Rb$_2$Mo$_2$O$_7$ Structure: A2B7C2_oC88_40_abc_2b6c_a3b-001
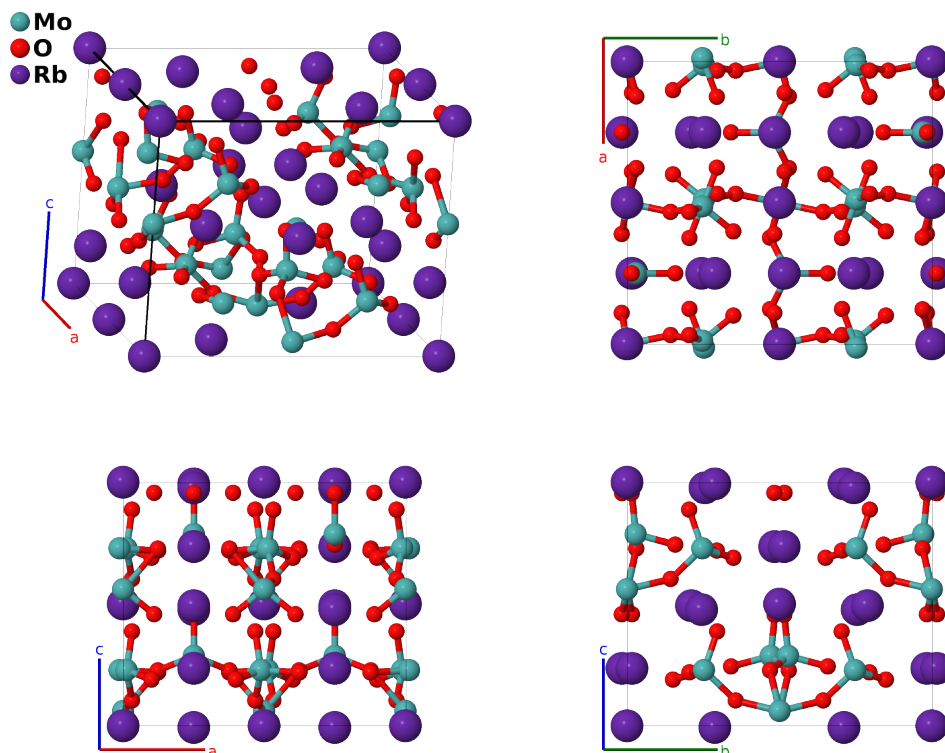
This structure originally had the label `A2B7C2_oC88_40_abc_2b6c_a3b`. Calls to that address will be redirected here.

https://aflow.org/p/CBWE

https://aflow.org/p/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
Pearson symbol	oC88
Space group number	40
Space group symbol	$Ama2$
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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$

$$\mathbf{a_3} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
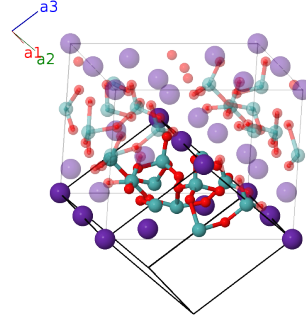
Basis vectors

		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
$\mathbf{B_2}$	$=$	$\tfrac{1}{2}\mathbf{a_1} - z_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Mo I
$\mathbf{B_3}$	$=$	$-z_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$cz_2\,\hat{\mathbf{z}}$	(4a)	Rb I
$\mathbf{B_4}$	$=$	$\tfrac{1}{2}\mathbf{a_1} - z_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Rb I
$\mathbf{B_5}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_3 - z_3)\,\mathbf{a_2} + (y_3 + z_3)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Mo II
$\mathbf{B_6}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_3 + z_3)\,\mathbf{a_2} - (y_3 - z_3)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4b)	Mo II
$\mathbf{B_7}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_4 - z_4)\,\mathbf{a_2} + (y_4 + z_4)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_8}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_4 + z_4)\,\mathbf{a_2} - (y_4 - z_4)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B_9}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_5 - z_5)\,\mathbf{a_2} + (y_5 + z_5)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_{10}}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_5 + z_5)\,\mathbf{a_2} - (y_5 - z_5)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B_{11}}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_6 - z_6)\,\mathbf{a_2} + (y_6 + z_6)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4b)	Rb II
$\mathbf{B_{12}}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_6 + z_6)\,\mathbf{a_2} - (y_6 - z_6)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4b)	Rb II
$\mathbf{B_{13}}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_7 - z_7)\,\mathbf{a_2} + (y_7 + z_7)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4b)	Rb III
$\mathbf{B_{14}}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_7 + z_7)\,\mathbf{a_2} - (y_7 - z_7)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4b)	Rb III
$\mathbf{B_{15}}$	$=$	$\tfrac{1}{4}\mathbf{a_1} + (y_8 - z_8)\,\mathbf{a_2} + (y_8 + z_8)\,\mathbf{a_3}$	$=$	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4b)	Rb IV
$\mathbf{B_{16}}$	$=$	$\tfrac{3}{4}\mathbf{a_1} - (y_8 + z_8)\,\mathbf{a_2} - (y_8 - z_8)\,\mathbf{a_3}$	$=$	$\tfrac{3}{4}a\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{19}}$	$=$	$\left(x_9 + \tfrac{1}{2}\right)\mathbf{a_1} - (y_9 + z_9)\,\mathbf{a_2} - (y_9 - z_9)\,\mathbf{a_3}$	$=$	$a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8c)	Mo III
$\mathbf{B_{20}}$	$=$	$-\left(x_9 - \tfrac{1}{2}\right)\mathbf{a_1} + (y_9 - z_9)\,\mathbf{a_2} + (y_9 + z_9)\,\mathbf{a_3}$	$=$	$-a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{23}}$	$=$	$\left(x_{10} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{10} + z_{10})\,\mathbf{a_2} - (y_{10} - z_{10})\,\mathbf{a_3}$	$=$	$a\left(x_{10} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8c)	O III
$\mathbf{B_{24}}$	$=$	$-\left(x_{10} - \tfrac{1}{2}\right)\mathbf{a_1} + (y_{10} - z_{10})\,\mathbf{a_2} + (y_{10} + z_{10})\,\mathbf{a_3}$	$=$	$-a\left(x_{10} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8c)	O III

$$\mathbf{B_{25}} = \begin{array}{l} x_{11}\,\mathbf{a_1} + (y_{11} - z_{11})\,\mathbf{a_2} + \\ (y_{11} + z_{11})\,\mathbf{a_3} \end{array} = ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O IV}$$

$$\mathbf{B_{26}} = \begin{array}{l} -x_{11}\,\mathbf{a_1} - (y_{11} + z_{11})\,\mathbf{a_2} - \\ (y_{11} - z_{11})\,\mathbf{a_3} \end{array} = -ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O IV}$$

$$\mathbf{B_{27}} = \begin{array}{l} \left(x_{11} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{11} + z_{11})\,\mathbf{a_2} - \\ (y_{11} - z_{11})\,\mathbf{a_3} \end{array} = a\left(x_{11} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O IV}$$

$$\mathbf{B_{28}} = \begin{array}{l} -\left(x_{11} - \tfrac{1}{2}\right)\mathbf{a_1} + \\ (y_{11} - z_{11})\,\mathbf{a_2} + (y_{11} + z_{11})\,\mathbf{a_3} \end{array} = -a\left(x_{11} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O IV}$$

$$\mathbf{B_{29}} = \begin{array}{l} x_{12}\,\mathbf{a_1} + (y_{12} - z_{12})\,\mathbf{a_2} + \\ (y_{12} + z_{12})\,\mathbf{a_3} \end{array} = ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O V}$$

$$\mathbf{B_{30}} = \begin{array}{l} -x_{12}\,\mathbf{a_1} - (y_{12} + z_{12})\,\mathbf{a_2} - \\ (y_{12} - z_{12})\,\mathbf{a_3} \end{array} = -ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O V}$$

$$\mathbf{B_{31}} = \begin{array}{l} \left(x_{12} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{12} + z_{12})\,\mathbf{a_2} - \\ (y_{12} - z_{12})\,\mathbf{a_3} \end{array} = a\left(x_{12} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O V}$$

$$\mathbf{B_{32}} = \begin{array}{l} -\left(x_{12} - \tfrac{1}{2}\right)\mathbf{a_1} + \\ (y_{12} - z_{12})\,\mathbf{a_2} + (y_{12} + z_{12})\,\mathbf{a_3} \end{array} = -a\left(x_{12} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O V}$$

$$\mathbf{B_{33}} = \begin{array}{l} x_{13}\,\mathbf{a_1} + (y_{13} - z_{13})\,\mathbf{a_2} + \\ (y_{13} + z_{13})\,\mathbf{a_3} \end{array} = ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VI}$$

$$\mathbf{B_{34}} = \begin{array}{l} -x_{13}\,\mathbf{a_1} - (y_{13} + z_{13})\,\mathbf{a_2} - \\ (y_{13} - z_{13})\,\mathbf{a_3} \end{array} = -ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VI}$$

$$\mathbf{B_{35}} = \begin{array}{l} \left(x_{13} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{13} + z_{13})\,\mathbf{a_2} - \\ (y_{13} - z_{13})\,\mathbf{a_3} \end{array} = a\left(x_{13} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VI}$$

$$\mathbf{B_{36}} = \begin{array}{l} -\left(x_{13} - \tfrac{1}{2}\right)\mathbf{a_1} + \\ (y_{13} - z_{13})\,\mathbf{a_2} + (y_{13} + z_{13})\,\mathbf{a_3} \end{array} = -a\left(x_{13} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VI}$$

$$\mathbf{B_{37}} = \begin{array}{l} x_{14}\,\mathbf{a_1} + (y_{14} - z_{14})\,\mathbf{a_2} + \\ (y_{14} + z_{14})\,\mathbf{a_3} \end{array} = ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VII}$$

$$\mathbf{B_{38}} = \begin{array}{l} -x_{14}\,\mathbf{a_1} - (y_{14} + z_{14})\,\mathbf{a_2} - \\ (y_{14} - z_{14})\,\mathbf{a_3} \end{array} = -ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VII}$$

$$\mathbf{B_{39}} = \begin{array}{l} \left(x_{14} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{14} + z_{14})\,\mathbf{a_2} - \\ (y_{14} - z_{14})\,\mathbf{a_3} \end{array} = a\left(x_{14} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VII}$$

$$\mathbf{B_{40}} = \begin{array}{l} -\left(x_{14} - \tfrac{1}{2}\right)\mathbf{a_1} + \\ (y_{14} - z_{14})\,\mathbf{a_2} + (y_{14} + z_{14})\,\mathbf{a_3} \end{array} = -a\left(x_{14} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VII}$$

$$\mathbf{B_{41}} = \begin{array}{l} x_{15}\,\mathbf{a_1} + (y_{15} - z_{15})\,\mathbf{a_2} + \\ (y_{15} + z_{15})\,\mathbf{a_3} \end{array} = ax_{15}\,\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VIII}$$

$$\mathbf{B_{42}} = \begin{array}{l} -x_{15}\,\mathbf{a_1} - (y_{15} + z_{15})\,\mathbf{a_2} - \\ (y_{15} - z_{15})\,\mathbf{a_3} \end{array} = -ax_{15}\,\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VIII}$$

$$\mathbf{B_{43}} = \begin{array}{l} \left(x_{15} + \tfrac{1}{2}\right)\mathbf{a_1} - (y_{15} + z_{15})\,\mathbf{a_2} - \\ (y_{15} - z_{15})\,\mathbf{a_3} \end{array} = a\left(x_{15} + \tfrac{1}{2}\right)\hat{\mathbf{x}} - by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VIII}$$

$$\mathbf{B_{44}} = \begin{array}{l} -\left(x_{15} - \tfrac{1}{2}\right)\mathbf{a_1} + \\ (y_{15} - z_{15})\,\mathbf{a_2} + (y_{15} + z_{15})\,\mathbf{a_3} \end{array} = -a\left(x_{15} - \tfrac{1}{2}\right)\hat{\mathbf{x}} + by_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} \qquad (8c) \qquad \text{O VIII}$$

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.