

La₃NbO₇ Structure:

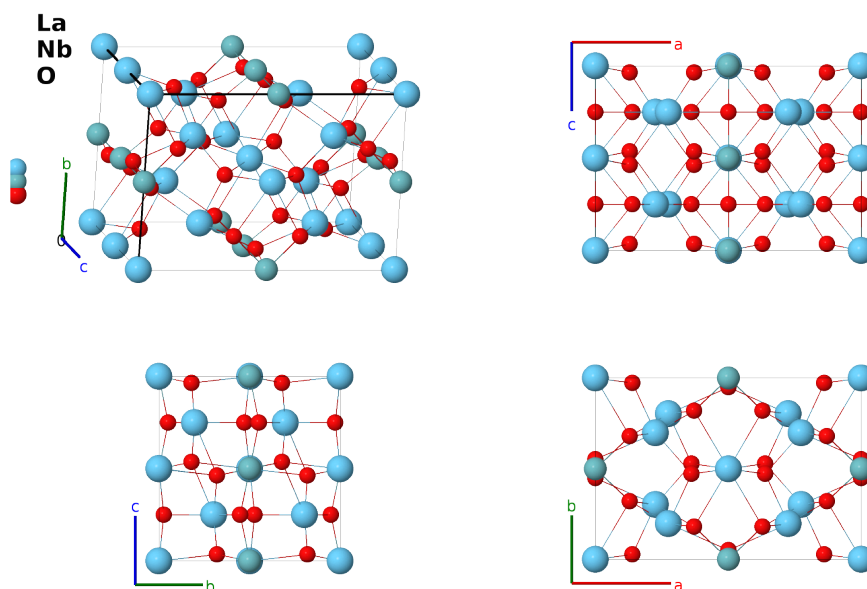
A3BC7_oC44_63_ag_b_cgh-001

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<https://aflow.org/prototype-encyclopedia/U2R2>

https://aflow.org/prototype-encyclopedia/A3BC7_oC44_63_ag_b_cgh-001



Prototype	La ₃ NbO ₇
AFLOW prototype label	A3BC7_oC44_63_ag_b_cgh-001
ICSD	10058
CCDC	1594943
Pearson symbol	oC44
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A3BC7_oC44_63_ag_b_cgh-001</code> <code>--params=a, b/a, c/a, y₃, x₄, y₄, x₅, y₅, x₆, y₆, z₆</code>

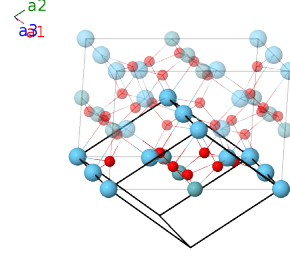
Other compounds with this structure

Eu₃IrO₇, Nd₃NbO₇, Pr₃IrO₇

- (Rossell, 1979) give $z_6 = -0.036$ for the O III (16h) site, but the corresponding CIF in the ICSD entry sets $z_6 = +0.036$. We use the ICSD value. In reality the difference in position is only about 0.5Å.

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
$\mathbf{B}_1$	$=$	0	$=$	0	La I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$	La I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	Nb I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	Nb I
$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	O I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	O I
$\mathbf{B}_7$	$=$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	La II
$\mathbf{B}_8$	$=$	$-(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	La II
$\mathbf{B}_9$	$=$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	La II
$\mathbf{B}_{10}$	$=$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	La II
$\mathbf{B}_{11}$	$=$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	O II
$\mathbf{B}_{12}$	$=$	$-(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	O II
$\mathbf{B}_{13}$	$=$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	O II
$\mathbf{B}_{14}$	$=$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	O II
$\mathbf{B}_{15}$	$=$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	O III
$\mathbf{B}_{16}$	$=$	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	O III
$\mathbf{B}_{17}$	$=$	$-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	O III
$\mathbf{B}_{18}$	$=$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	O III
$\mathbf{B}_{19}$	$=$	$-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	O III
$\mathbf{B}_{20}$	$=$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	O III
$\mathbf{B}_{21}$	$=$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	O III

$$\mathbf{B}_{22} = - (x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3 = -ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (16h) \quad \text{O III}$$

References

- [1] H. J. Rossell, *Fluorite-related phases* Ln_3MO_7 , Ln = *rare earth*, Y or Sc, M = Nb, Sb, or Ta: II. Structure determination, J. Solid State Chem. **27**, 115–122 (1979), doi:10.1016/0022-4596(79)90150-6.

Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 10058.

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