β-$NbPd_3$ Structure: AB3_oP24_59_ae_befg-001

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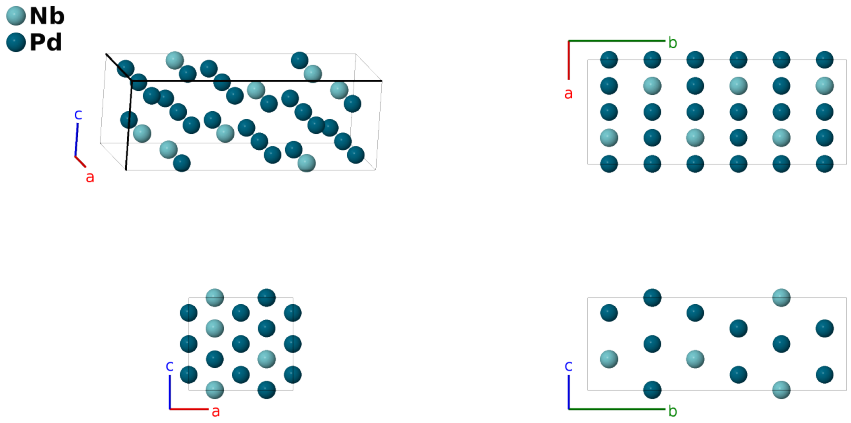
https://aflow.org/p/5BSF

https://aflow.org/p/AB3_oP24_59_ae_befg-001

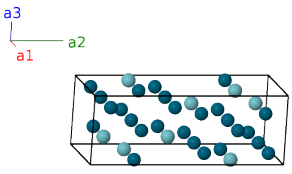


Prototype	$NbPd_3$
AFLOW prototype label	AB3_oP24_59_ae_befg-001
ICSD	105193
Pearson symbol	oP24
Space group number	59
Space group symbol	$Pmmn$
AFLOW prototype command	`aflow --proto=AB3_oP24_59_ae_befg-001 --params=`$a, b/a, c/a, z_1, z_2, y_3, z_3, y_4, z_4, x_5, z_5, x_6, y_6, z_6$

- Although β-$NbPd_3$ and α-$NbPd_3$, which has the $D0_{22}$ structure, coexist over a wide range of temperatures, it is thought that α-$NbPd_3$ is the ground state (Chandrasekharaiah, 1988).
- (Giessen, 1964) state that their coordinates are given in the $Pmmn$ setting of space group #59, but it is apparent that they actually use the $Pmnm$ setting. We transformed this to $Pmmn$.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Pd I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2b)	Pd I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	Pd II
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4e)	Pd II
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	Pd II
$\mathbf{B_{12}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4e)	Pd II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4f)	Pd III
$\mathbf{B_{14}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4f)	Pd III
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4f)	Pd III
$\mathbf{B_{16}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4f)	Pd III
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{18}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{20}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{22}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV
$\mathbf{B_{24}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8g)	Pd IV

References

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