VN (Low-temperature) Structure: AB_tP8_111_n_n-001

This structure previously used the label(s) `AB_tP8_111_n_n`. 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.

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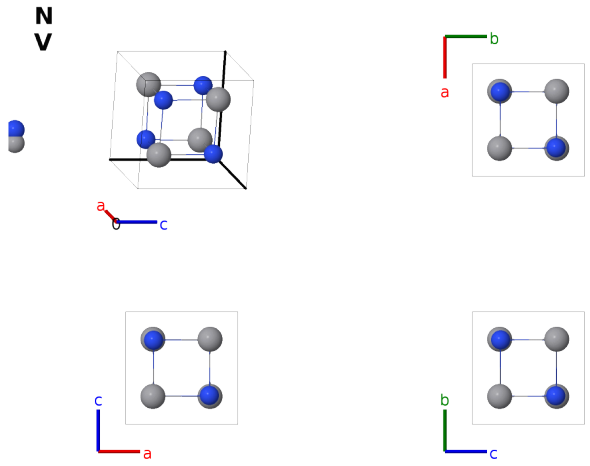
https://aflow.org/prototype-encyclopedia/GUN1

https://aflow.org/prototype-encyclopedia/AB_tP8_111_n_n-001

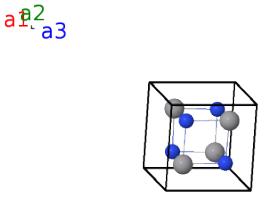


Prototype	NV
AFLOW prototype label	AB_tP8_111_n_n-001
Pearson symbol	tP8
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	`aflow --proto=AB_tP8_111_n_n-001 --params=`$a, c/a, x_1, z_1, x_2, z_2$

- Above 205K vanadium nitride transforms into the rock salt ($B1$) structure.
- We use the data taken at 150K.
- (Kubel, 1988) place this structure in space group $P\bar{4}2m$ #111, but since $c/a \approx 1$ the default tolerance of AFLOW places this in the cubic space group $P\bar{4}3m$ #215. It is likely that first-principles calculations will place this compound in the higher symmetry space group.
- The $P\bar{4}2m$ structure may be recovered from AFLOW using the commmand
- aflow --proto=AB_tP8_111_n_n:N:V --params=a,c/a,x_1,z_1,x_2,z_2 --tolerance=0.001 .
- We could not find an ICSD entry for (Kubel, 1988).

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4n)	N I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4n)	N I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4n)	N I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4n)	N I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4n)	V I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4n)	V I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4n)	V I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4n)	V I

References

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Found in

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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