NbAs Structure: AB_tI8_109_a_a-001

This structure previously used the label(s) `AB_tI8_109_a_a`. Calls to these addresses will be redirected here.

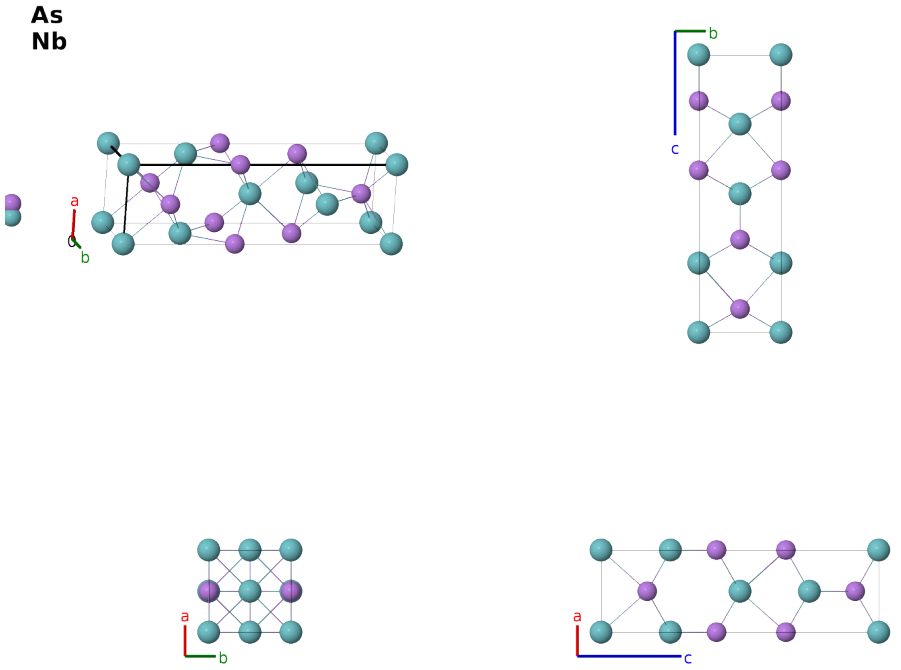
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/M2PT

https://aflow.org/prototype-encyclopedia/AB_tI8_109_a_a-001



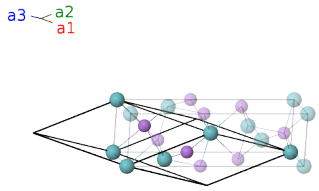
Prototype	AsNb
AFLOW prototype label	AB_tI8_109_a_a-001
ICSD	16585
CCDC	1597144
Pearson symbol	tI8
Space group number	109
Space group symbol	$I4_1md$
AFLOW prototype command	`aflow --proto=AB_tI8_109_a_a-001 --params=`$a, c/a, z_1, z_2$

Other compounds with this structure
TaAs, β-TaP, β-NbP

- Space group $I4_1md$ #109 allows an arbitary placement of the z-axis origin. Here we chose to place a niobium atom at the origin.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_2}$	=	$\left(z_1+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_1+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_1+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	As I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	Nb I
$\mathbf{B_4}$	=	$\left(z_2+\frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_2+\frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Nb I

References

[1] S. Furuseth and A. Kjekshus, *On the Arsendies and Antimonides of Niobium*, Acta Chem. Scand. **18**, 1180–1195 (1964), doi:10.3891/acta.chem.scand.18-1180.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043