

ϵ -WO₃ (low-temperature) Structure: A3B_mP16_7_6a_2a-001

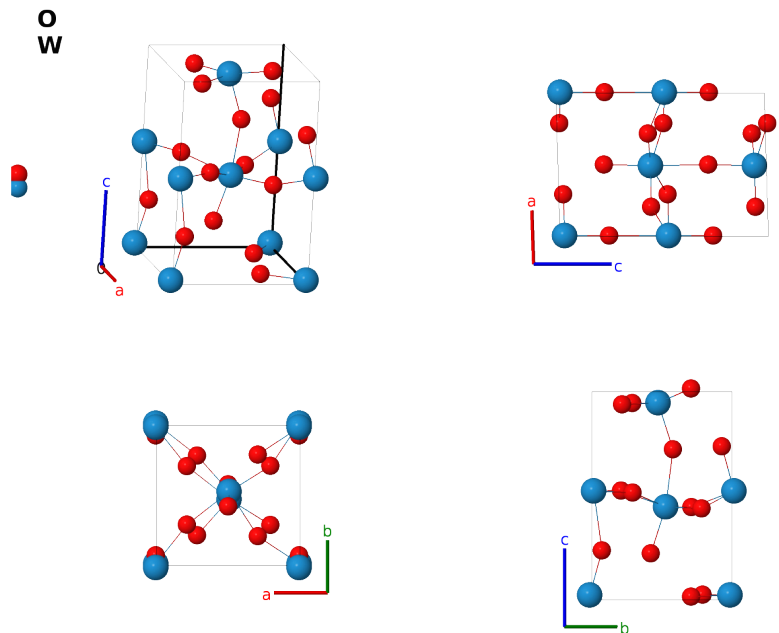
This structure previously used the label(s) **A3B_mP16_7_6a_2a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/SUKZ>

https://aflow.org/prototype-encyclopedia/A3B_mP16_7_6a_2a-001



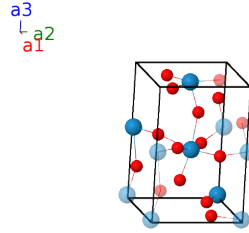
Prototype	O ₃ W
AFLOW prototype label	A3B_mP16_7_6a_2a-001
ICSD	84139
CCDC	1644153
Pearson symbol	mP16
Space group number	7
Space group symbol	<i>Pc</i>
AFLOW prototype command	<pre>aflow --proto=A3B_mP16_7_6a_2a-001 --params=a, b/a, c/a, β, $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$</pre>

- All stable phases of WO₃ are distortions of the cubic α -ReO₃ (*D*_{0h}) 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) (this structure)
- 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 - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937) superseded by δ -WO₃
 - The original β -WO₃ (Salje, 1977)
 - Hexagonal WO₃, presumably metastable, found by (Gerand, 1979) while dehydrating WO₃·H₂O
- The data for the current structure was taken by (Woodward, 1997) at 15K via neutron diffraction.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_6$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_8$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{10}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O VI

$$\begin{aligned}
\mathbf{B}_{12} &= x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_6 + c \left(z_6 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(2a) &\quad \text{O VI} \\
\mathbf{B}_{13} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} &(2a) &\quad \text{W I} \\
\mathbf{B}_{14} &= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_7 + c \left(z_7 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(2a) &\quad \text{W I} \\
\mathbf{B}_{15} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} &(2a) &\quad \text{W II} \\
\mathbf{B}_{16} &= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_8 + c \left(z_8 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} &(2a) &\quad \text{W II}
\end{aligned}$$

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