

Ni₁₂P₅ Structure:

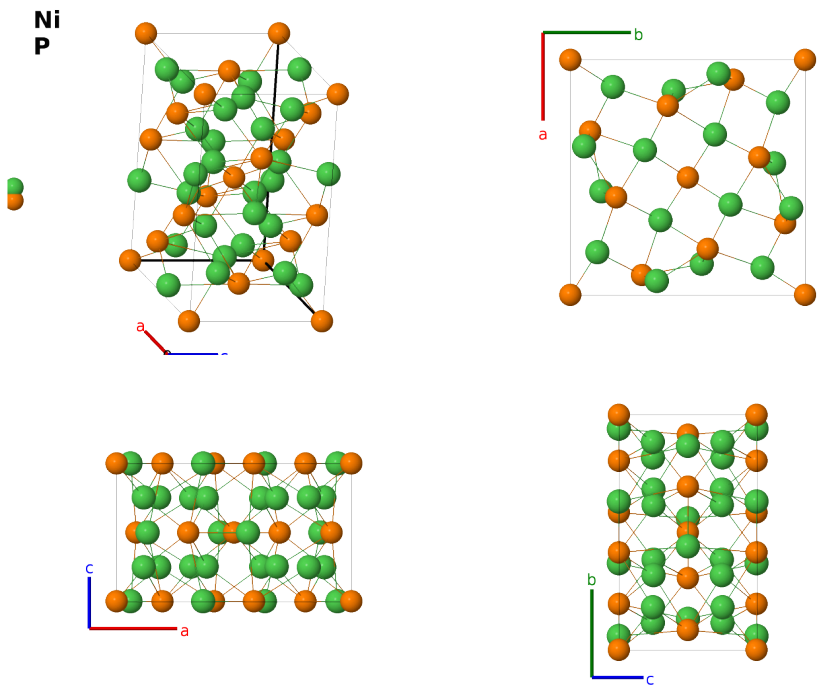
A12B5_tI34_87_hi_ah-001

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<https://aflow.org/prototype-encyclopedia/13WH>

https://aflow.org/prototype-encyclopedia/A12B5_tI34_87_hi_ah-001



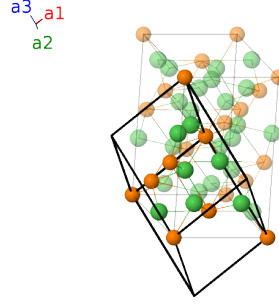
Prototype	Ni ₁₂ P ₅
AFLOW prototype label	A12B5_tI34_87_hi_ah-001
ICSD	108640
CCDC	1666299
Pearson symbol	tI34
Space group number	87
Space group symbol	I4/m
AFLOW prototype command	<code>aflow --proto=A12B5_tI34_87_hi_ah-001</code> <code>--params=a, c/a, x₂, y₂, x₃, y₃, x₄, y₄, z₄</code>

Other compounds with this structure

Pt₁₂Si₅

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) P I
$\mathbf{B}_2$	=	$y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}}$	(8h) Ni I
$\mathbf{B}_3$	=	$-y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}}$	(8h) Ni I
$\mathbf{B}_4$	=	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8h) Ni I
$\mathbf{B}_5$	=	$-x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3$	=	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8h) Ni I
$\mathbf{B}_6$	=	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(8h) P II
$\mathbf{B}_7$	=	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(8h) P II
$\mathbf{B}_8$	=	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(8h) P II
$\mathbf{B}_9$	=	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(8h) P II
$\mathbf{B}_{10}$	=	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{11}$	=	$-(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{12}$	=	$(x_4 + z_4) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	=	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{13}$	=	$-(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	=	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{14}$	=	$-(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{15}$	=	$(y_4 - z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{16}$	=	$-(x_4 + z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	=	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16i) Ni II
$\mathbf{B}_{17}$	=	$(x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	=	$-ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(16i) Ni II

References

- [1] S. Rundqvist and E. Larsson, *The Crystal Structure of Ni₁₂P₅*, Acta Chem. Scand. **13**, 551–560 (1959), doi:10.3891/acta.chem.scand.13-0551.

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