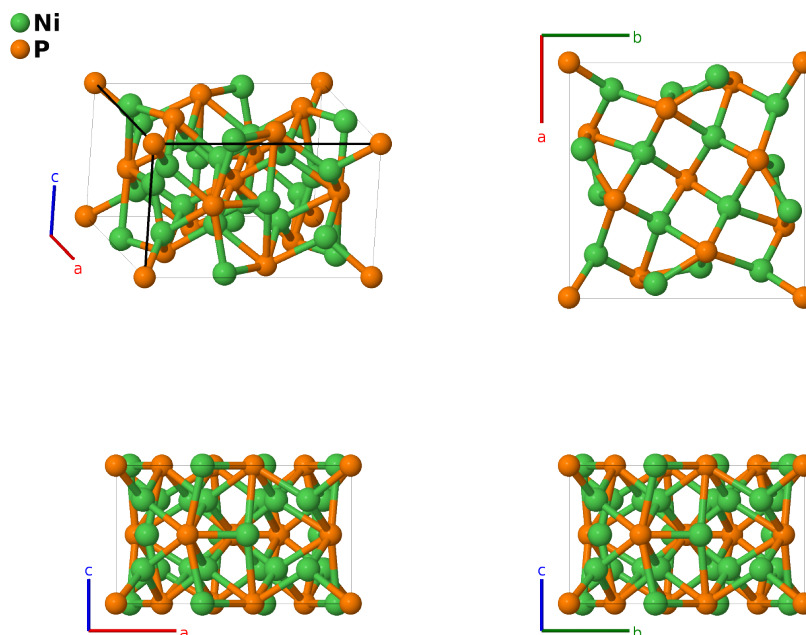


# Ni<sub>12</sub>P<sub>5</sub> Structure: A12B5\_tI34\_87\_hi\_ah-001

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<https://aflow.org/p/13WH>

[https://aflow.org/p/A12B5\\_tI34\\_87\\_hi\\_ah-001](https://aflow.org/p/A12B5_tI34_87_hi_ah-001)

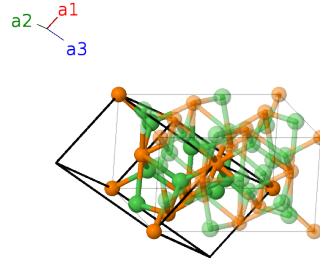


Prototype	Ni <sub>12</sub> P <sub>5</sub>
AFLOW prototype label	A12B5_tI34_87_hi_ah-001
ICSD	108640
Pearson symbol	tI34
Space group number	87
Space group symbol	<i>I4/m</i>
AFLOW prototype command	<code>aflow --proto=A12B5_tI34_87_hi_ah-001 --params=a, c/a, x<sub>2</sub>, y<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub></code>

## Other compounds with this structure

Pt<sub>12</sub>Si<sub>5</sub>

## 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 Ni<sub>12</sub>P<sub>5</sub>*, Acta Chem. Scand. **13**, 551–560 (1959), doi:10.3891/acta.chem.scand.13-0551.