

Mo₄P₃ Structure:

A4B3_oP56_62_8c_6c-001

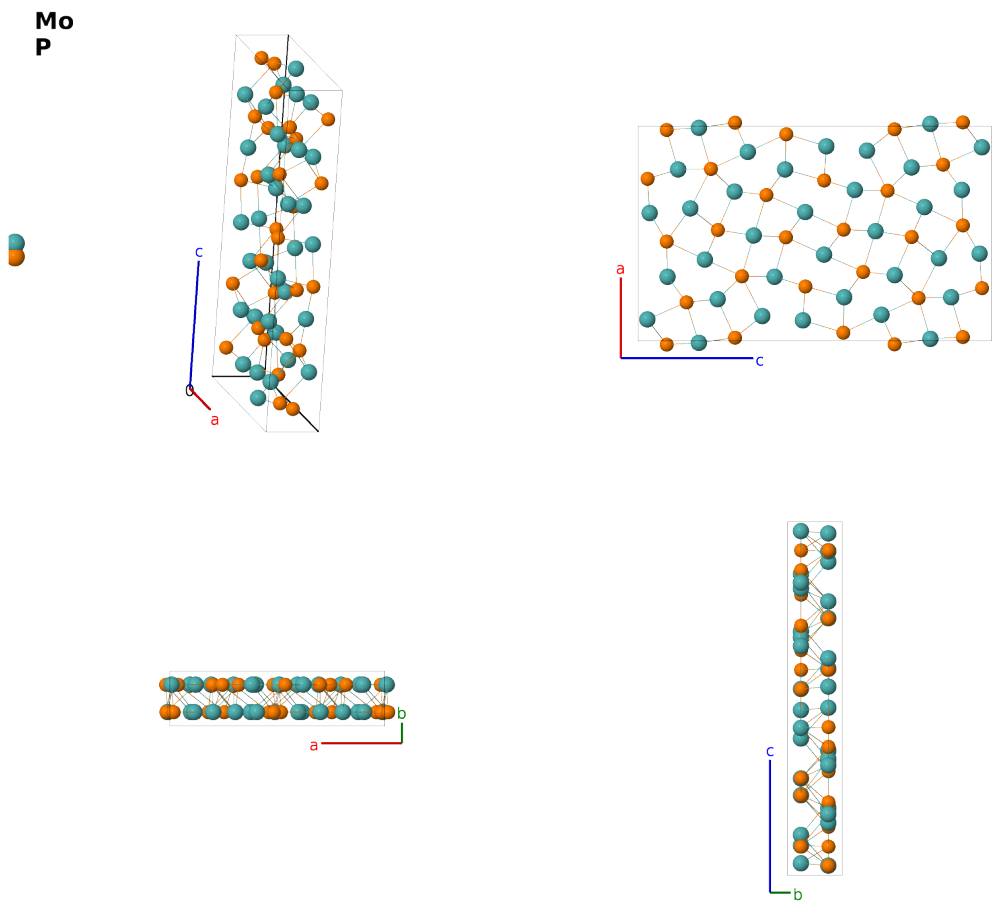
This structure previously used the label(s) **A4B3_oP56_62_8c_6c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/S9HM>

https://aflow.org/prototype-encyclopedia/A4B3_oP56_62_8c_6c-001



Prototype	Mo ₄ P ₃
AFLOW prototype label	A4B3_oP56_62_8c_6c-001
ICSD	43237
CCDC	1612759
Pearson symbol	oP56
Space group number	62

Space group symbol

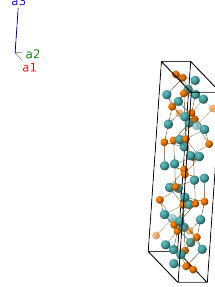
Pnma

AFLOW prototype command

afLOW --proto=A4B3_oP56_62_8c_6c-001
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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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_2$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_4$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo I
$\mathbf{B}_5$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Mo II
$\mathbf{B}_6$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo II
$\mathbf{B}_7$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Mo II
$\mathbf{B}_8$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo 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)	Mo V
$\mathbf{B}_{18}$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo 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)	Mo V
$\mathbf{B}_{20}$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Mo V

$$\begin{aligned}
\mathbf{B}_{53} &= x_{14} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= ax_{14} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} &(4c) &\text{P VI} \\
\mathbf{B}_{54} &= -\left(x_{14} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_{14} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{P VI} \\
&\quad \left(z_{14} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{55} &= -x_{14} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= -ax_{14} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} &(4c) &\text{P VI} \\
\mathbf{B}_{56} &= \left(x_{14} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a\left(x_{14} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{P VI} \\
&\quad \left(z_{14} - \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

References

[1] S. Rundqvist, *The Crystal Structure of Mo_4P_3* , Acta Chem. Scand. **19**, 393–400 (1965), doi:10.3891/acta.chem.scand.19-0393.

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