VN (Low-temperature) Structure: AB_tP8_111_n_n-001

This structure originally had the label `AB_tP8_111_n_n`. Calls to that address will be redirected here.

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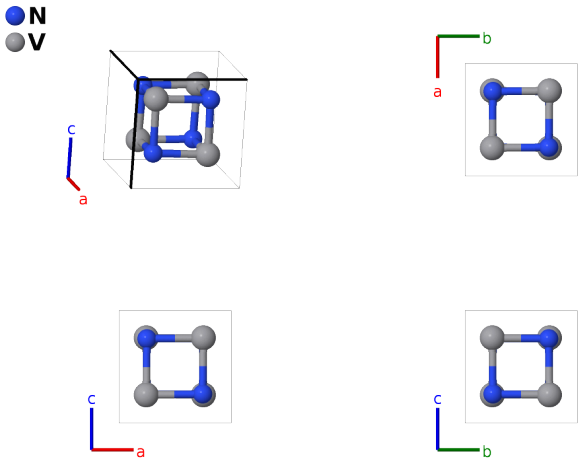
https://aflow.org/p/GUN1

https://aflow.org/p/AB_tP8_111_n_n-001

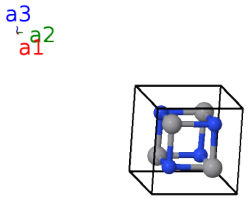


Prototype	NV
AFLOW prototype label	AB_tP8_111_n_n-001
ICSD	none
Pearson symbol	tP8
Space group number	111
Space group symbol	$P\bar{4}2m$
AFLOW prototype command	`aflow --proto=AB_tP8_111_n_n-001 --params=`$a, c/a, x_1, z_1, x_2, z_2$

- 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

[1] F. Kubel, W. Lengauer, K. Yvon, K. Knorr, and A. Junod, *Structural phase transition at 205 K in stoichiometric vanadium nitride*, Phys. Rev. B **38**, 12908–12912 (1988), doi:10.1103/PhysRevB.38.12908.

[2] H. T. Stokes and D. M. Hatch, FINDSYM*: program for identifying the space-group symmetry of a crystal*, J. App. Crystallogr. **38**, 237–238 (2005), doi:10.1107/S0021889804031528.

[3] D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.

[4] A. L. Speck, *Single-crystal structure validation with the program PLATON*, J. App. Crystallogr. **36**, 7–13 (2003), doi:10.1107/S0021889802022112.

Found in

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