

δ -WO₃ Structure:

A3B_aP32_2_12i_4i-001

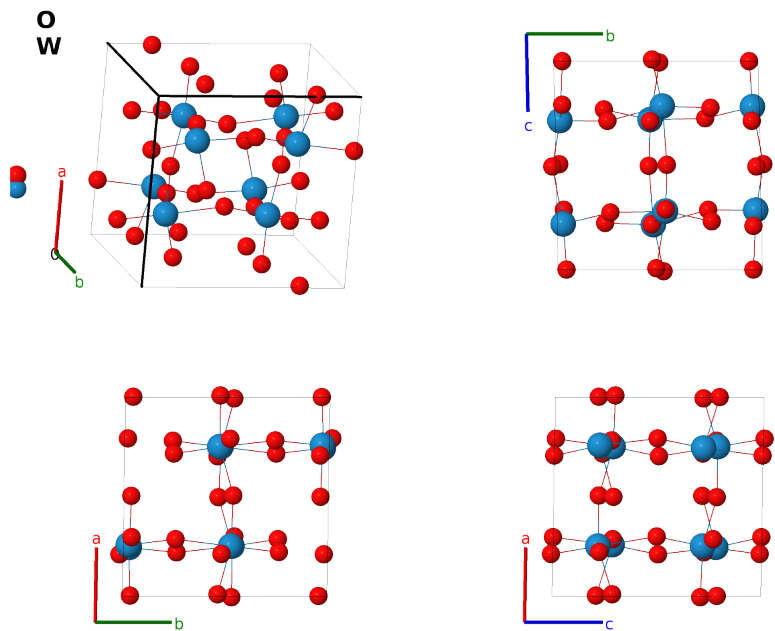
This structure previously used the label(s) **A3B_aP32_2_12i_4i**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/9JTN>

https://aflow.org/prototype-encyclopedia/A3B_aP32_2_12i_4i-001

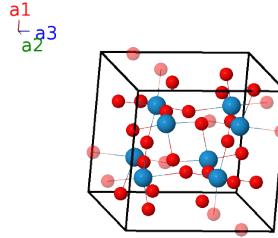


Prototype	O ₃ W
AFLOW prototype label	A3B_aP32_2_12i_4i-001
ICSD	1620
CCDC	1591700
Pearson symbol	aP32
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=A3B_aP32_2_12i_4i-001 --params=a,b/a,c/a,α,β,γ,$x_1,y_1,z_1,x_2,y_2,z_2,x_3,y_3,z_3,x_4,y_4,z_4,x_5,y_5,z_5,x_6,y_6,z_6,x_7,y_7,z_7,x_8,y_8,z_8,x_9,y_9,z_9,x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15},y_{15},z_{15},x_{16},y_{16},z_{16}$</pre>

- All stable phases of WO_3 are distortions of the cubic $\alpha\text{-ReO}_3$ ($D0_9$) phase. Based on (Woodward, 1997 and Vogt, 1999), the known stable phases and their approximate temperature ranges are:
 - $\alpha\text{-WO}_3$ (1010-1170 K) (Vogt, 1999)
 - $\beta\text{-WO}_3$ (600-1170 K) (Vogt, 1999)
 - $\gamma\text{-WO}_3$ (290-600 K) (Vogt, 1999)
 - $\delta\text{-WO}_3$ (230-290 K) (Diehl, 1978) (this structure)
 - $\epsilon\text{-WO}_3$ (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 - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by $\delta\text{-WO}_3$
 - The original $\beta\text{-WO}_3$ (Salje, 1977)
 - Hexagonal WO_3 , presumably metastable, found by (Gerand, 1979) while dehydrating $\text{WO}_3 \cdot \text{H}_2\text{O}$
- The structure of near-room-temperature WO_3 was first solved by (Bräkken, 1931), who proposed a triclinic structure which was half the size of the current structure. This structure was very close to an orthorhombic structure leading (Hermann, 1937) to interpreted it as such, giving it the $D0_{10}$ *Strukturbericht* designation. (Diehl, 1978) refined these results to give the present structure.

Triclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
 c_x &= c \cos \beta \\
 c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
 c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	O IV

$\mathbf{B}_8$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B}_9$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B}_{10}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B}_{11}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B}_{12}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B}_{13}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	O VII
$\mathbf{B}_{14}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	O VII
$\mathbf{B}_{15}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	O VIII
$\mathbf{B}_{16}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$	(2i)	O VIII
$\mathbf{B}_{17}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(2i)	O IX
$\mathbf{B}_{18}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$	(2i)	O IX
$\mathbf{B}_{19}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(2i)	O X
$\mathbf{B}_{20}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}}$	(2i)	O X
$\mathbf{B}_{21}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(2i)	O XI
$\mathbf{B}_{22}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}}$	(2i)	O XI
$\mathbf{B}_{23}$	$=$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} + (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}}$	(2i)	O XII
$\mathbf{B}_{24}$	$=$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} - (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} - c_z z_{12} \hat{\mathbf{z}}$	(2i)	O XII
$\mathbf{B}_{25}$	$=$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} + (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} + c_z z_{13} \hat{\mathbf{z}}$	(2i)	W I
$\mathbf{B}_{26}$	$=$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} - (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} - c_z z_{13} \hat{\mathbf{z}}$	(2i)	W I
$\mathbf{B}_{27}$	$=$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} + (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} + c_z z_{14} \hat{\mathbf{z}}$	(2i)	W II
$\mathbf{B}_{28}$	$=$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} - (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} - c_z z_{14} \hat{\mathbf{z}}$	(2i)	W II
$\mathbf{B}_{29}$	$=$	$x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} + (by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} + c_z z_{15} \hat{\mathbf{z}}$	(2i)	W III
$\mathbf{B}_{30}$	$=$	$-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} - (by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} - c_z z_{15} \hat{\mathbf{z}}$	(2i)	W III
$\mathbf{B}_{31}$	$=$	$x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} + (by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} + c_z z_{16} \hat{\mathbf{z}}$	(2i)	W IV

$$\mathbf{B}_{32} = -x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3 = - (ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} - (by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} - c_z z_{16} \hat{\mathbf{z}} \quad (2i) \quad \text{W IV}$$

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 WO₃*, 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 WO₃*, 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 WO₃*, 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.

Found in

- [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.

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.