δ-WO_3 Structure: A3B_aP32_2_12i_4i-001

This structure originally had the label `A3B_aP32_2_12i_4i`. Calls to that address will be redirected here.

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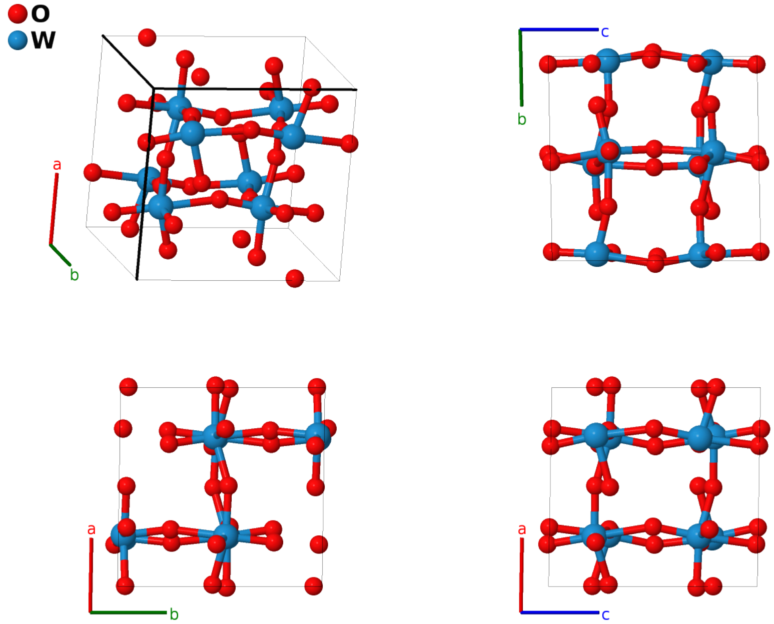
https://aflow.org/p/9JTN

https://aflow.org/p/A3B_aP32_2_12i_4i-001



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Pearson symbol	aP32
Space group number	2
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- 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) (this structure)
– ϵ-WO_3 (below 23 K) (Woodward, 1997)

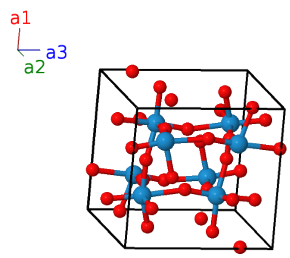
- Woodward notes that "The transition temperatures display large hysteresis effects and universal agreement is not found in the literature."

- 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  – The original $D0_{10}$ structure (Bräkken, 1931; Hermann, 1937), superseded by δ-WO_3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 $WO_3{\cdot}H_2O$

- 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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + by_1\cos\gamma + c_xz_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_yz_1)\,\hat{\mathbf{y}} + c_zz_1\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + by_1\cos\gamma + c_xz_1)\,\hat{\mathbf{x}} - (by_1\sin\gamma + c_yz_1)\,\hat{\mathbf{y}} - c_zz_1\,\hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_xz_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_yz_2)\,\hat{\mathbf{y}} + c_zz_2\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + by_2\cos\gamma + c_xz_2)\,\hat{\mathbf{x}} - (by_2\sin\gamma + c_yz_2)\,\hat{\mathbf{y}} - c_zz_2\,\hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} + c_zz_3\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} - c_zz_3\,\hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} + c_zz_4\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} - c_zz_4\,\hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} + c_zz_5\,\hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} - c_zz_5\,\hat{\mathbf{z}}$	(2i)	O V

$\mathbf{B_{11}}$	=	$x_{6}\,\mathbf{a}_{1}+y_{6}\,\mathbf{a}_{2}+z_{6}\,\mathbf{a}_{3}$	=	$\left(ax_{6}+by_{6}\cos\gamma+c_{x}z_{6}\right)\,\mathbf{\hat{x}}+\left(by_{6}\sin\gamma+c_{y}z_{6}\right)\,\mathbf{\hat{y}}+c_{z}z_{6}\,\mathbf{\hat{z}}$	(2i)	O VI
$\mathbf{B_{12}}$	=	$-x_{6}\,\mathbf{a}_{1}-y_{6}\,\mathbf{a}_{2}-z_{6}\,\mathbf{a}_{3}$	=	$-\left(ax_{6}+by_{6}\cos\gamma+c_{x}z_{6}\right)\,\mathbf{\hat{x}}-\left(by_{6}\sin\gamma+c_{y}z_{6}\right)\,\mathbf{\hat{y}}-c_{z}z_{6}\,\mathbf{\hat{z}}$	(2i)	O VI
$\mathbf{B_{13}}$	=	$x_{7}\,\mathbf{a}_{1}+y_{7}\,\mathbf{a}_{2}+z_{7}\,\mathbf{a}_{3}$	=	$\left(ax_{7}+by_{7}\cos\gamma+c_{x}z_{7}\right)\,\mathbf{\hat{x}}+\left(by_{7}\sin\gamma+c_{y}z_{7}\right)\,\mathbf{\hat{y}}+c_{z}z_{7}\,\mathbf{\hat{z}}$	(2i)	O VII
$\mathbf{B_{14}}$	=	$-x_{7}\,\mathbf{a}_{1}-y_{7}\,\mathbf{a}_{2}-z_{7}\,\mathbf{a}_{3}$	=	$-\left(ax_{7}+by_{7}\cos\gamma+c_{x}z_{7}\right)\,\mathbf{\hat{x}}-\left(by_{7}\sin\gamma+c_{y}z_{7}\right)\,\mathbf{\hat{y}}-c_{z}z_{7}\,\mathbf{\hat{z}}$	(2i)	O VII
$\mathbf{B_{15}}$	=	$x_{8}\,\mathbf{a}_{1}+y_{8}\,\mathbf{a}_{2}+z_{8}\,\mathbf{a}_{3}$	=	$\left(ax_{8}+by_{8}\cos\gamma+c_{x}z_{8}\right)\,\mathbf{\hat{x}}+\left(by_{8}\sin\gamma+c_{y}z_{8}\right)\,\mathbf{\hat{y}}+c_{z}z_{8}\,\mathbf{\hat{z}}$	(2i)	O VIII
$\mathbf{B_{16}}$	=	$-x_{8}\,\mathbf{a}_{1}-y_{8}\,\mathbf{a}_{2}-z_{8}\,\mathbf{a}_{3}$	=	$-\left(ax_{8}+by_{8}\cos\gamma+c_{x}z_{8}\right)\,\mathbf{\hat{x}}-\left(by_{8}\sin\gamma+c_{y}z_{8}\right)\,\mathbf{\hat{y}}-c_{z}z_{8}\,\mathbf{\hat{z}}$	(2i)	O VIII
$\mathbf{B_{17}}$	=	$x_{9}\,\mathbf{a}_{1}+y_{9}\,\mathbf{a}_{2}+z_{9}\,\mathbf{a}_{3}$	=	$\left(ax_{9}+by_{9}\cos\gamma+c_{x}z_{9}\right)\,\mathbf{\hat{x}}+\left(by_{9}\sin\gamma+c_{y}z_{9}\right)\,\mathbf{\hat{y}}+c_{z}z_{9}\,\mathbf{\hat{z}}$	(2i)	O IX
$\mathbf{B_{18}}$	=	$-x_{9}\,\mathbf{a}_{1}-y_{9}\,\mathbf{a}_{2}-z_{9}\,\mathbf{a}_{3}$	=	$-\left(ax_{9}+by_{9}\cos\gamma+c_{x}z_{9}\right)\,\mathbf{\hat{x}}-\left(by_{9}\sin\gamma+c_{y}z_{9}\right)\,\mathbf{\hat{y}}-c_{z}z_{9}\,\mathbf{\hat{z}}$	(2i)	O IX
$\mathbf{B_{19}}$	=	$x_{10}\,\mathbf{a}_{1}+y_{10}\,\mathbf{a}_{2}+z_{10}\,\mathbf{a}_{3}$	=	$\left(ax_{10}+by_{10}\cos\gamma+c_{x}z_{10}\right)\,\mathbf{\hat{x}}+\left(by_{10}\sin\gamma+c_{y}z_{10}\right)\,\mathbf{\hat{y}}+c_{z}z_{10}\,\mathbf{\hat{z}}$	(2i)	O X
$\mathbf{B_{20}}$	=	$-x_{10}\,\mathbf{a}_{1}-y_{10}\,\mathbf{a}_{2}-z_{10}\,\mathbf{a}_{3}$	=	$-\left(ax_{10}+by_{10}\cos\gamma+c_{x}z_{10}\right)\,\mathbf{\hat{x}}-\left(by_{10}\sin\gamma+c_{y}z_{10}\right)\,\mathbf{\hat{y}}-c_{z}z_{10}\,\mathbf{\hat{z}}$	(2i)	O X
$\mathbf{B_{21}}$	=	$x_{11}\,\mathbf{a}_{1}+y_{11}\,\mathbf{a}_{2}+z_{11}\,\mathbf{a}_{3}$	=	$\left(ax_{11}+by_{11}\cos\gamma+c_{x}z_{11}\right)\,\mathbf{\hat{x}}+\left(by_{11}\sin\gamma+c_{y}z_{11}\right)\,\mathbf{\hat{y}}+c_{z}z_{11}\,\mathbf{\hat{z}}$	(2i)	O XI
$\mathbf{B_{22}}$	=	$-x_{11}\,\mathbf{a}_{1}-y_{11}\,\mathbf{a}_{2}-z_{11}\,\mathbf{a}_{3}$	=	$-\left(ax_{11}+by_{11}\cos\gamma+c_{x}z_{11}\right)\,\mathbf{\hat{x}}-\left(by_{11}\sin\gamma+c_{y}z_{11}\right)\,\mathbf{\hat{y}}-c_{z}z_{11}\,\mathbf{\hat{z}}$	(2i)	O XI
$\mathbf{B_{23}}$	=	$x_{12}\,\mathbf{a}_{1}+y_{12}\,\mathbf{a}_{2}+z_{12}\,\mathbf{a}_{3}$	=	$\left(ax_{12}+by_{12}\cos\gamma+c_{x}z_{12}\right)\,\mathbf{\hat{x}}+\left(by_{12}\sin\gamma+c_{y}z_{12}\right)\,\mathbf{\hat{y}}+c_{z}z_{12}\,\mathbf{\hat{z}}$	(2i)	O XII
$\mathbf{B_{24}}$	=	$-x_{12}\,\mathbf{a}_{1}-y_{12}\,\mathbf{a}_{2}-z_{12}\,\mathbf{a}_{3}$	=	$-\left(ax_{12}+by_{12}\cos\gamma+c_{x}z_{12}\right)\,\mathbf{\hat{x}}-\left(by_{12}\sin\gamma+c_{y}z_{12}\right)\,\mathbf{\hat{y}}-c_{z}z_{12}\,\mathbf{\hat{z}}$	(2i)	O XII
$\mathbf{B_{25}}$	=	$x_{13}\,\mathbf{a}_{1}+y_{13}\,\mathbf{a}_{2}+z_{13}\,\mathbf{a}_{3}$	=	$\left(ax_{13}+by_{13}\cos\gamma+c_{x}z_{13}\right)\,\mathbf{\hat{x}}+\left(by_{13}\sin\gamma+c_{y}z_{13}\right)\,\mathbf{\hat{y}}+c_{z}z_{13}\,\mathbf{\hat{z}}$	(2i)	W I
$\mathbf{B_{26}}$	=	$-x_{13}\,\mathbf{a}_{1}-y_{13}\,\mathbf{a}_{2}-z_{13}\,\mathbf{a}_{3}$	=	$-\left(ax_{13}+by_{13}\cos\gamma+c_{x}z_{13}\right)\,\mathbf{\hat{x}}-\left(by_{13}\sin\gamma+c_{y}z_{13}\right)\,\mathbf{\hat{y}}-c_{z}z_{13}\,\mathbf{\hat{z}}$	(2i)	W I
$\mathbf{B_{27}}$	=	$x_{14}\,\mathbf{a}_{1}+y_{14}\,\mathbf{a}_{2}+z_{14}\,\mathbf{a}_{3}$	=	$\left(ax_{14}+by_{14}\cos\gamma+c_{x}z_{14}\right)\,\mathbf{\hat{x}}+\left(by_{14}\sin\gamma+c_{y}z_{14}\right)\,\mathbf{\hat{y}}+c_{z}z_{14}\,\mathbf{\hat{z}}$	(2i)	W II
$\mathbf{B_{28}}$	=	$-x_{14}\,\mathbf{a}_{1}-y_{14}\,\mathbf{a}_{2}-z_{14}\,\mathbf{a}_{3}$	=	$-\left(ax_{14}+by_{14}\cos\gamma+c_{x}z_{14}\right)\,\mathbf{\hat{x}}-\left(by_{14}\sin\gamma+c_{y}z_{14}\right)\,\mathbf{\hat{y}}-c_{z}z_{14}\,\mathbf{\hat{z}}$	(2i)	W II
$\mathbf{B_{29}}$	=	$x_{15}\,\mathbf{a}_{1}+y_{15}\,\mathbf{a}_{2}+z_{15}\,\mathbf{a}_{3}$	=	$\left(ax_{15}+by_{15}\cos\gamma+c_{x}z_{15}\right)\,\mathbf{\hat{x}}+\left(by_{15}\sin\gamma+c_{y}z_{15}\right)\,\mathbf{\hat{y}}+c_{z}z_{15}\,\mathbf{\hat{z}}$	(2i)	W III
$\mathbf{B_{30}}$	=	$-x_{15}\,\mathbf{a}_{1}-y_{15}\,\mathbf{a}_{2}-z_{15}\,\mathbf{a}_{3}$	=	$-\left(ax_{15}+by_{15}\cos\gamma+c_{x}z_{15}\right)\,\mathbf{\hat{x}}-\left(by_{15}\sin\gamma+c_{y}z_{15}\right)\,\mathbf{\hat{y}}-c_{z}z_{15}\,\mathbf{\hat{z}}$	(2i)	W III
$\mathbf{B_{31}}$	=	$x_{16}\,\mathbf{a}_{1}+y_{16}\,\mathbf{a}_{2}+z_{16}\,\mathbf{a}_{3}$	=	$\left(ax_{16}+by_{16}\cos\gamma+c_{x}z_{16}\right)\,\mathbf{\hat{x}}+\left(by_{16}\sin\gamma+c_{y}z_{16}\right)\,\mathbf{\hat{y}}+c_{z}z_{16}\,\mathbf{\hat{z}}$	(2i)	W IV
$\mathbf{B_{32}}$	=	$-x_{16}\,\mathbf{a}_{1}-y_{16}\,\mathbf{a}_{2}-z_{16}\,\mathbf{a}_{3}$	=	$-\left(ax_{16}+by_{16}\cos\gamma+c_{x}z_{16}\right)\,\mathbf{\hat{x}}-\left(by_{16}\sin\gamma+c_{y}z_{16}\right)\,\mathbf{\hat{y}}-c_{z}z_{16}\,\mathbf{\hat{z}}$	(2i)	W IV

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Found in

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