Nb_4As_3 Structure: A3B4_oC56_63_2c2f_ac3f-001

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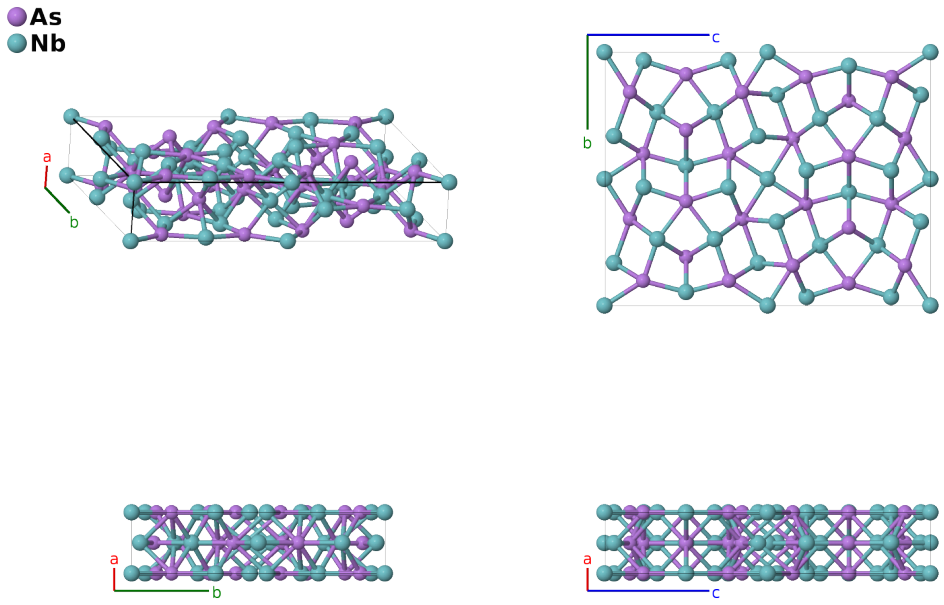
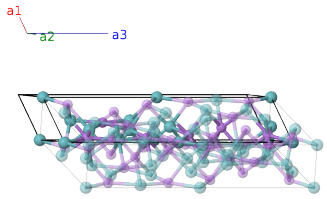


Prototype	As_3Nb_4
AFLOW prototype label	A3B4_oC56_63_2c2f_ac3f-001
ICSD	15032
Pearson symbol	oC56
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A3B4_oC56_63_2c2f_ac3f-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8, y_9, z_9$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Nb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	As II
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	As II
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_9}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	As III
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	As III
$\mathbf{B_{11}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	As III
$\mathbf{B_{12}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	As III
$\mathbf{B_{13}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8f)	As IV
$\mathbf{B_{14}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	As IV
$\mathbf{B_{15}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	As IV
$\mathbf{B_{16}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8f)	As IV
$\mathbf{B_{17}}$	=	$-y_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8f)	Nb III
$\mathbf{B_{18}}$	=	$y_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb III
$\mathbf{B_{19}}$	=	$-y_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb III
$\mathbf{B_{20}}$	=	$y_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8f)	Nb III
$\mathbf{B_{21}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8f)	Nb IV
$\mathbf{B_{22}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb IV
$\mathbf{B_{23}}$	=	$-y_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb IV
$\mathbf{B_{24}}$	=	$y_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8f)	Nb IV
$\mathbf{B_{25}}$	=	$-y_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8f)	Nb V
$\mathbf{B_{26}}$	=	$y_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb V
$\mathbf{B_{27}}$	=	$-y_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Nb V
$\mathbf{B_{28}}$	=	$y_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(8f)	Nb V

References

[1] B. Carlsson and S. Rundqvist, *The Crystal Structure of* Nb_4As_3, Acta Chem. Scand. **25**, 1742–1752 (1971), doi:10.3891/acta.chem.scand.25-1742.