$D0_{10}$ (WO_3) Structure (*Obsolete*): A3B_oP16_57_a2d_d-001

This structure previously used the label(s) `A3B_oP16_57_a2d_d`. Calls to these addresses will be redirected here.

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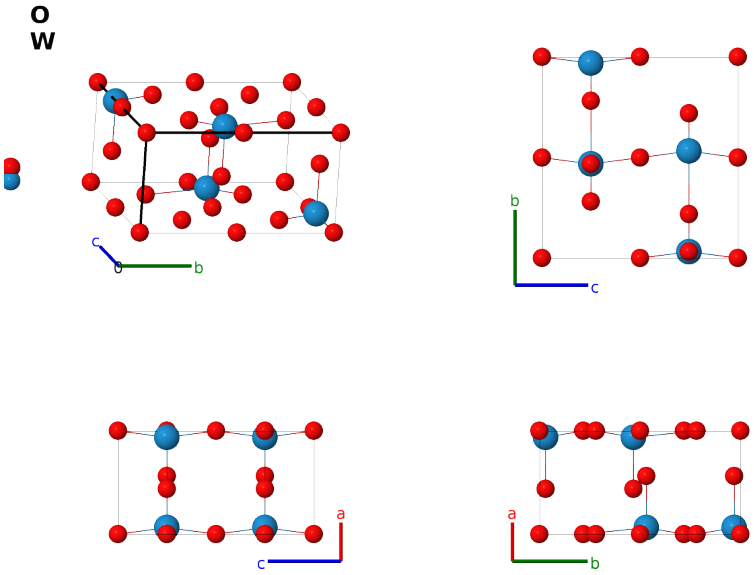
https://aflow.org/prototype-encyclopedia/5B3E

https://aflow.org/prototype-encyclopedia/A3B_oP16_57_a2d_d-001



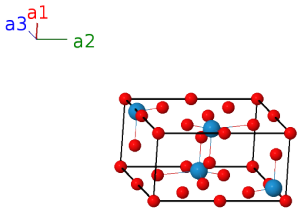
Prototype	O_3W
AFLOW prototype label	A3B_oP16_57_a2d_d-001
***Strukturbericht* designation**	$D0_{10}$
ICSD	36168
CCDC	1607946
Pearson symbol	oP16
Space group number	57
Space group symbol	*Pbcm*
AFLOW prototype command	`aflow --proto=A3B_oP16_57_a2d_d-001 --params=`$a, b/a, c/a, x_2, y_2, x_3, y_3, x_4, y_4$

- 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)
  - 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  - The original $D0_{10}$ structure (Bräkken, 1931), (Hermann, 1937) (this structure), superseded by δ-WO_3
  - The original β-WO_3 (Salje, 1977)
  - Hexagonal WO_3, presumably metastable, found by (Gerand, 1979) while dehydrating $WO_3 \cdot H_2O$
- (Bräkken, 1931) found a triclinic unit cell for WO_3 (this structure), and this is what the structure given in the ICSD. As it was nearly orthorhombic, (Hermann, 1937) approximated it with the structure shown here and gave it the *Strukturbericht* symbol $D0_{10}$. Later (Diehl, 1978) showed that the near-room-temperature phase of WO_3 was indeed a triclinic crystal, but the unit cell was double that of Bräkken and is in fact a pseudo-cubic distorted perovskite.
- We retain this original structure for its historical interest.

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
$\mathbf{B_1}$	=	0	=	0	(4a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	O I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O III
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	O III

$$\mathbf{B_{13}} = x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}} \quad \text{(4d)} \quad \text{W I}$$

$$\mathbf{B_{14}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}} \quad \text{(4d)} \quad \text{W I}$$

$$\mathbf{B_{15}} = -x_4\,\mathbf{a}_1 + \left(y_4 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}} \quad \text{(4d)} \quad \text{W I}$$

$$\mathbf{B_{16}} = x_4\,\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}} \quad \text{(4d)} \quad \text{W I}$$

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