W_3O_{10} ($WO_3 \cdot \frac{1}{3}H_2O$) Structure: A10B3_oF52_42_2abce_ab-001

This structure originally had the label `A10B3_oF52_42_2abce_ab`. Calls to that address will be redirected here.

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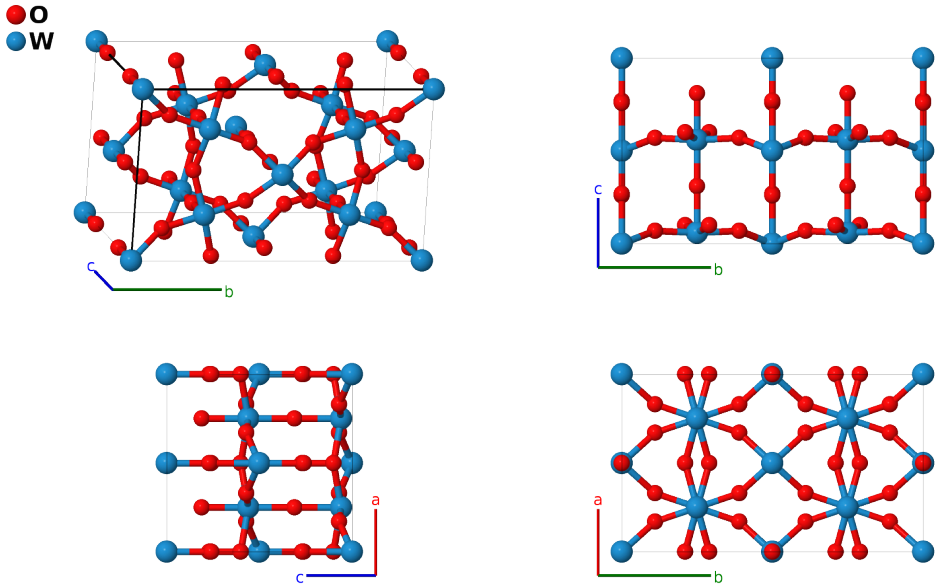
https://aflow.org/p/TH7F

https://aflow.org/p/A10B3_oF52_42_2abce_ab-001

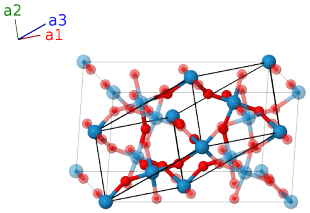


Prototype	$O_{10}W_3$
AFLOW prototype label	A10B3_oF52_42_2abce_ab-001
ICSD	15514
Pearson symbol	oF52
Space group number	42
Space group symbol	$Fmm2$
AFLOW prototype command	`aflow --proto=A10B3_oF52_42_2abce_ab-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, z_4, z_5, y_6, z_6, x_7, y_7, z_7$

- The designation of this structure is somewhat confusing. (Gerand, 1981) call this structure $WO_3 \cdot \frac{1}{3}H_2O$, more properly written as $W_3O_9 \cdot H_2O$, but they do not give the positions of the hydrogen atoms, which are presumably associated with the O-V [O(2) in (Gerand, 1981)] atoms. Without further guidance we have left the hydrogens out of this study.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B_4}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_5}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_6}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8b)	W II
$\mathbf{B_7}$	=	$\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	W II
$\mathbf{B_8}$	=	$(y_6 + z_6)\,\mathbf{a}_1 - (y_6 - z_6)\,\mathbf{a}_2 + (y_6 - z_6)\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_9}$	=	$-(y_6 - z_6)\,\mathbf{a}_1 + (y_6 + z_6)\,\mathbf{a}_2 - (y_6 + z_6)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8c)	O IV
$\mathbf{B_{10}}$	=	$(-x_7 + y_7 + z_7)\,\mathbf{a}_1 + (x_7 - y_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7 - z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16e)	O V
$\mathbf{B_{11}}$	=	$(x_7 - y_7 + z_7)\,\mathbf{a}_1 + (-x_7 + y_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7 + z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16e)	O V
$\mathbf{B_{12}}$	=	$-(x_7 + y_7 - z_7)\,\mathbf{a}_1 + (x_7 + y_7 + z_7)\,\mathbf{a}_2 + (x_7 - y_7 - z_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16e)	O V
$\mathbf{B_{13}}$	=	$(x_7 + y_7 + z_7)\,\mathbf{a}_1 - (x_7 + y_7 - z_7)\,\mathbf{a}_2 - (x_7 - y_7 + z_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16e)	O V

References

[1] B. Gerand, G. Nowogrocki, and M. Figlarz, *A new tungsten trioxide hydrate, $WO_3 \cdot \frac{1}{3}H_2O$: Preparation, characterization, and crystallographic study*, J. Solid State Chem. **38**, 312–320 (1981), doi:10.1016/0022-4596(81)90062-1.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.