

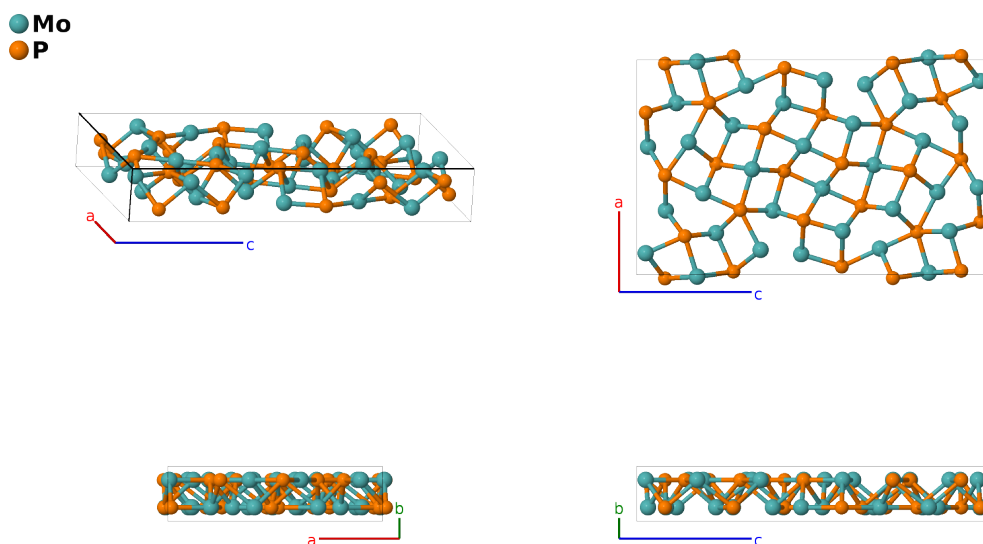
Mo₄P₃ Structure: A4B3_oP56_62_8c_6c-001

This structure originally had the label **A4B3_oP56_62_8c_6c**. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/S9HM>

https://aflow.org/p/A4B3_oP56_62_8c_6c-001



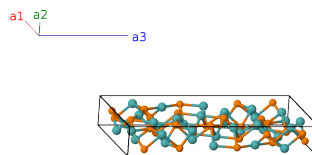
Prototype	Mo ₄ P ₃
AFLOW prototype label	A4B3_oP56_62_8c_6c-001
ICSD	43237
Pearson symbol	oP56
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	aflow --proto=A4B3_oP56_62_8c_6c-001 --params= <i>a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, z₈, x₉, z₉, x₁₀, z₁₀, x₁₁, z₁₁, x₁₂, z₁₂, x₁₃, z₁₃, x₁₄, z₁₄</i>

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



$$\begin{aligned}
\mathbf{B}_{33} &= x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(4c) & \text{P I} \\
\mathbf{B}_{34} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P I} \\
&\quad \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= -x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(4c) & \text{P I} \\
\mathbf{B}_{36} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P I} \\
\mathbf{B}_{37} &= x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(4c) & \text{P II} \\
\mathbf{B}_{38} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P II} \\
&\quad \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{39} &= -x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} &(4c) & \text{P II} \\
\mathbf{B}_{40} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P II} \\
&\quad \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{41} &= x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= ax_{11} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(4c) & \text{P III} \\
\mathbf{B}_{42} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P III} \\
&\quad \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{43} &= -x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= -ax_{11} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(4c) & \text{P III} \\
\mathbf{B}_{44} &= \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a\left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P III} \\
&\quad \left(z_{11} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{45} &= x_{12} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= ax_{12} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} &(4c) & \text{P IV} \\
\mathbf{B}_{46} &= -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_{12} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P IV} \\
&\quad \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{47} &= -x_{12} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= -ax_{12} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}} &(4c) & \text{P IV} \\
\mathbf{B}_{48} &= \left(x_{12} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a\left(x_{12} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P IV} \\
&\quad \left(z_{12} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{49} &= x_{13} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= ax_{13} \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} &(4c) & \text{P V} \\
\mathbf{B}_{50} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + &= -a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P V} \\
&\quad \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{51} &= -x_{13} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= -ax_{13} \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}} &(4c) & \text{P V} \\
\mathbf{B}_{52} &= \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - &= a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{P V} \\
&\quad \left(z_{13} - \frac{1}{2}\right) \mathbf{a}_3 \\
\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 Mo₄P₃*, Acta Chem. Scand. **19**, 393–400 (1965), doi:10.3891/acta.chem.scand.19-0393.