

Ni₃P (*D*0₃) Structure:

A3B_tI32_82_3g_g-001

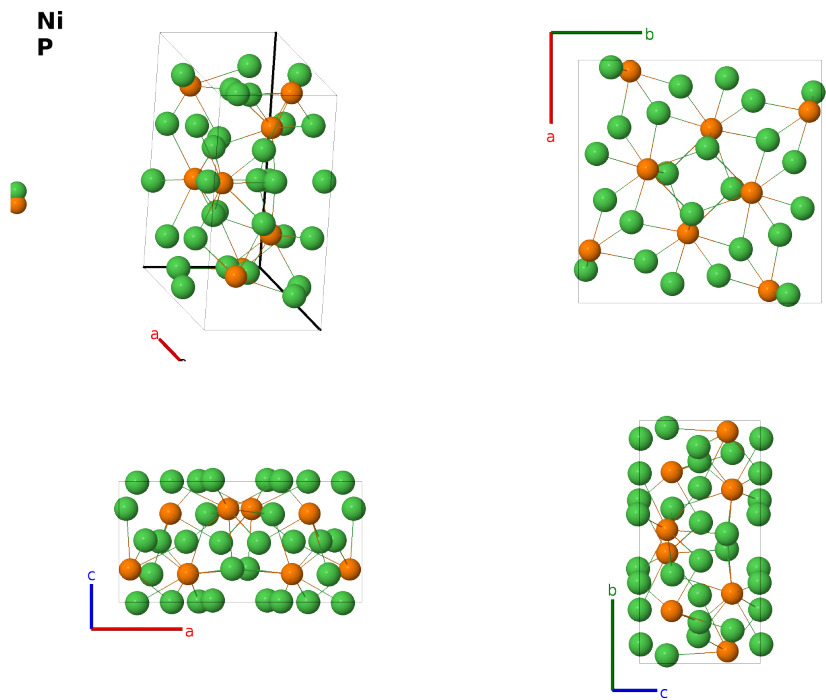
This structure previously used the label(s) **A3B_tI32_82_3g_g**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WHNY>

https://aflow.org/prototype-encyclopedia/A3B_tI32_82_3g_g-001



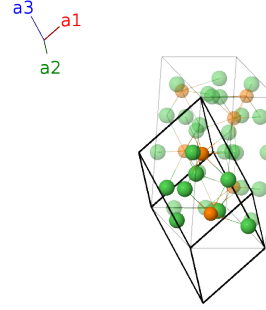
Prototype	Ni ₃ P
AFLOW prototype label	A3B_tI32_82_3g_g-001
<i>Strukturbericht</i> designation	<i>D</i> 0 ₃
ICSD	626503
CCDC	1752037
Pearson symbol	tI32
Space group number	82
Space group symbol	<i>I</i> $\bar{4}$
AFLOW prototype command	<code>aflow --proto=A3B_tI32_82_3g_g-001</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

Other compounds with this structure

Cr₃P, Fe₃B, Fe₃P, Mn₃P, Mo₃P, Ti₃P, V₃P

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
$\mathbf{B}_1$	$(y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8g)	Ni I
$\mathbf{B}_2$	$-(y_1 - z_1) \mathbf{a}_1 - (x_1 - z_1) \mathbf{a}_2 - (x_1 + y_1) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8g)	Ni I
$\mathbf{B}_3$	$-(x_1 + z_1) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 - (x_1 - y_1) \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8g)	Ni I
$\mathbf{B}_4$	$(x_1 - z_1) \mathbf{a}_1 - (y_1 + z_1) \mathbf{a}_2 + (x_1 - y_1) \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8g)	Ni I
$\mathbf{B}_5$	$(y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8g)	Ni II
$\mathbf{B}_6$	$-(y_2 - z_2) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8g)	Ni II
$\mathbf{B}_7$	$-(x_2 + z_2) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3$	=	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8g)	Ni II
$\mathbf{B}_8$	$(x_2 - z_2) \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8g)	Ni II
$\mathbf{B}_9$	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	Ni III
$\mathbf{B}_{10}$	$-(y_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8g)	Ni III
$\mathbf{B}_{11}$	$-(x_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	Ni III
$\mathbf{B}_{12}$	$(x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8g)	Ni III
$\mathbf{B}_{13}$	$(y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_{14}$	$-(y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	P I
$\mathbf{B}_{15}$	$-(x_4 + z_4) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	=	$ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	P I

$$\mathbf{B}_{16} = \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} \quad (8g) \quad \text{P I}$$

References

- [1] S. Rundqvist, E. Hassler, and L. Lundvik, *Refinement of the Ni_3P Structure*, Acta Chem. Scand. **16**, 242–243 (1962), doi:10.3891/acta.chem.scand.16-0242.

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