α-WO_3 Structure: A3B_tP16_130_cf_c-001

This structure previously used the label(s) `A3B_tP16_130_cf_c`. Calls to these addresses will be redirected here.

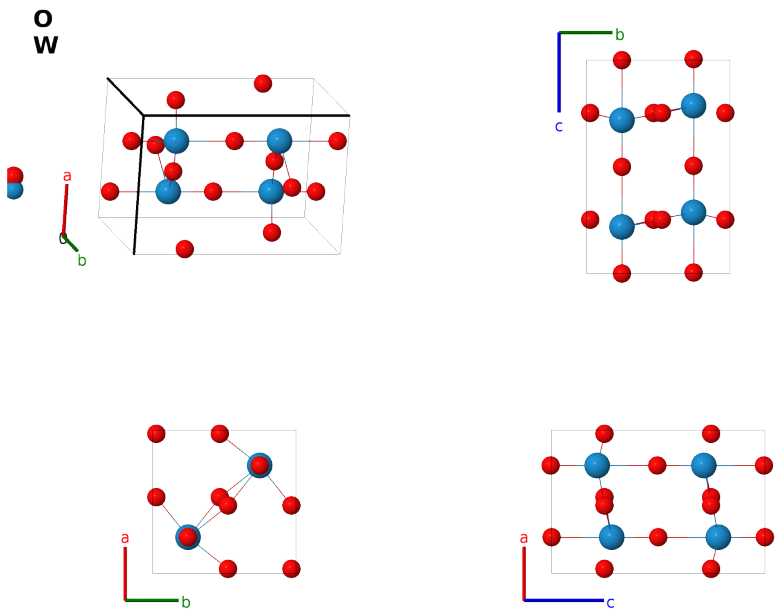
Cite this page as:

- 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.

---

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

https://aflow.org/prototype-encyclopedia/A3B_tP16_130_cf_c-001



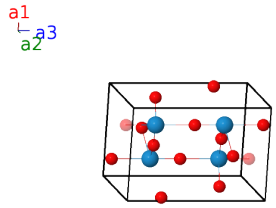
Prototype	O_3W
AFLOW prototype label	A3B_tP16_130_cf_c-001
ICSD	50732
CCDC	1615636
Pearson symbol	tP16
Space group number	130
Space group symbol	$P4/ncc$
AFLOW prototype command	`aflow --proto=A3B_tP16_130_cf_c-001 --params=`$a, c/a, z_1, z_2, x_3$

- 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) (this structure)
  - β-WO_3 (600-1170 K) (Vogt, 1999)
  - 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  - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by δ-WO_3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 $WO_3 \cdot H_2O$.
- We use the α-WO_3 data taken by (Vogt, 1999) at 800°C (1073K).
- (Kehl, 1952) originally put this structure in space group $P4/nmm$ #129, with a c-lattice constant set to half of the current value. This structure was corrected by (Vogh, 1999).

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	W I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{11}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	O II

$$\mathbf{B_{14}} = \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{3}{4}\mathbf{a}_3 = a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\hat{\mathbf{z}} \quad \text{(8f)} \quad \text{O II}$$

$$\mathbf{B_{15}} = -\left(x_3 - \tfrac{1}{2}\right)\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \tfrac{3}{4}\mathbf{a}_3 = -a\left(x_3 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\hat{\mathbf{z}} \quad \text{(8f)} \quad \text{O II}$$

$$\mathbf{B_{16}} = x_3\,\mathbf{a}_1 + \left(x_3 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{3}{4}\mathbf{a}_3 = ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{3}{4}c\hat{\mathbf{z}} \quad \text{(8f)} \quad \text{O II}$$

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.

First cited in

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.