

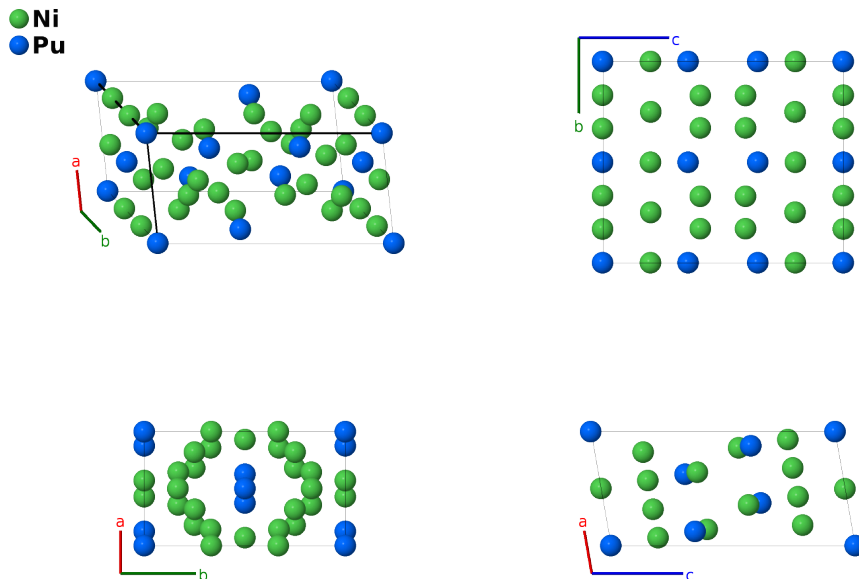
PuNi₄ Structure:

A4B_mC30_12_gi2j_ai-001

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<https://aflow.org/p/WBF9>

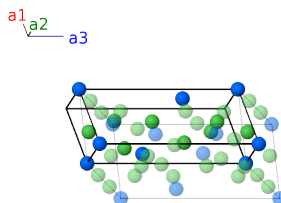
https://aflow.org/p/A4B_mC30_12_gi2j_ai-001



Prototype	Ni ₄ Pu
AFLOW prototype label	A4B_mC30_12_gi2j_ai-001
ICSD	105322
Pearson symbol	mC30
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A4B_mC30_12_gi2j_ai-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>y</i> ₂ , <i>x</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>z</i> ₄ , <i>x</i> ₅ , <i>y</i> ₅ , <i>z</i> ₅ , <i>x</i> ₆ , <i>y</i> ₆ , <i>z</i> ₆

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(2a) Pu I
\mathbf{B}_2	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(4g) Ni I
\mathbf{B}_3	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-by_2 \hat{\mathbf{y}}$	(4g) Ni I
\mathbf{B}_4	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ni II
\mathbf{B}_5	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Ni II
\mathbf{B}_6	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Pu II
\mathbf{B}_7	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Pu II
\mathbf{B}_8	$=$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j) Ni III
\mathbf{B}_9	$=$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j) Ni III
\mathbf{B}_{10}	$=$	$-(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j) Ni III
\mathbf{B}_{11}	$=$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j) Ni III
\mathbf{B}_{12}	$=$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) Ni IV
\mathbf{B}_{13}	$=$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) Ni IV
\mathbf{B}_{14}	$=$	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) Ni IV
\mathbf{B}_{15}	$=$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j) Ni IV

References

- [1] D. T. Cromer and A. C. Larson, *The crystal structure of PuNi₄*, Acta Cryst. **13**, 909–912 (1960), doi:10.1107/S0365110X60002223.