

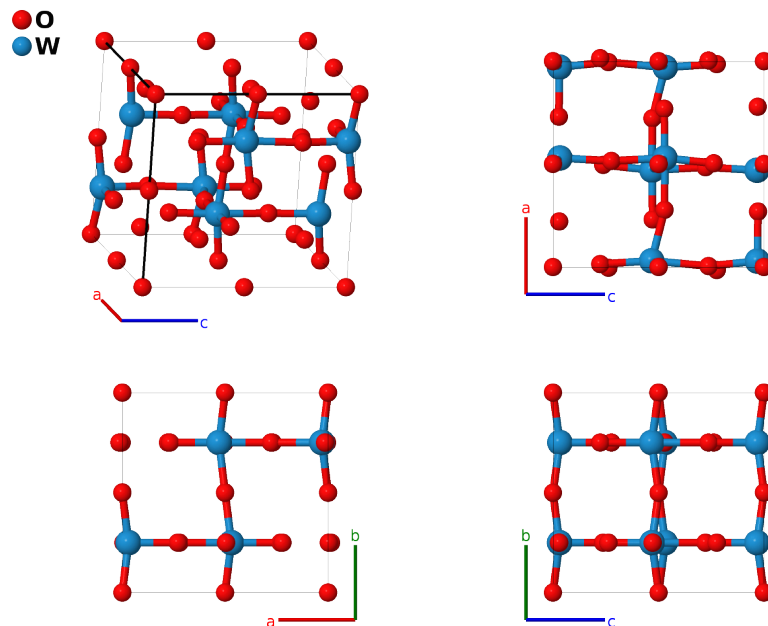
Original β -WO₃ Structure (*Obsolete*): A3B_oP32_62_ab4c_2c-001

This structure originally had the label A3B_oP32_62_ab4c_2c. Calls to that address will be redirected here.

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<https://aflow.org/p/KPH8>

https://aflow.org/p/A3B_oP32_62_ab4c_2c-001



Prototype	O ₃ W
AFLOW prototype label	A3B_oP32_62_ab4c_2c-001
ICSD	836
Pearson symbol	oP32
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=A3B_oP32_62_ab4c_2c-001 --params=a, b/a, c/a, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈</code>

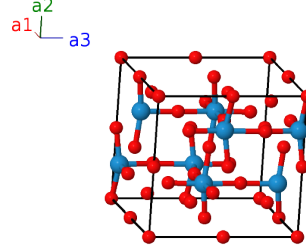
- All stable phases of WO₃ are distortions of the cubic α -ReO₃ (*D*0₉) phase. Based on (Woodward, 1997 and Vogt, 1999), the known stable phases and their approximate temperature ranges are:

- α -WO₃ (1010-1170 K) (Vogt, 1999)
- β -WO₃ (600-1170 K) (Vogt, 1999)
- γ -WO₃ (290-600 K) (Vogt, 1999)
- δ -WO₃ (230-290 K) (Diehl, 1978)

- ϵ -WO₃ (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 - The original $D0_{10}$ structure (Brækken, 1931; Hermann, 1937), superseded by δ -WO₃
 - The original β -WO₃ (Salje, 1977) (this structure)
 - Hexagonal WO₃, presumably metastable, found by (Gerand, 1979) while dehydrating WO₃·H₂O

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$=$	0	$=$	0	(4a) O I
\mathbf{B}_2	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) O I
\mathbf{B}_3	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} b \hat{\mathbf{y}}$	(4a) O I
\mathbf{B}_4	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) O I
\mathbf{B}_5	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(4b) O II
\mathbf{B}_6	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(4b) O II
\mathbf{B}_7	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4b) O II
\mathbf{B}_8	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(4b) O II
\mathbf{B}_9	$=$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c) O III
\mathbf{B}_{10}	$=$	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c) O III
\mathbf{B}_{11}	$=$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c) O III
\mathbf{B}_{12}	$=$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c) O III
\mathbf{B}_{13}	$=$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c) O IV
\mathbf{B}_{14}	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c) O IV
\mathbf{B}_{15}	$=$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c) O IV
\mathbf{B}_{16}	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c) O IV
\mathbf{B}_{17}	$=$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c) O V
\mathbf{B}_{18}	$=$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c) O V
\mathbf{B}_{19}	$=$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c) O V

$$\begin{aligned}
\mathbf{B}_{20} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3 = a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{O V} \\
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (4c) & \text{O VI} \\
\mathbf{B}_{22} &= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 = -a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{O VI} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (4c) & \text{O VI} \\
\mathbf{B}_{24} &= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 = a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{O VI} \\
\mathbf{B}_{25} &= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3 = ax_7 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (4c) & \text{W I} \\
\mathbf{B}_{26} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{W I} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (4c) & \text{W I} \\
\mathbf{B}_{28} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 = a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{W I} \\
\mathbf{B}_{29} &= x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (4c) & \text{W II} \\
\mathbf{B}_{30} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{W II} \\
\mathbf{B}_{31} &= -x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (4c) & \text{W II} \\
\mathbf{B}_{32} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (4c) & \text{W II}
\end{aligned}$$

References

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Found in

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