β-WO_3 Structure: A3B_oP32_60_3d_d-001

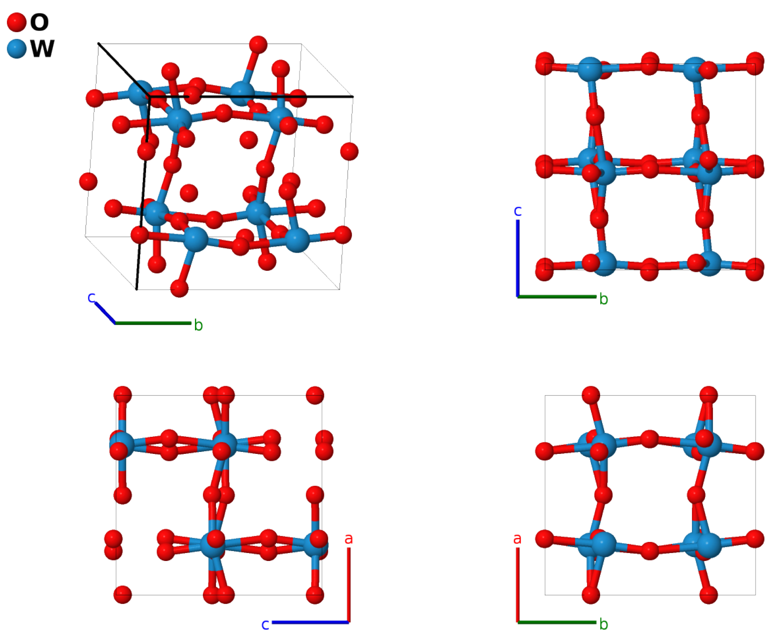
This structure originally had the label `A3B_oP32_60_3d_d`. Calls to that address will be redirected here.

Cite this page as: 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

---

https://aflow.org/p/S00Q

https://aflow.org/p/A3B_oP32_60_3d_d-001



Prototype	O_3W
AFLOW prototype label	A3B_oP32_60_3d_d-001
ICSD	50729
Pearson symbol	oP32
Space group number	60
Space group symbol	*Pbcn*
AFLOW prototype command	`aflow --proto=A3B_oP32_60_3d_d-001` `--params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4$

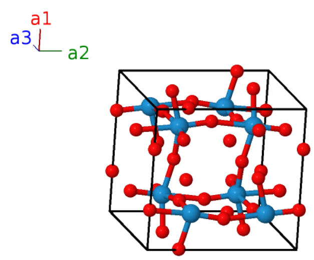
- All stable phases of WO_3 are distortions of the cubic α-ReO_3 ($D0_9$) phase. Based on (Woodward, 1997 and Vogt, 1999), the known stable phases and their approximate temperature ranges are:
  - α-WO_3 (1010-1170 K) (Vogt, 1999)
  - β-WO_3 (600-1170 K) (Vogt, 1999) (this structure)
  - γ-WO_3 (290-600 K) (Vogt, 1999)
  - δ-WO_3 (230-290 K) (Diehl, 1978)

  - ϵ-WO_3 (below 23 K) (Woodward, 1997)

- Woodward notes that "The transition temperatures display large hysteresis effects and universal agreement is not found in the literature."
- In addition, several other structures have been proposed and/or found:
  - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by δ-WO_3
  - The original β-WO_3 (Salje, 1977)
  - Hexagonal WO_3, presumably metastable, found by (Gerand, 1979) while dehydrating $WO_3{\cdot}H_2O$
- (Salje, 1977) originally found this structure to be in space group *Pnma* #62, but a redetermination by (Vogh, 1999) places it in the *Pbcn* #60 space group.
- (Vogt, 1999) give the structure in the *Pcnb* setting of space group #60. We used FINDSYM to translate this to the standard *Pbcn* setting.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8d)	O I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{12}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II

$\mathbf{B_{15}}$	=	$x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} - by_2\,\mathbf{\hat{y}} + c\left(z_2 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{16}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_2 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_2\,\mathbf{\hat{z}}$	(8d)	O II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} + cz_3\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{18}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_3 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{19}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + by_3\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{20}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_3 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_3\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} - cz_3\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{22}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_3 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_3 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{23}}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} - by_3\,\mathbf{\hat{y}} + c\left(z_3 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{24}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_3 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_3\,\mathbf{\hat{z}}$	(8d)	O III
$\mathbf{B_{25}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{26}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{27}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + by_4\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{28}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - b\left(y_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{29}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{30}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - c\left(z_4 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{31}}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} - by_4\,\mathbf{\hat{y}} + c\left(z_4 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8d)	W I
$\mathbf{B_{32}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + b\left(y_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(8d)	W I

References

[1] P. M. Woodward, A. W. Sleight, and T. Vogt, *Ferroelectric Tungsten Trioxide*, J. Solid State Chem. **131**, 9–17 (1997), doi:10.1006/jssc.1997.7268.

[2] T. Vogt, P. M. Woodward, and B. A. Hunter, *The High-Temperature Phases of WO_3*, J. Solid State Chem. **144**, 209–215 (1999), doi:10.1006/jssc.1999.8173.

[3] R. Diehl, G. Brandt, and E. Salje, *The Crystal Structure of Triclinic WO_3*, Acta Crystallogr. Sect. B **34**, 1105–1111 (1978), doi:10.1107/S0567740878005014.

[4] H. Bräkken, *Die Kristallstrukturen der Trioxyde von Chrom, Molybdän und Wolfram*, Z. Kristallogr. **78**, 484–488 (1931), doi:10.1524/zkri.1931.78.1.484.

[5] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[6] E. Salje, *The Orthorhombic Phase of WO_3*, Acta Crystallogr. Sect. B **33**, 574–577 (1977), doi:10.1107/S0567740877004130.

[7] B. Gerand, G. Nowogrocki, J. Guenot, and M. Figlarz, *Structural study of a new hexagonal form of tungsten trioxide*, J. Solid State Chem. **29**, 429–434 (1979), doi:10.1016/0022-4596(79)90199-3.