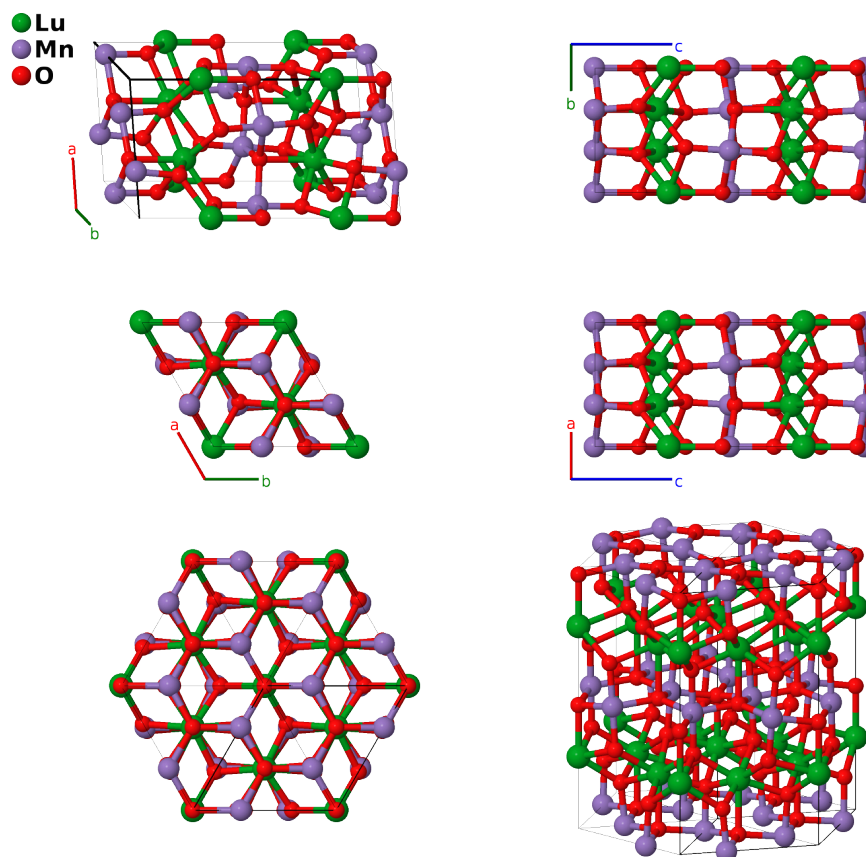


LuMnO₃ Structure: ABC3_hP30_185_ab_c_ab2c-001

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<https://aflow.org/p/YGS5>

https://aflow.org/p/ABC3_hP30_185_ab_c_ab2c-001



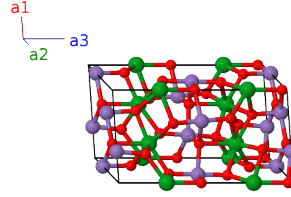
Prototype	LuMnO ₃
AFLOW prototype label	ABC3_hP30_185_ab_c_ab2c-001
ICSD	54767
Pearson symbol	hP30
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	<code>aflow --proto=ABC3_hP30_185_ab_c_ab2c-001 --params=a, c/a, z₁, z₂, z₃, z₄, x₅, z₅, x₆, z₆, x₇, z₇</code>

Other compounds with this structure

DyMnO₃, EuMnO₃, LuFeO₃, GdMnO₃, HoMnO₃, InMnO₃, TmFeO₃, YMnO₃

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Lu I
\mathbf{B}_2	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Lu I
\mathbf{B}_3	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_4	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_5	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Lu II
\mathbf{B}_6	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Lu II
\mathbf{B}_7	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	Lu II
\mathbf{B}_8	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4b)	Lu II
\mathbf{B}_9	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	O II
\mathbf{B}_{10}	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O II
\mathbf{B}_{11}	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4b)	O II
\mathbf{B}_{12}	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4b)	O II
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{14}	$= x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{15}	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + c z_5 \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{16}	$= -x_5 \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{17}	$= -x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_5 \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{18}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Mn I
\mathbf{B}_{19}	$= x_6 \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{20}	$= x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{21}	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} + c z_6 \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_6 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_6 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_6 \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{24}	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O III
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{26}	$= x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{27}	$= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} + c z_7 \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{28}	$= -x_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_7 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{29}	$= -x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_7 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O IV
\mathbf{B}_{30}	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	O IV

References

- [1] B. B. van Aken, A. Meetsma, and T. T. M. Palstra, *Hexagonal LuMnO₃ Structure*, Acta Crystallogr. Sect. E **57**, i101–i03 (2001), doi:10.1107/S1600536801015896.