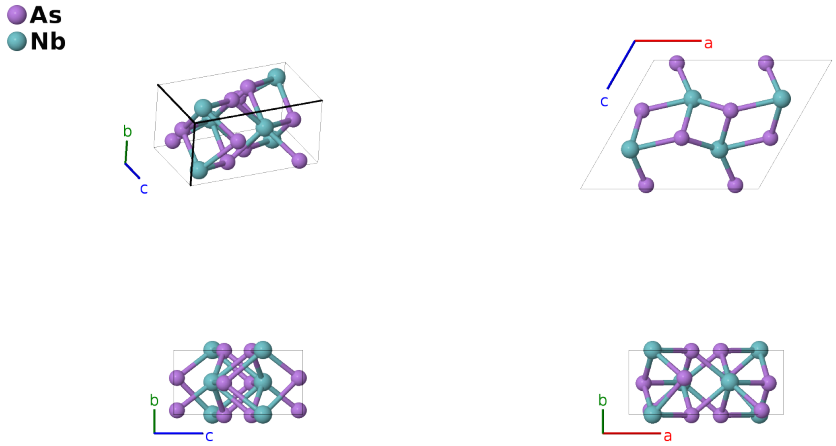
$NbAs_2$ Structure: A2B_mC12_5_2c_c-001

This structure originally had the label `A2B_mC12_5_2c_c`. Calls to that address will be redirected here.

Cite this page as: 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/p/0898

https://aflow.org/p/A2B_mC12_5_2c_c-001



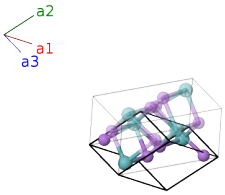
Prototype	As_2Nb
AFLOW prototype label	A2B_mC12_5_2c_c-001
ICSD	18143
Pearson symbol	mC12
Space group number	5
Space group symbol	$C2$
AFLOW prototype command	`aflow --proto=A2B_mC12_5_2c_c-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3$

Other compounds with this structure
$MoAs_2$, $TaAs_2$, $NbSb_2$, $TaSb_2$

- The zero of the y-axis can be chosen arbitrarily in space group $C2$ #5. Here we choose it so that $y_3 = \frac{1}{2}$ for the niobium atom.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(x_1 - y_1)\,\mathbf{a}_1 + (x_1 + y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_2}$	=	$-(x_1 + y_1)\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4c)	As I
$\mathbf{B_3}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4c)	As II
$\mathbf{B_4}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4c)	As II
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4c)	Nb I
$\mathbf{B_6}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4c)	Nb I

References

[1] S. Furuseth and A. Kjeeshus, *The Crystal Structures of $NbAs_2$ and $NbSb_2$*, Acta Cryst. **18**, 320–324 (1965), doi:10.1107/S0365110X65000750.