Hypothetical SiO_2-like WN_2 structure: A2B_cI36_229_h_d-001

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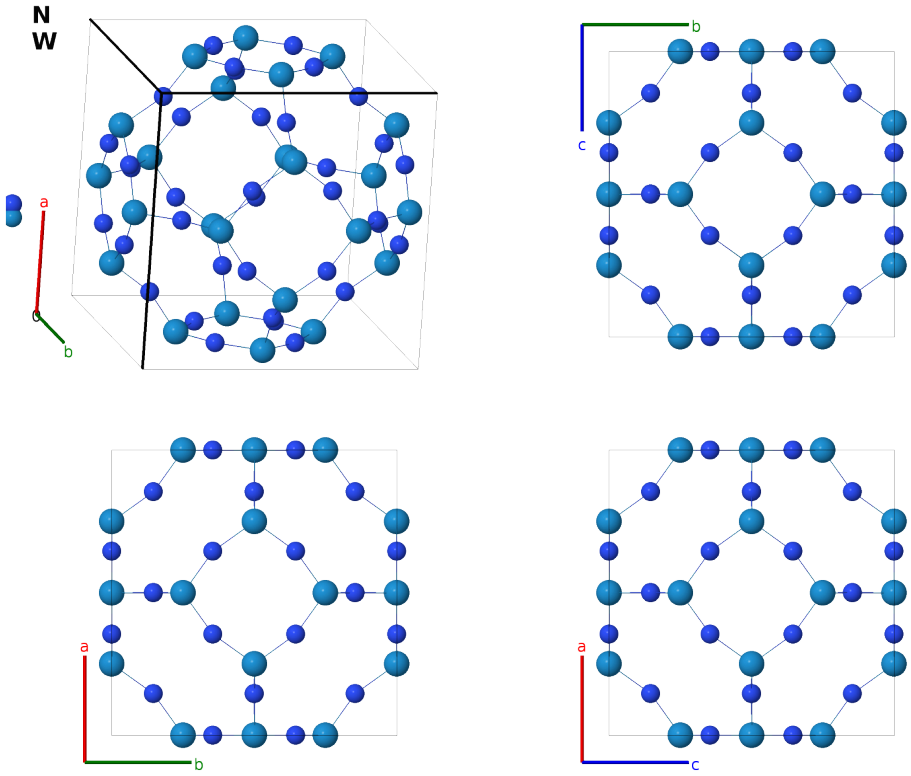
https://aflow.org/prototype-encyclopedia/C4JM

https://aflow.org/prototype-encyclopedia/A2B_cI36_229_h_d-001



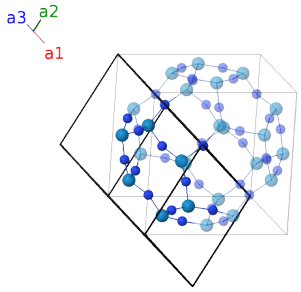
Prototype	N_2W
AFLOW prototype label	A2B_cI36_229_h_d-001
Pearson symbol	cI36
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B_cI36_229_h_d-001 --params=`a, y_2

- This structure was studied by (Mehl, 2015) as part of an effort to understand vacancy formation in the $N_{1-x}W_x$ system. It was produced by removing 4 nitrogen and 10 tungsten atoms from a 64-atom supercell of the rock salt ($B1$) structure. The resulting structure leaves four nitrogen atoms forming a tetrahedron around each tungsten atom, with the perfect regular tetrahedron occuring when $y_2 = 1/\sqrt{8}$ with an N-W-N bond angle of 109.47°. It is similar to the idealized β-cristobalite SiO_2 structure, although the current structure has never been reported for any compound.

- The y_2-value for this structure reported in (Mehl, 2015) Table VI should be replaced by 1/2 - y_2, as we do here.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	W I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12d)	W I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(12d)	W I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	W I
$\mathbf{B_5}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	W I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	W I
$\mathbf{B_7}$	=	$2y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_9}$	=	$-y_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{10}}$	=	$-2y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{11}}$	=	$y_2\,\mathbf{a}_1 + 2y_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{13}}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{14}}$	=	$-y_2\,\mathbf{a}_1 - 2y_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24h)	N I
$\mathbf{B_{15}}$	=	$y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + 2y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(24h)	N I
$\mathbf{B_{16}}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2$	=	$-ay_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$	(24h)	N I
$\mathbf{B_{17}}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2$	=	$ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(24h)	N I
$\mathbf{B_{18}}$	=	$-y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - 2y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$	(24h)	N I

References

[1] M. J. Mehl, D. Finkenstadt, C. Dane, G. L. W. Hart, and S. Curtarolo, *Finding the stable structures of $N_{1-x}W_x$ with an* ab initio *high-throughput approach*, Phys. Rev. B **91**, 184110 (2015), doi:10.1103/PhysRevB.91.184110.

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