

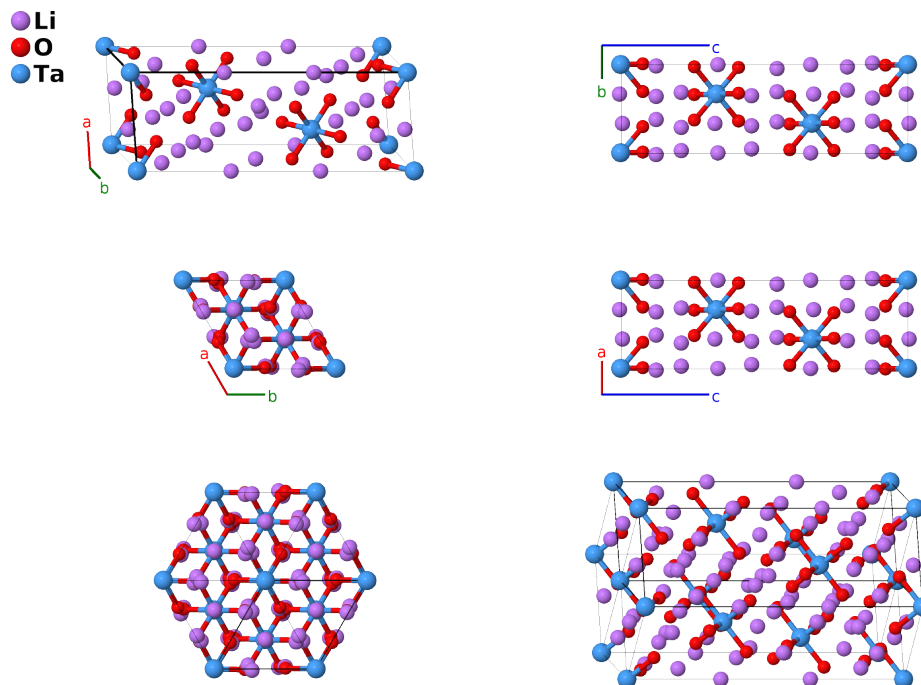
Li₇TaO₆ Structure: A8B6C_hR15_148_cf_f_a-001

This structure originally had the label A8B6C_hR15_148_cf_f_a. Calls to that address will be redirected here.

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<https://afLOW.org/p/L1GH>

https://afLOW.org/p/A8B6C_hR15_148_cf_f_a-001

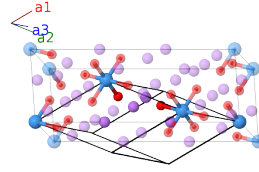


Prototype	Li ₇ O ₆ Ta
AFLOW prototype label	A8B6C_hR15_148_cf_f_a-001
ICSD	74949
Pearson symbol	hR15
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<pre>afLOW --proto=A8B6C_hR15_148_cf_f_a-001 --params=a, c/a, x₂, x₃, y₃, z₃, x₄, y₄, z₄</pre>

- The Li-I (2c) site is half-occupied.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(1a)	Ta I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Li I
\mathbf{B}_3	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Li I
\mathbf{B}_4	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_5	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_6	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_7	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_8	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_9	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	Li II
\mathbf{B}_{10}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{11}	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{12}	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{13}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{14}	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I
\mathbf{B}_{15}	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O I

References

- [1] G. Wehrum and R. Hoppe, *Zur Kenntnis 'Kationen-reicher' Tantalate Über $\text{Li}_7[\text{TaO}_6]$* , Z. Anorganische und Allgemeine Chemie **620**, 659–664 (1994), doi:10.1002/zaac.19946200414.

Found in

- [1] L. Kahle, X. Cheng, T. Binninger, S. D. Lacey, A. Marcolongo, F. Zipoli, E. Gilardi, C. Villevieille, M. E. Kazzi, N. Marzari, and D. Pergolesi, *The solid-state Li-ion conductor Li_7TaO_6 : A combined computational and experimental study*, Solid State Ion. **347**, 115226 (2020), doi:10.1016/j.ssi.2020.115226.