β-Np (A_d) Structure: A_tP4_129_ac-001

This structure originally had the label `A_tP4_129_ac`. Calls to that address will be redirected here.

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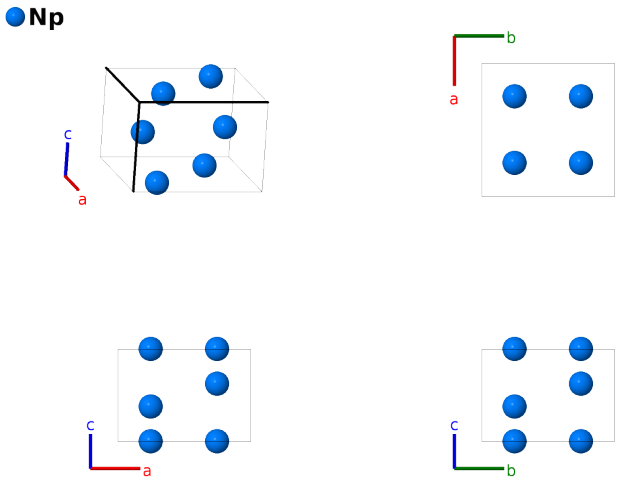
https://aflow.org/p/UNPK

https://aflow.org/p/A_tP4_129_ac-001

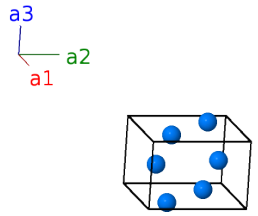


Prototype	Np
AFLOW prototype label	A_tP4_129_ac-001
***Strukturbericht* designation**	A_d
ICSD	44379
Pearson symbol	tP4
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=A_tP4_129_ac-001 --params=`$a, c/a, z_2$

- 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 ($A2$) 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 $P42_1c$ #113. However, as noted by Structure Reports 15, 121 (1951), the correct space group is $P4/nmm$ #129. $P42_1c$ is a subgroup of $P4/nmm$.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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, Tornoto, 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).