NbP ("40") Structure: AB_tI8_141_a_b-001

This structure originally had the label `AB_tI8_141_a_b`. Calls to that address will be redirected here.

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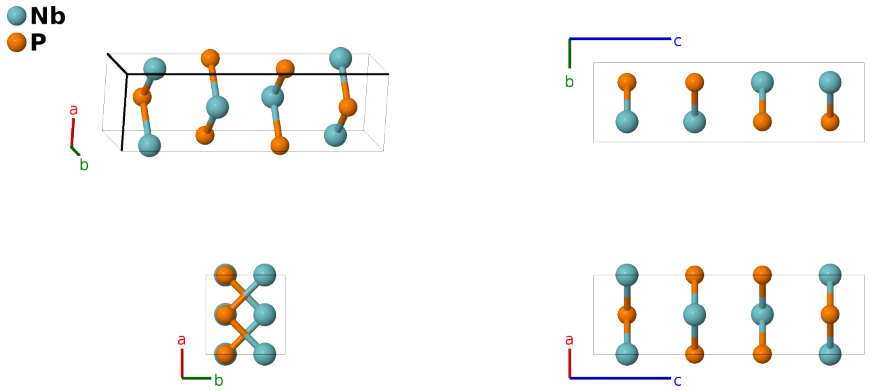
https://aflow.org/p/R06D

https://aflow.org/p/AB_tI8_141_a_b-001

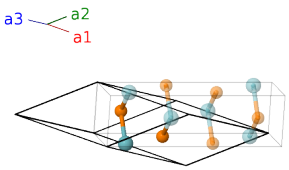


Prototype	NbP
AFLOW prototype label	AB_tI8_141_a_b-001
***Strukturbericht* designation**	"40"
ICSD	76027
Pearson symbol	tI8
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=AB_tI8_141_a_b-001 --params=`$a, c/a$

- When $c/a = 2$, the atoms in this lattice are on the sites of the face-centered cubic lattice. Thus (Lu, 1991) use this lattice for their structural stability studies, and arbitrarily assign this lattice a Strukturbericht designation of "40." Note that (Schönberg, 1954) gives the space group as $I4_122$ #98 but, as (Villars, 1991) notes, the coordinates given increase the symmetry to $I4_1/amd$ #141.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_2}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_3}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_4}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4b)	P I

References

[1] N. Schönberg, *An X-Ray Investigation of Transition Metal Phosphides*, Acta Chem. Scand. **8**, 226–239 (1954), doi:10.3891/acta.chem.scand.08-0221.

[2] Z. W. Lu, S.-H. Wei, and A. Zunger, *Long-Range Order in Binary Late-Transition-Metal Alloys*, Phys. Rev. Lett. **66**, 1753–1756 (1991), doi:10.1103/PhysRevLett.66.1753.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.