

Rb₂Mo₂O₇ Structure:

A2B7C2_oC88_40_abc_2b6c_a3b-001

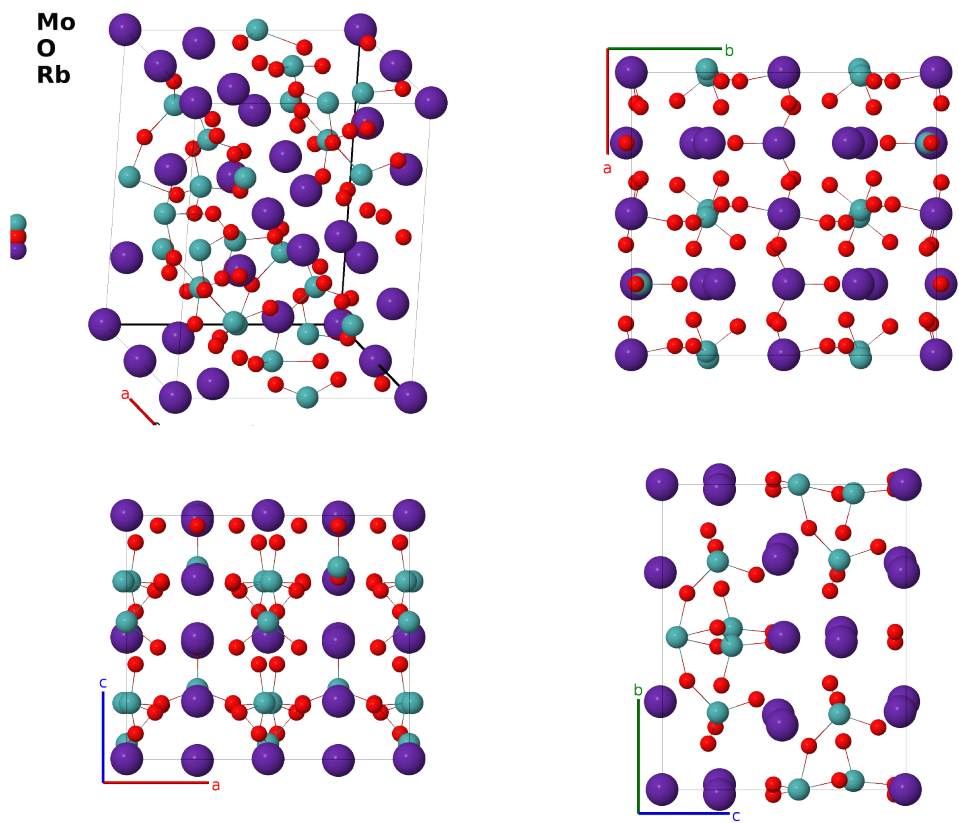
This structure previously used the label(s) **A2B7C2_oC88_40_abc_2b6c_a3b**. Calls to these addresses will be redirected here.

Cite this page as:

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

https://aflow.org/prototype-encyclopedia/A2B7C2_oC88_40_abc_2b6c_a3b-001

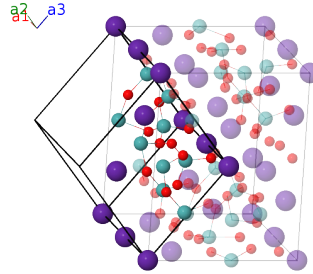


Prototype	Mo ₂ O ₇ Rb ₂
AFLOW prototype label	A2B7C2_oC88_40_abc_2b6c_a3b-001
ICSD	249126
CCDC	1715487
Pearson symbol	oC88
Space group number	40
Space group symbol	<i>Ama</i> 2

AFLOW prototype command aflow --proto=A2B7C2_oC88_40_abc_2b6c_a3b-001
 --params= $a, b/a, c/a, z_1, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, y_7, z_7, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(4a)	Mo I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_1 \hat{\mathbf{z}}$	(4a)	Mo I
$\mathbf{B}_3$	$= -z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4a)	Rb I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(4a)	Rb I
$\mathbf{B}_5$	$= \frac{1}{4} \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	Mo II
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	Mo II
$\mathbf{B}_7$	$= \frac{1}{4} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + (y_6 - z_6) \mathbf{a}_2 + (y_6 + z_6) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4b)	Rb II
$\mathbf{B}_{12}$	$= \frac{3}{4} \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 - (y_6 - z_6) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4b)	Rb II
$\mathbf{B}_{13}$	$= \frac{1}{4} \mathbf{a}_1 + (y_7 - z_7) \mathbf{a}_2 + (y_7 + z_7) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4b)	Rb III
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 - (y_7 + z_7) \mathbf{a}_2 - (y_7 - z_7) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4b)	Rb III
$\mathbf{B}_{15}$	$= \frac{1}{4} \mathbf{a}_1 + (y_8 - z_8) \mathbf{a}_2 + (y_8 + z_8) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4b)	Rb IV
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 - (y_8 + z_8) \mathbf{a}_2 - (y_8 - z_8) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4b)	Rb IV
$\mathbf{B}_{17}$	$= x_9 \mathbf{a}_1 + (y_9 - z_9) \mathbf{a}_2 + (y_9 + z_9) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Mo III
$\mathbf{B}_{18}$	$= -x_9 \mathbf{a}_1 - (y_9 + z_9) \mathbf{a}_2 - (y_9 - z_9) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Mo III
$\mathbf{B}_{19}$	$= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 + z_9) \mathbf{a}_2 - (y_9 - z_9) \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Mo III
$\mathbf{B}_{20}$	$= -(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 - z_9) \mathbf{a}_2 + (y_9 + z_9) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8c)	Mo III
$\mathbf{B}_{21}$	$= x_{10} \mathbf{a}_1 + (y_{10} - z_{10}) \mathbf{a}_2 + (y_{10} + z_{10}) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B}_{22}$	$= -x_{10} \mathbf{a}_1 - (y_{10} + z_{10}) \mathbf{a}_2 - (y_{10} - z_{10}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8c)	O III

$$\begin{aligned}
\mathbf{B}_{23} &= \begin{pmatrix} x_{10} + \frac{1}{2} \\ y_{10} - z_{10} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{10} + z_{10} \\ y_{10} - z_{10} \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 = a \left(x_{10} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{24} &= \begin{pmatrix} -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{10} - z_{10}) \mathbf{a}_2 + (y_{10} + z_{10}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{10} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{25} &= \begin{pmatrix} x_{11} \mathbf{a}_1 + (y_{11} - z_{11}) \mathbf{a}_2 + \\ (y_{11} + z_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{26} &= \begin{pmatrix} -x_{11} \mathbf{a}_1 - (y_{11} + z_{11}) \mathbf{a}_2 - \\ (y_{11} - z_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{27} &= \begin{pmatrix} \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_1 - (y_{11} + z_{11}) \mathbf{a}_2 - \\ (y_{11} - z_{11}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{11} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{28} &= \begin{pmatrix} -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{11} - z_{11}) \mathbf{a}_2 + (y_{11} + z_{11}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{11} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{29} &= \begin{pmatrix} x_{12} \mathbf{a}_1 + (y_{12} - z_{12}) \mathbf{a}_2 + \\ (y_{12} + z_{12}) \mathbf{a}_3 \end{pmatrix} = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{30} &= \begin{pmatrix} -x_{12} \mathbf{a}_1 - (y_{12} + z_{12}) \mathbf{a}_2 - \\ (y_{12} - z_{12}) \mathbf{a}_3 \end{pmatrix} = -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{31} &= \begin{pmatrix} \left(x_{12} + \frac{1}{2}\right) \mathbf{a}_1 - (y_{12} + z_{12}) \mathbf{a}_2 - \\ (y_{12} - z_{12}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{12} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{32} &= \begin{pmatrix} -\left(x_{12} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{12} - z_{12}) \mathbf{a}_2 + (y_{12} + z_{12}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{12} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{33} &= \begin{pmatrix} x_{13} \mathbf{a}_1 + (y_{13} - z_{13}) \mathbf{a}_2 + \\ (y_{13} + z_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{34} &= \begin{pmatrix} -x_{13} \mathbf{a}_1 - (y_{13} + z_{13}) \mathbf{a}_2 - \\ (y_{13} - z_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{35} &= \begin{pmatrix} \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_1 - (y_{13} + z_{13}) \mathbf{a}_2 - \\ (y_{13} - z_{13}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{13} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{36} &= \begin{pmatrix} -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{13} - z_{13}) \mathbf{a}_2 + (y_{13} + z_{13}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{13} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{37} &= \begin{pmatrix} x_{14} \mathbf{a}_1 + (y_{14} - z_{14}) \mathbf{a}_2 + \\ (y_{14} + z_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{38} &= \begin{pmatrix} -x_{14} \mathbf{a}_1 - (y_{14} + z_{14}) \mathbf{a}_2 - \\ (y_{14} - z_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{39} &= \begin{pmatrix} \left(x_{14} + \frac{1}{2}\right) \mathbf{a}_1 - (y_{14} + z_{14}) \mathbf{a}_2 - \\ (y_{14} - z_{14}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{14} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{40} &= \begin{pmatrix} -\left(x_{14} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{14} - z_{14}) \mathbf{a}_2 + (y_{14} + z_{14}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{14} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{41} &= \begin{pmatrix} x_{15} \mathbf{a}_1 + (y_{15} - z_{15}) \mathbf{a}_2 + \\ (y_{15} + z_{15}) \mathbf{a}_3 \end{pmatrix} = ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{42} &= \begin{pmatrix} -x_{15} \mathbf{a}_1 - (y_{15} + z_{15}) \mathbf{a}_2 - \\ (y_{15} - z_{15}) \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{43} &= \begin{pmatrix} \left(x_{15} + \frac{1}{2}\right) \mathbf{a}_1 - (y_{15} + z_{15}) \mathbf{a}_2 - \\ (y_{15} - z_{15}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{15} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{44} &= \begin{pmatrix} -\left(x_{15} - \frac{1}{2}\right) \mathbf{a}_1 + \\ (y_{15} - z_{15}) \mathbf{a}_2 + (y_{15} + z_{15}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{15} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O VIII}
\end{aligned}$$

References

- [1] Z. A. Solodovnikova and S. F. Solodovnikov, *Rubidium dimolybdate, $Rb_2Mo_2O_7$, and caesium dimolybdate, $Cs_2Mo_2O_7$* , Acta Crystallogr. Sect. C **62**, i53–i56 (2006), doi:10.1107/S0108270106014880.

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