Hexagonal WO_3 Structure: A3B_hP12_191_gl_f-001

This structure originally had the label `A3B_hP12_191_gl_f`. Calls to that address will be redirected here.

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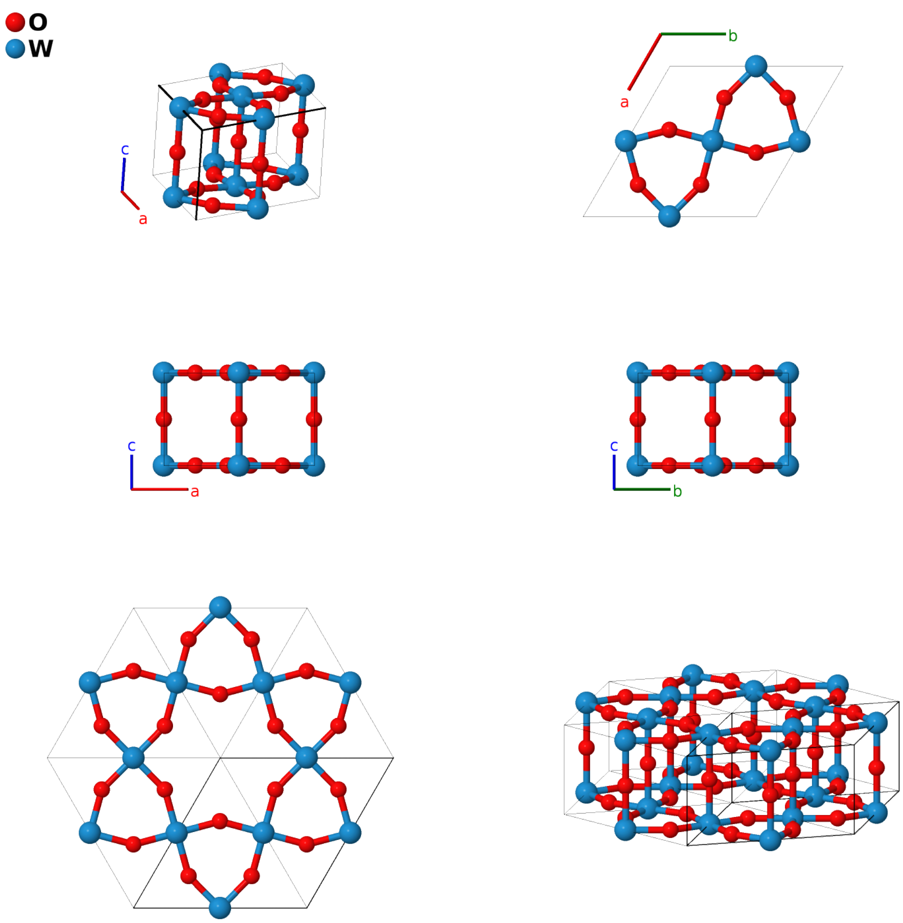
https://aflow.org/p/SQAX

https://aflow.org/p/A3B_hP12_191_gl_f-001

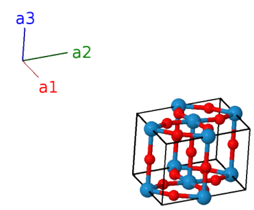


Prototype	O_3W
AFLOW prototype label	A3B_hP12_191_gl_f-001
ICSD	32001
Pearson symbol	hP12
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=A3B_hP12_191_gl_f-001` `--params=`$a, c/a, x_3$

- 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  - The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by δ-WO_3
  - The original β-WO_3 (Salje, 1977)
  - Hexagonal WO_3, presumably metastable, found by (Gerand, 1979) while dehydrating $WO_3 \cdot H_2O$ (this structure)
- (Gerand, 1979) determined the structure of hexagonal WO_3 by X-ray diffraction of powdered samples. They found evidence of super-reflection, indicating that the unit cell should be doubled along the c-axis, but were unable to determine the shift in atomic positions for the double unit cell. We report what they called the "half-cell" structure.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	W I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	W I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3f)	W I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	O I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_8}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{11}}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6l)	O II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}}$	(6l)	O II

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