

β -Np (A_d) Structure: A_tP4_129_ac-001

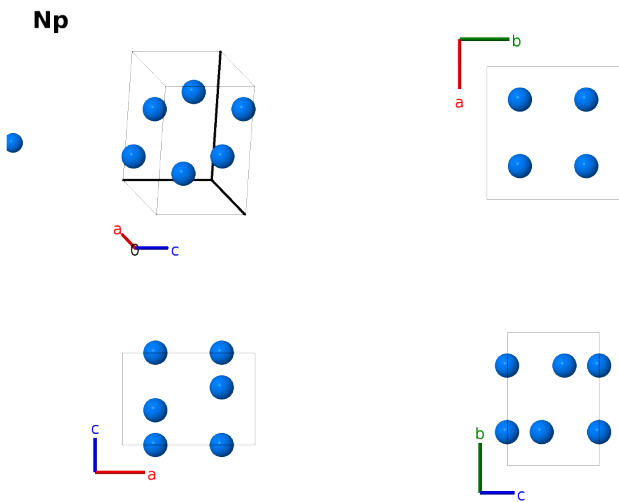
This structure previously used the label(s) **A.tP4_129_ac**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A_tP4_129_ac-001

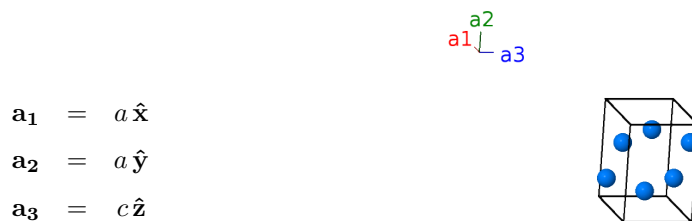


Prototype	Np
AFLOW prototype label	A_tP4_129_ac-001
<i>Strukturbericht</i> designation	A_d
ICSD	44379
CCDC	1613777
Pearson symbol	tP4
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<code>aflow --proto=A_tP4_129_ac-001 --params=a, c/a, z₂</code>

- Neptunium is found in three forms (Donohue, 1974):
 - The ground state, α -Np (A_c), stable below 280°C,
 - β -Np (A_d), stable in the range 280-577°C, (this structure) and
 - a body-centered cubic (A_2) structure above 577°C.

- When $z = 1/2$ the atoms in this structure are in the $L1_0$ (CuAu) or the $A6$ (indium) structure. This structure is identical to the $B10$ (PbO) structure. Pearson's Handbook, along with the original papers, give the space group as $P4_21c$ #113. However, as noted by Structure Reports 15, 121 (1951), the correct space group is $P4/nmm$ #129. $P4_21c$ is a subgroup of $P4/nmm$.

Simple Tetragonal primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	Np I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	Np I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Np II
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Np II

References

- [1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. XVIII. Crystal structure studies of neptunium metal at elevated temperatures*, Acta Cryst. **5**, 664–667 (1952), doi:10.1107/S0365110X52001805.
- [2] W. B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys* (Wiley Interscience, New York, London, Sydney, Toronto, 1972).
- [3] A. J. C. Wilson, ed., *Structure Reports for 1951*, vol. 15 (N.V.A. Oosthoek's Uitgevers, Utrecht, 1958).

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

First cited in

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