

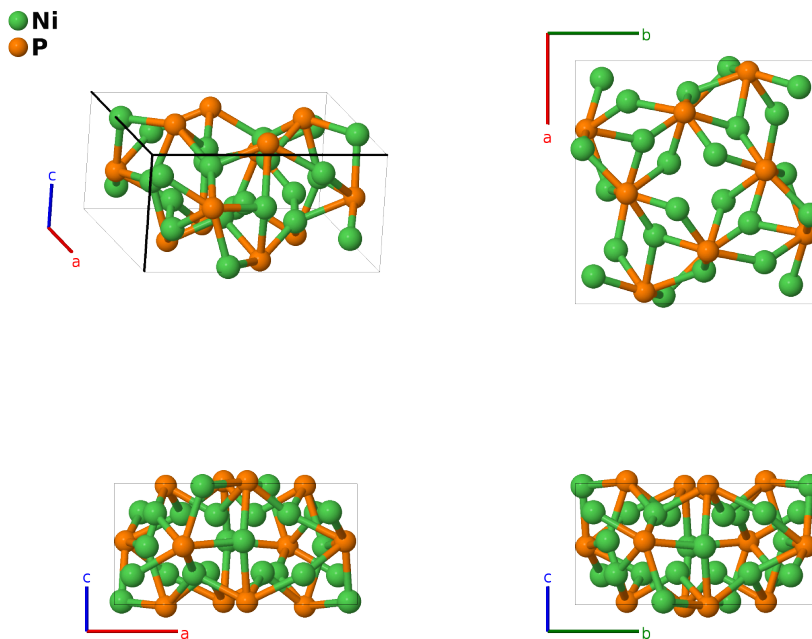
Ni₃P (*D*0_e) Structure: A3B_tI32_82_3g_g-001

This structure originally had the label A3B_tI32_82_3g_g. Calls to that address will be redirected here.

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<https://aflow.org/p/WHNY>

https://aflow.org/p/A3B_tI32_82_3g_g-001

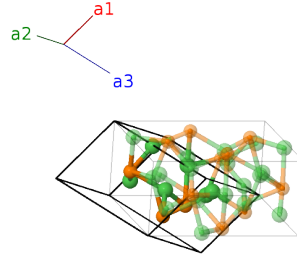


Prototype	Ni ₃ P
AFLOW prototype label	A3B_tI32_82_3g_g-001
<i>Strukturbericht</i> designation	<i>D</i> 0 ₃
ICSD	626503
Pearson symbol	tI32
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	aflow --proto=A3B_tI32_82_3g_g-001 --params= <i>a</i> , <i>c/a</i> , <i>x</i> ₁ , <i>y</i> ₁ , <i>z</i> ₁ , <i>x</i> ₂ , <i>y</i> ₂ , <i>z</i> ₂ , <i>x</i> ₃ , <i>y</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄

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}	$(x_4 - z_4)\mathbf{a}_1 - (y_4 + z_4)\mathbf{a}_2 + (x_4 - y_4)\mathbf{a}_3$	=	$-ay_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(8g)	P I

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.