

Na₂Mo₂O₇ Structure:

A2B2C7_oC88_64_ef_df_3f2g-001

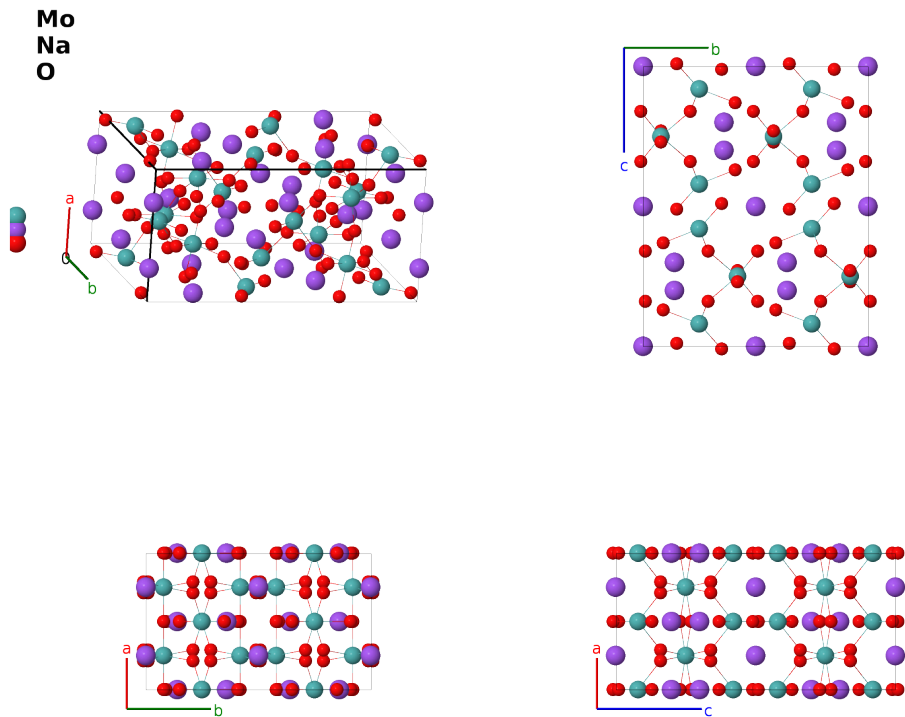
This structure previously used the label(s) **A2B2C7_oC88_64_ef_df_3f2g**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/0H5D>

https://aflow.org/prototype-encyclopedia/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
CCDC	1600096
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</code> <code>--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>

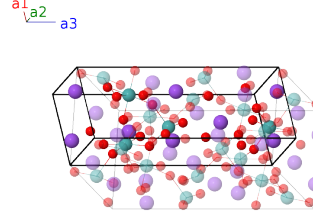
Other compounds with this structure

$\text{Na}_2\text{W}_2\text{O}_7$

- (Lindqvist, 1950) gives data for the prototype compound, $\text{Na}_2\text{Mo}_2\text{O}_7$, but the ICSD entry lists the compound as $\text{Na}_2\text{W}_2\text{O}_7$. Otherwise the data matches exactly with the prototype, so we use that ICSD entry here.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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

$\mathbf{B}_{18} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O I
	$(z_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{19} =$	$-(y_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O I
	$(z_5 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II
	$(z_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O II
	$(z_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{24} =$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8f)	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)	O III
$\mathbf{B}_{26} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O III
	$(z_7 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{27} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	O III
	$(z_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{29} =$	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 +$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(16g)	O IV
	$z_8 \mathbf{a}_3$				
$\mathbf{B}_{30} =$	$(-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_1 -$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O IV
	$(x_8 + y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$-(x_8 + y_8 - \frac{1}{2}) \mathbf{a}_1 +$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O IV
	$(-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{32} =$	$(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 -$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(16g)	O IV
	$z_8 \mathbf{a}_3$				
$\mathbf{B}_{33} =$	$-(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(16g)	O IV
	$z_8 \mathbf{a}_3$				
$\mathbf{B}_{34} =$	$(x_8 - y_8 + \frac{1}{2}) \mathbf{a}_1 +$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O IV
	$(x_8 + y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$(x_8 + y_8 + \frac{1}{2}) \mathbf{a}_1 +$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O IV
	$(x_8 - y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 +$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(16g)	O IV
	$z_8 \mathbf{a}_3$				
$\mathbf{B}_{37} =$	$(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 +$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(16g)	O V
	$z_9 \mathbf{a}_3$				
$\mathbf{B}_{38} =$	$(-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_1 -$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O V
	$(x_9 + y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{39} =$	$-(x_9 + y_9 - \frac{1}{2}) \mathbf{a}_1 +$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O V
	$(-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{40} =$	$(x_9 + y_9) \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 -$	$=$	$ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(16g)	O V
	$z_9 \mathbf{a}_3$				
$\mathbf{B}_{41} =$	$-(x_9 - y_9) \mathbf{a}_1 - (x_9 + y_9) \mathbf{a}_2 -$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(16g)	O V
	$z_9 \mathbf{a}_3$				
$\mathbf{B}_{42} =$	$(x_9 - y_9 + \frac{1}{2}) \mathbf{a}_1 +$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O V
	$(x_9 + y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$				

$$\begin{aligned}
\mathbf{B}_{43} &= \begin{pmatrix} (x_9 + y_9 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_9 + \frac{1}{2} \right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2} \right) \hat{\mathbf{z}} & (16g) & \text{O V} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 + \\ z_9 \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16g) & \text{O V}
\end{aligned}$$

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.

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