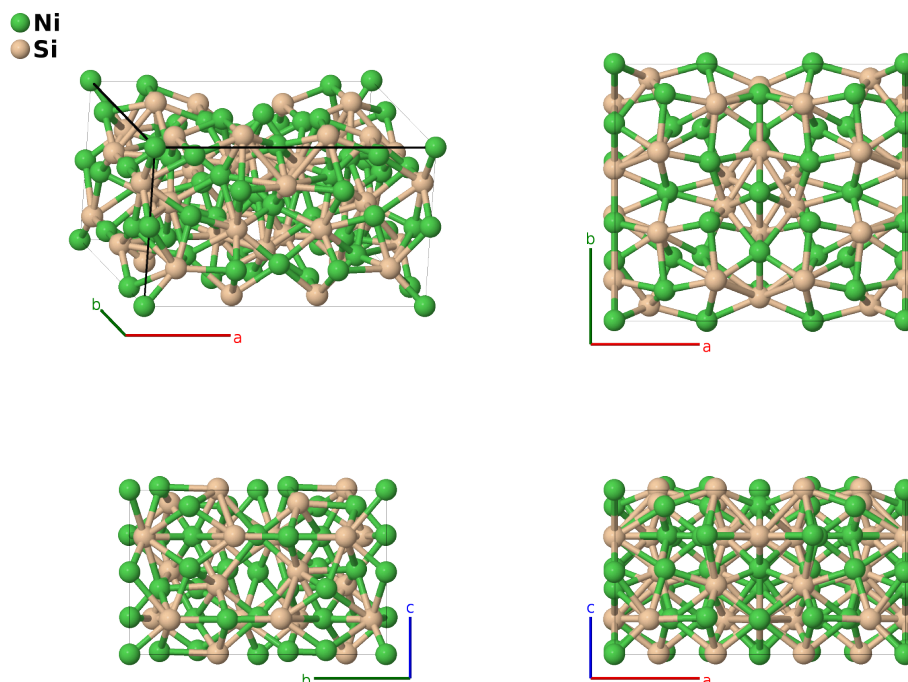# Ni₃Si₂ Structure: A3B2_oC80_36_4a4b_2a3b-001

This structure originally had the label `A3B2_oC80_36_4a4b_2a3b`. Calls to that address will be redirected here.

https://aflow.org/p/5H38

https://aflow.org/p/A3B2_oC80_36_4a4b_2a3b-001

Prototype	Ni₃Si₂
AFLOW prototype label	A3B2_oC80_36_4a4b_2a3b-001
ICSD	43561
Pearson symbol	oC80
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	aflow --proto=A3B2_oC80_36_4a4b_2a3b-001 --params=$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

Base-centered Orthorhombic primitive vectors

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

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

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
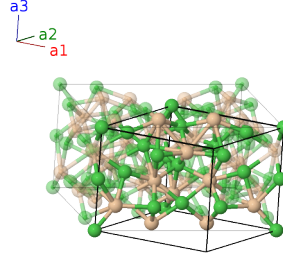
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ni I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} + \left(z_1 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Ni I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Ni II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Ni II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Ni III
$\mathbf{B_6}$	=	$y_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Ni III
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	Ni IV
$\mathbf{B_8}$	=	$y_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Ni IV
$\mathbf{B_9}$	=	$-y_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	Si II
$\mathbf{B_{12}}$	=	$y_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4a)	Si II
$\mathbf{B_{13}}$	=	$(x_7 - y_7)\,\mathbf{a_1} + (x_7 + y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	Ni V
$\mathbf{B_{14}}$	=	$-(x_7 - y_7)\,\mathbf{a_1} - (x_7 + y_7)\,\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Ni V
$\mathbf{B_{15}}$	=	$(x_7 + y_7)\,\mathbf{a_1} + (x_7 - y_7)\,\mathbf{a_2} + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Ni V
$\mathbf{B_{16}}$	=	$-(x_7 + y_7)\,\mathbf{a_1} - (x_7 - y_7)\,\mathbf{a_2} + z_7\,\mathbf{a_3}$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	Ni V
$\mathbf{B_{17}}$	=	$(x_8 - y_8)\,\mathbf{a_1} + (x_8 + y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8b)	Ni VI
$\mathbf{B_{18}}$	=	$-(x_8 - y_8)\,\mathbf{a_1} - (x_8 + y_8)\,\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Ni VI
$\mathbf{B_{19}}$	=	$(x_8 + y_8)\,\mathbf{a_1} + (x_8 - y_8)\,\mathbf{a_2} + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Ni VI
$\mathbf{B_{20}}$	=	$-(x_8 + y_8)\,\mathbf{a_1} - (x_8 - y_8)\,\mathbf{a_2} + z_8\,\mathbf{a_3}$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8b)	Ni VI
$\mathbf{B_{21}}$	=	$(x_9 - y_9)\,\mathbf{a_1} + (x_9 + y_9)\,\mathbf{a_2} + z_9\,\mathbf{a_3}$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8b)	Ni VII
$\mathbf{B_{22}}$	=	$-(x_9 - y_9)\,\mathbf{a_1} - (x_9 + y_9)\,\mathbf{a_2} + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(8b)	Ni VII

$$\mathbf{B_{23}} = \begin{array}{c}(x_9+y_9)\,\mathbf{a_1} + (x_9-y_9)\,\mathbf{a_2} + \\ \left(z_9+\frac{1}{2}\right)\mathbf{a_3}\end{array} = ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VII}$$

$$\mathbf{B_{24}} = \begin{array}{c}-(x_9+y_9)\,\mathbf{a_1} - (x_9-y_9)\,\mathbf{a_2} + \\ z_9\,\mathbf{a_3}\end{array} = -ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VII}$$

$$\mathbf{B_{25}} = \begin{array}{c}(x_{10}-y_{10})\,\mathbf{a_1} + \\ (x_{10}+y_{10})\,\mathbf{a_2} + z_{10}\,\mathbf{a_3}\end{array} = ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VIII}$$

$$\mathbf{B_{26}} = \begin{array}{c}-(x_{10}-y_{10})\,\mathbf{a_1} - \\ (x_{10}+y_{10})\,\mathbf{a_2} + \left(z_{10}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = -ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VIII}$$

$$\mathbf{B_{27}} = \begin{array}{c}(x_{10}+y_{10})\,\mathbf{a_1} + \\ (x_{10}-y_{10})\,\mathbf{a_2} + \left(z_{10}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VIII}$$

$$\mathbf{B_{28}} = \begin{array}{c}-(x_{10}+y_{10})\,\mathbf{a_1} - \\ (x_{10}-y_{10})\,\mathbf{a_2} + z_{10}\,\mathbf{a_3}\end{array} = -ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Ni VIII}$$

$$\mathbf{B_{29}} = \begin{array}{c}(x_{11}-y_{11})\,\mathbf{a_1} + \\ (x_{11}+y_{11})\,\mathbf{a_2} + z_{11}\,\mathbf{a_3}\end{array} = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si III}$$

$$\mathbf{B_{30}} = \begin{array}{c}-(x_{11}-y_{11})\,\mathbf{a_1} - \\ (x_{11}+y_{11})\,\mathbf{a_2} + \left(z_{11}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si III}$$

$$\mathbf{B_{31}} = \begin{array}{c}(x_{11}+y_{11})\,\mathbf{a_1} + \\ (x_{11}-y_{11})\,\mathbf{a_2} + \left(z_{11}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si III}$$

$$\mathbf{B_{32}} = \begin{array}{c}-(x_{11}+y_{11})\,\mathbf{a_1} - \\ (x_{11}-y_{11})\,\mathbf{a_2} + z_{11}\,\mathbf{a_3}\end{array} = -ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si III}$$

$$\mathbf{B_{33}} = \begin{array}{c}(x_{12}-y_{12})\,\mathbf{a_1} + \\ (x_{12}+y_{12})\,\mathbf{a_2} + z_{12}\,\mathbf{a_3}\end{array} = ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si IV}$$

$$\mathbf{B_{34}} = \begin{array}{c}-(x_{12}-y_{12})\,\mathbf{a_1} - \\ (x_{12}+y_{12})\,\mathbf{a_2} + \left(z_{12}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = -ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si IV}$$

$$\mathbf{B_{35}} = \begin{array}{c}(x_{12}+y_{12})\,\mathbf{a_1} + \\ (x_{12}-y_{12})\,\mathbf{a_2} + \left(z_{12}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si IV}$$

$$\mathbf{B_{36}} = \begin{array}{c}-(x_{12}+y_{12})\,\mathbf{a_1} - \\ (x_{12}-y_{12})\,\mathbf{a_2} + z_{12}\,\mathbf{a_3}\end{array} = -ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si IV}$$

$$\mathbf{B_{37}} = \begin{array}{c}(x_{13}-y_{13})\,\mathbf{a_1} + \\ (x_{13}+y_{13})\,\mathbf{a_2} + z_{13}\,\mathbf{a_3}\end{array} = ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si V}$$

$$\mathbf{B_{38}} = \begin{array}{c}-(x_{13}-y_{13})\,\mathbf{a_1} - \\ (x_{13}+y_{13})\,\mathbf{a_2} + \left(z_{13}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = -ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si V}$$

$$\mathbf{B_{39}} = \begin{array}{c}(x_{13}+y_{13})\,\mathbf{a_1} + \\ (x_{13}-y_{13})\,\mathbf{a_2} + \left(z_{13}+\frac{1}{2}\right)\mathbf{a_3}\end{array} = ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si V}$$

$$\mathbf{B_{40}} = \begin{array}{c}-(x_{13}+y_{13})\,\mathbf{a_1} - \\ (x_{13}-y_{13})\,\mathbf{a_2} + z_{13}\,\mathbf{a_3}\end{array} = -ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8b) \qquad \text{Si V}$$

References

[1] G. Pilström, *The Crystal Structure of Ni_3Si_2 with some Notes on Ni_5Si_2*, Acta Chem. Scand. **15**, 893–902 (1961), doi:10.3891/acta.chem.scand.15-0893.