

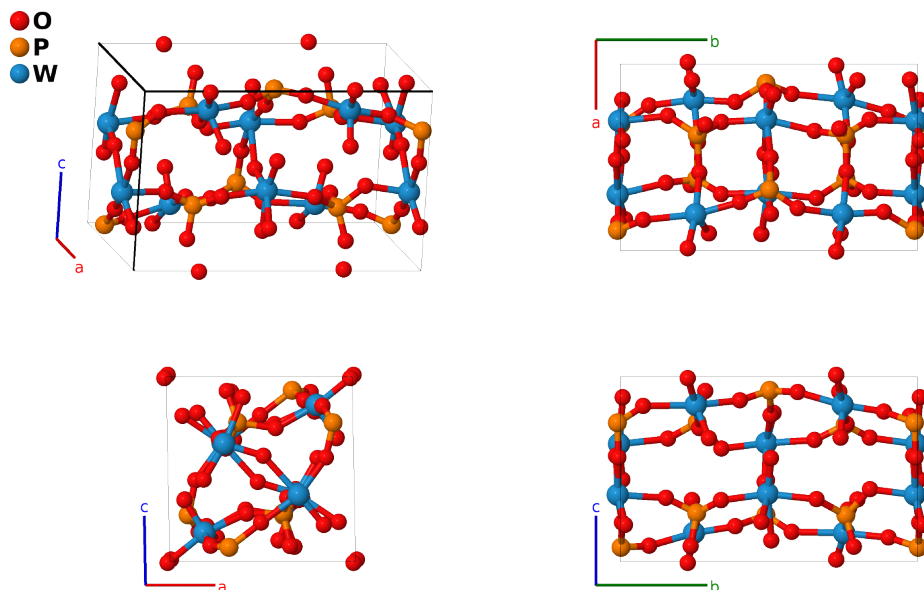
W₂O₃(PO₄)₂ Structure: A11B2C2_mP60_4_22a_4a_4a-001

This structure originally had the label A11B2C2_mP60_4_22a_4a_4a. Calls to that address will be redirected here.

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<https://aflow.org/p/Z0HK>

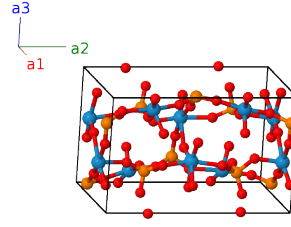
https://aflow.org/p/A11B2C2_mP60_4_22a_4a_4a-001



Prototype	O ₁₁ P ₄ W ₄
AFLOW prototype label	A11B2C2_mP60_4_22a_4a_4a-001
ICSD	36103
Pearson symbol	mP60
Space group number	4
Space group symbol	P2 ₁
AFLOW prototype command	<pre>aflow --proto=A11B2C2_mP60_4_22a_4a_4a-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅, y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉,x₂₀,y₂₀,z₂₀,x₂₁,y₂₁,z₂₁,x₂₂,y₂₂, z₂₂,x₂₃,y₂₃,z₂₃,x₂₄,y₂₄,z₂₄,x₂₅,y₂₅,z₂₅,x₂₆,y₂₆,z₂₆,x₂₇,y₂₇,z₂₇,x₂₈,y₂₈,z₂₈,x₂₉,y₂₉,z₂₉, x₃₀,y₃₀,z₃₀</pre>

Simple Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_3	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
\mathbf{B}_4	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
\mathbf{B}_6	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
\mathbf{B}_7	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
\mathbf{B}_8	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
\mathbf{B}_9	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
\mathbf{B}_{10}	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
\mathbf{B}_{11}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O VI
\mathbf{B}_{12}	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O VI
\mathbf{B}_{13}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O VII
\mathbf{B}_{14}	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O VII
\mathbf{B}_{15}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O VIII
\mathbf{B}_{16}	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O VIII
\mathbf{B}_{17}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O IX
\mathbf{B}_{18}	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O IX
\mathbf{B}_{19}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O X
\mathbf{B}_{20}	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	=	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O X
\mathbf{B}_{21}	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2a)	O XI
\mathbf{B}_{22}	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	=	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(2a)	O XI
\mathbf{B}_{23}	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(2a)	O XII

$$\begin{aligned}
\mathbf{B}_{54} &= -x_{27} \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 - z_{27} \mathbf{a}_3 = -\left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{27} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W I} \\
\mathbf{B}_{55} &= x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3 = \left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W II} \\
\mathbf{B}_{56} &= -x_{28} \mathbf{a}_1 + \left(y_{28} + \frac{1}{2}\right) \mathbf{a}_2 - z_{28} \mathbf{a}_3 = -\left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W II} \\
\mathbf{B}_{57} &= x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + z_{29} \mathbf{a}_3 = \left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W III} \\
\mathbf{B}_{58} &= -x_{29} \mathbf{a}_1 + \left(y_{29} + \frac{1}{2}\right) \mathbf{a}_2 - z_{29} \mathbf{a}_3 = -\left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{29} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W III} \\
\mathbf{B}_{59} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 = \left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W IV} \\
\mathbf{B}_{60} &= -x_{30} \mathbf{a}_1 + \left(y_{30} + \frac{1}{2}\right) \mathbf{a}_2 - z_{30} \mathbf{a}_3 = -\left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{30} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{W IV}
\end{aligned}$$

References

- [1] P. Kierkegaard and S. Åsbrink, *The Crystal Structure of $W_2O_3(PO_4)_2$. Determination of a Superstructure by Means of Least-Squares Calculations*, Acta Chem. Scand. **18**, 2329–2338 (1964), doi:10.3891/acta.chem.scand.18-2329.