α-$LiIO_3$ Structure: ABC3_hP10_173_b_a_c-001

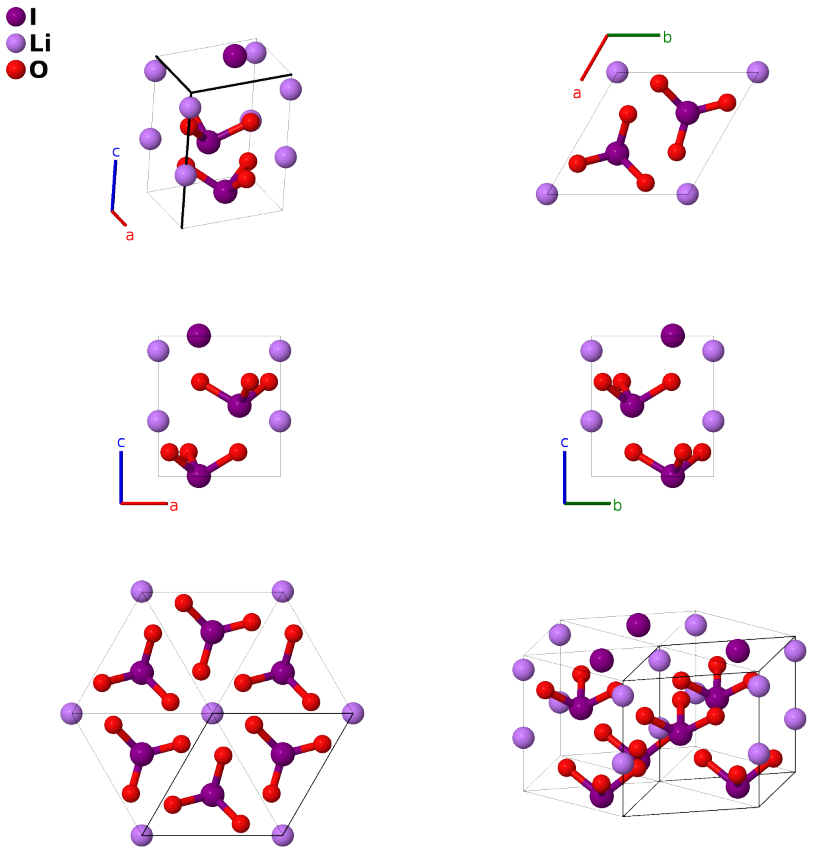
This structure originally had the label `ABC3_hP10_173_b_a_c`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/p/DF6Y

https://aflow.org/p/ABC3_hP10_173_b_a_c-001



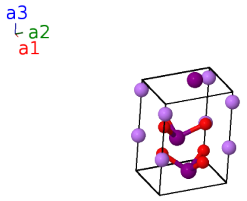
Prototype	$ILiO_3$
AFLOW prototype label	ABC3_hP10_173_b_a_c-001
ICSD	14377
Pearson symbol	hP10
Space group number	173
Space group symbol	$P6_3$
AFLOW prototype command	`aflow --proto=ABC3_hP10_173_b_a_c-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, z_3$

- $LiIO_3$ is known to exist in three forms:

- α-$LiIO_3$, stable below 470K:
  - (Zachariasen, 1931) originally determined that the structure of α-$LiIO_3$ was in space group $P6_322$ #182, which (Hermann, 1937) designated *Strukturbericht* $E2_3$.
  - (Rosenzweig, 1966) subsequently determined that this structure was incorrect because of the small sample size, and determined that the true structure was in space group $P6_3$ #173. (this structure)
- β-$LiIO_3$, stable from 573K up to the melting point at 708K.
- γ-$LiIO_3$, stable between the α- and β-phases, with an orthorhombic structure in space group $Pna2_1$ #33.
- The ICSD entry uses a = 5.485Å rather than the value 5.1815Å found in (Rosenzweig, 1966). This is perhaps influenced bo (De Boer, 1966) (ICSD 14344) and the original work of (Zachariasen, 1931), who both found values nearer 5.48Å. For now we will continue to use 5.1815Å.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	I I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	I I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_7}$	=	$-(x_3-y_3)\,\mathbf{a}_1-x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I
$\mathbf{B_{10}}$	=	$(x_3-y_3)\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O I

References

[1] A. Rosenzweig and B. Morosin, *A reinvestigation of the crystal structure of $LiIO_3$*, Acta Cryst. **20**, 758–761 (1966), doi:10.1107/S0365110X66001804.

[2] W. H. Zachariasen and F. A. Barta, *Crystal Structure of Lithium Iodate*, Phys. Rev. **37**, 1626–1630 (1931), doi:10.1103/PhysRev.37.1626.

[3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[4] J. L. D. Boer, F. van Bolhuis, and R. V. Olthof-Hazekamp, *Re-investigation of the crystal structure of lithium iodate*, Acta Crystallographica **21**, 841–843 (1966), doi:10.1107/S0365110X66004031.