

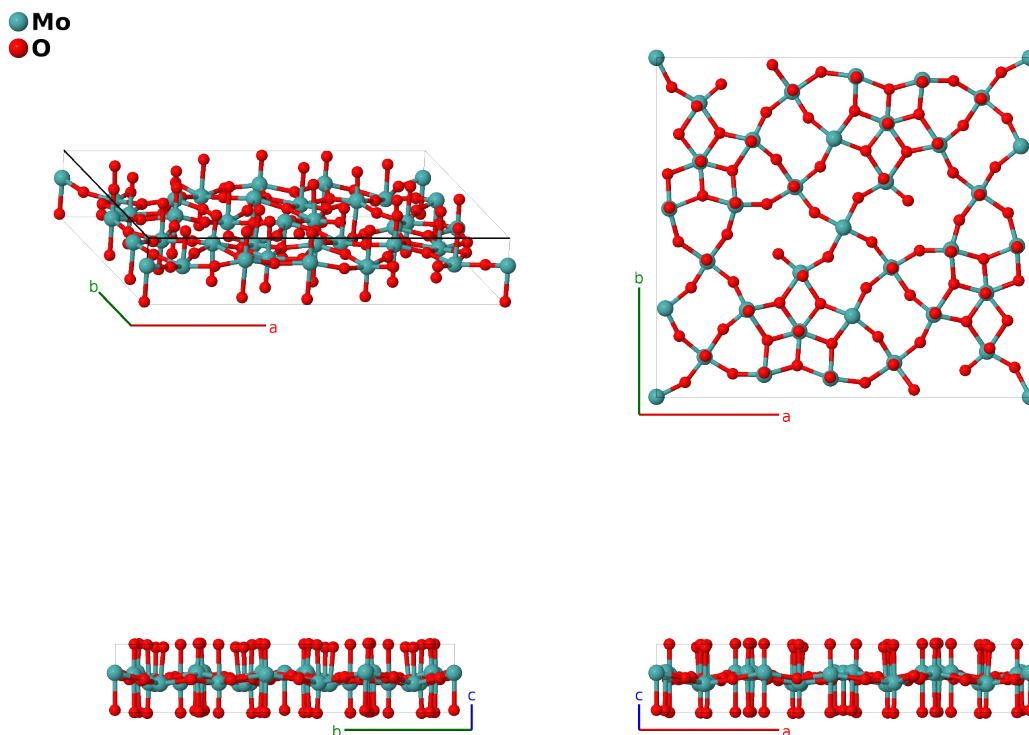
Mo₁₇O₄₇ Structure: A17B47_oP128_32_a8c_a23c-001

This structure originally had the label A17B47_oP128_32_a8c_a23c. Calls to that address will be redirected here.

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<https://aflow.org/p/484W>

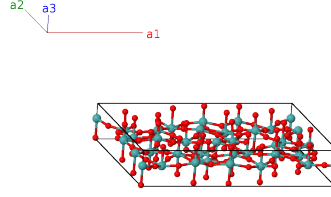
https://aflow.org/p/A17B47_oP128_32_a8c_a23c-001



Prototype	Mo ₁₇ O ₄₇
AFLOW prototype label	A17B47_oP128_32_a8c_a23c-001
ICSD	28333
Pearson symbol	oP128
Space group number	32
Space group symbol	<i>Pba</i> 2
AFLOW prototype command	<pre>aflow --proto=A17B47_oP128_32_a8c_a23c-001 --params=a, b/a, c/a, z1, 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, x31, y31, z31, x32, y32, z32, x33, y33, z33</pre>

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	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Mo I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	Mo I
\mathbf{B}_3	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Mo II
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Mo II
\mathbf{B}_7	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Mo II
\mathbf{B}_8	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Mo II
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Mo III
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Mo III
\mathbf{B}_{11}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Mo III
\mathbf{B}_{12}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Mo III
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Mo IV
\mathbf{B}_{14}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Mo IV
\mathbf{B}_{15}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Mo IV
\mathbf{B}_{16}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Mo IV
\mathbf{B}_{17}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Mo V
\mathbf{B}_{18}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Mo V
\mathbf{B}_{19}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Mo V
\mathbf{B}_{20}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Mo V
\mathbf{B}_{21}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Mo VI
\mathbf{B}_{22}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Mo VI
\mathbf{B}_{23}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Mo VI
\mathbf{B}_{24}	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Mo VI
\mathbf{B}_{25}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4c)	Mo VII

$$\begin{aligned}
\mathbf{B}_{117} &= x_{31} \mathbf{a}_1 + y_{31} \mathbf{a}_2 + z_{31} \mathbf{a}_3 &= ax_{31} \hat{\mathbf{x}} + by_{31} \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}} & (4c) & \text{O XXII} \\
\mathbf{B}_{118} &= -x_{31} \mathbf{a}_1 - y_{31} \mathbf{a}_2 + z_{31} \mathbf{a}_3 &= -ax_{31} \hat{\mathbf{x}} - by_{31} \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}} & (4c) & \text{O XXII} \\
\mathbf{B}_{119} &= \left(x_{31} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{31} - \frac{1}{2}\right) \mathbf{a}_2 + z_{31} \mathbf{a}_3 &= a \left(x_{31} + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_{31} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}} & (4c) & \text{O XXII} \\
\mathbf{B}_{120} &= -\left(x_{31} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{31} + \frac{1}{2}\right) \mathbf{a}_2 + z_{31} \mathbf{a}_3 &= -a \left(x_{31} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{31} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{31} \hat{\mathbf{z}} & (4c) & \text{O XXII} \\
\mathbf{B}_{121} &= x_{32} \mathbf{a}_1 + y_{32} \mathbf{a}_2 + z_{32} \mathbf{a}_3 &= ax_{32} \hat{\mathbf{x}} + by_{32} \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}} & (4c) & \text{O XXIII} \\
\mathbf{B}_{122} &= -x_{32} \mathbf{a}_1 - y_{32} \mathbf{a}_2 + z_{32} \mathbf{a}_3 &= -ax_{32} \hat{\mathbf{x}} - by_{32} \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}} & (4c) & \text{O XXIII} \\
\mathbf{B}_{123} &= \left(x_{32} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{32} - \frac{1}{2}\right) \mathbf{a}_2 + z_{32} \mathbf{a}_3 &= a \left(x_{32} + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_{32} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}} & (4c) & \text{O XXIII} \\
\mathbf{B}_{124} &= -\left(x_{32} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{32} + \frac{1}{2}\right) \mathbf{a}_2 + z_{32} \mathbf{a}_3 &= -a \left(x_{32} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{32} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{32} \hat{\mathbf{z}} & (4c) & \text{O XXIII} \\
\mathbf{B}_{125} &= x_{33} \mathbf{a}_1 + y_{33} \mathbf{a}_2 + z_{33} \mathbf{a}_3 &= ax_{33} \hat{\mathbf{x}} + by_{33} \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}} & (4c) & \text{O XXIV} \\
\mathbf{B}_{126} &= -x_{33} \mathbf{a}_1 - y_{33} \mathbf{a}_2 + z_{33} \mathbf{a}_3 &= -ax_{33} \hat{\mathbf{x}} - by_{33} \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}} & (4c) & \text{O XXIV} \\
\mathbf{B}_{127} &= \left(x_{33} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{33} - \frac{1}{2}\right) \mathbf{a}_2 + z_{33} \mathbf{a}_3 &= a \left(x_{33} + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_{33} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}} & (4c) & \text{O XXIV} \\
\mathbf{B}_{128} &= -\left(x_{33} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{33} + \frac{1}{2}\right) \mathbf{a}_2 + z_{33} \mathbf{a}_3 &= -a \left(x_{33} - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_{33} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{33} \hat{\mathbf{z}} & (4c) & \text{O XXIV}
\end{aligned}$$

References

- [1] L. Kihlberg, *Least Squares Refinement of the Structure of Mo₁₇O₄₇*, Acta Chem. Scand. **17**, 1485–1487 (1963), doi:10.3891/acta.chem.scand.17-1485.