

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

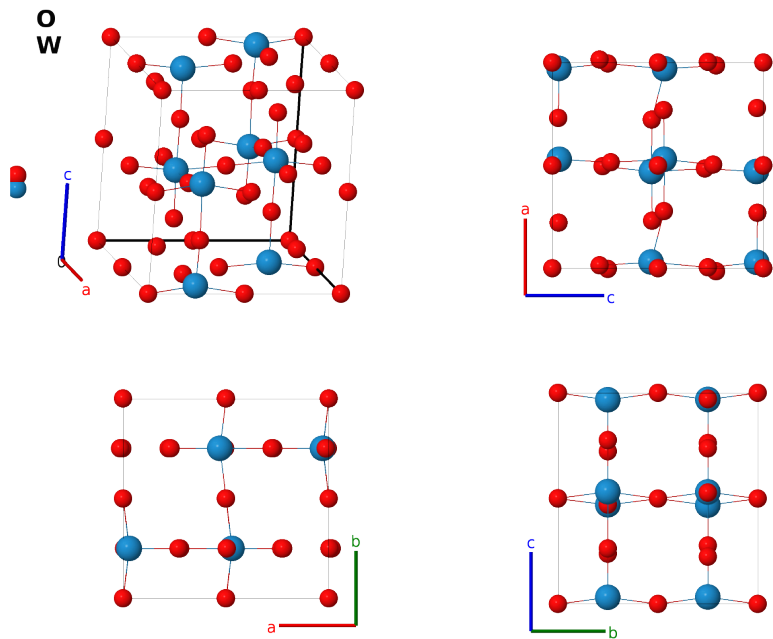
This structure previously used the label(s) A3B_oP32_62_ab4c_2c. Calls to these addresses will be redirected here.

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/KPH8>

https://aflow.org/prototype-encyclopedia/A3B_oP32_62_ab4c_2c-001



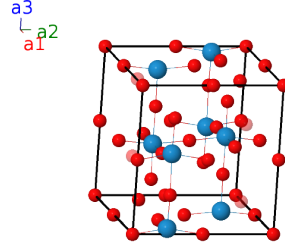
Prototype	O ₃ W
AFLOW prototype label	A3B_oP32_62_ab4c_2c-001
ICSD	836
CCDC	1591084
Pearson symbol	oP32
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=A3B_oP32_62_ab4c_2c-001</code> <code>--params=a, b/a, c/a, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈</code>

- All stable phases of WO₃ are distortions of the cubic α -ReO₃ (*D*_{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)
- 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 - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by δ -WO₃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) (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
$\mathbf{B}_{18} =$	$-\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{20} =$	$\left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	O VI
$\mathbf{B}_{22} =$	$-\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	O VI
$\mathbf{B}_{24} =$	$\left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	W I
$\mathbf{B}_{26} =$	$-\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_7 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	W I
$\mathbf{B}_{28} =$	$\left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	W II
$\mathbf{B}_{30} =$	$-\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$ $\left(z_8 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	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)	W II
$\mathbf{B}_{32} =$	$\left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	W 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 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] 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.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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.