

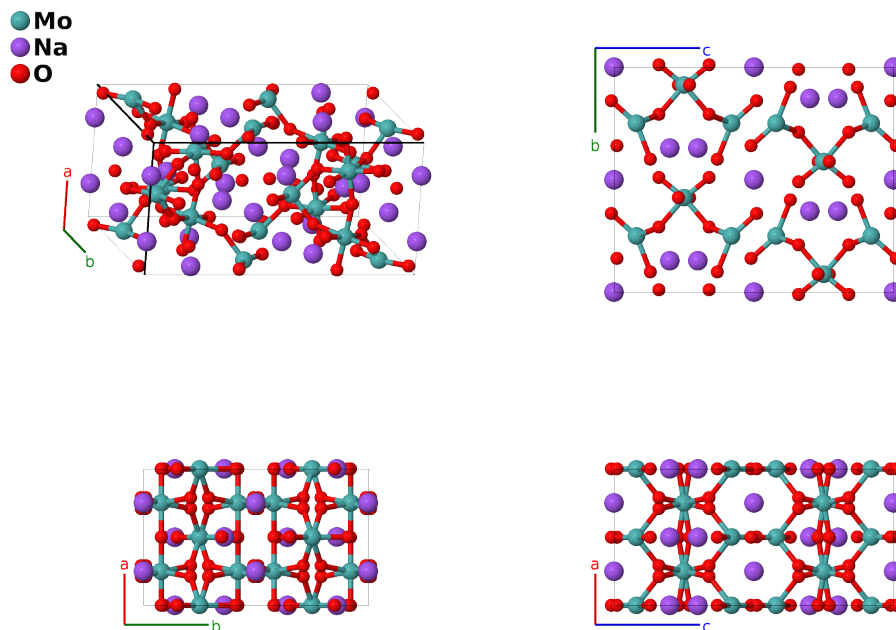
Na₂Mo₂O₇ Structure: A2B2C7_oC88_64_ef_df_3f2g-001

This structure originally had the label A2B2C7_oC88_64_ef_df_3f2g. 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/0H5D>

https://aflow.org/p/A2B2C7_oC88_64_ef_df_3f2g-001



Prototype	Mo ₂ Na ₂ O ₇
AFLOW prototype label	A2B2C7_oC88_64_ef_df_3f2g-001
ICSD	24041
Pearson symbol	oC88
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A2B2C7_oC88_64_ef_df_3f2g-001 --params=a, b/a, c/a, x1, y2, y3, z3, y4, z4, y5, z5, y6, z6, y7, z7, x8, y8, z8, x9, y9, z9</code>

Other compounds with this structure

Na₂W₂O₇

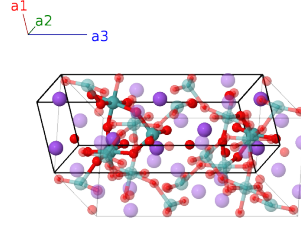
- (Lindqvist, 1950) gives data for the prototype compound, Na₂Mo₂O₇, but the ICSD entry lists the compound as Na₂W₂O₇. Otherwise the data matches exactly with the prototype, so we use that ICSD entry here.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}}$	(8d)	Na I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Na I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}}$	(8d)	Na I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8d)	Na I
\mathbf{B}_5	$= -\left(y_2 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	Mo I
\mathbf{B}_6	$= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	Mo I
\mathbf{B}_7	$= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	Mo I
\mathbf{B}_8	$= -\left(y_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	Mo I
\mathbf{B}_9	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	Mo II
\mathbf{B}_{10}	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Mo II
\mathbf{B}_{11}	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Mo II
\mathbf{B}_{12}	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	Mo II
\mathbf{B}_{13}	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	Na II
\mathbf{B}_{14}	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Na II
\mathbf{B}_{15}	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Na II
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	Na II
\mathbf{B}_{17}	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{18}	$= \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{19}	$= -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{20}	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f)	O I
\mathbf{B}_{21}	$= -y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8f)	O II
\mathbf{B}_{22}	$= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O II

$$\begin{aligned}
\mathbf{B}_{23} &= -\left(y_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O II} \\
\mathbf{B}_{24} &= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (8f) & \text{O II} \\
\mathbf{B}_{25} &= -y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8f) & \text{O III} \\
\mathbf{B}_{26} &= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O III} \\
\mathbf{B}_{27} &= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= & \frac{1}{2}a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O III} \\
\mathbf{B}_{28} &= y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & -by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (8f) & \text{O III} \\
\mathbf{B}_{29} &= (x_8 - y_8) \mathbf{a}_1 + (x_8 + 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}} & (16g) & \text{O IV} \\
\mathbf{B}_{30} &= (-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_1 - (x_8 + y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= & -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{31} &= -(x_8 + y_8 - \frac{1}{2}) \mathbf{a}_1 + (-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 &= & -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{32} &= (x_8 + y_8) \mathbf{a}_1 + (x_8 - 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}} & (16g) & \text{O IV} \\
\mathbf{B}_{33} &= -(x_8 - y_8) \mathbf{a}_1 - (x_8 + 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}} & (16g) & \text{O IV} \\
\mathbf{B}_{34} &= (x_8 - y_8 + \frac{1}{2}) \mathbf{a}_1 + (x_8 + y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 &= & a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{35} &= (x_8 + y_8 + \frac{1}{2}) \mathbf{a}_1 + (x_8 - y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 &= & a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O IV} \\
\mathbf{B}_{36} &= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - 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}} & (16g) & \text{O IV} \\
\mathbf{B}_{37} &= (x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{38} &= (-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_1 - (x_9 + y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= & -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{39} &= -(x_9 + y_9 - \frac{1}{2}) \mathbf{a}_1 + (-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 &= & -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{40} &= (x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{41} &= -(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{42} &= (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_1 + (x_9 + y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 &= & a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{43} &= (x_9 + y_9 + \frac{1}{2}) \mathbf{a}_1 + (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 &= & a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{44} &= -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16g) & \text{O V}
\end{aligned}$$

References

- [1] I. Lindqvist, *Crystal Structure Studies on Anhydrous Sodium Molybdates and Tungstates*, Acta Chem. Scand. **4**, 1066–1074 (1950), doi:10.3891/acta.chem.scand.04-1066.