$E2_3$ ($LiIO_3$) Structure (*Obsolete*): ABC3_hP10_182_c_b_g-001

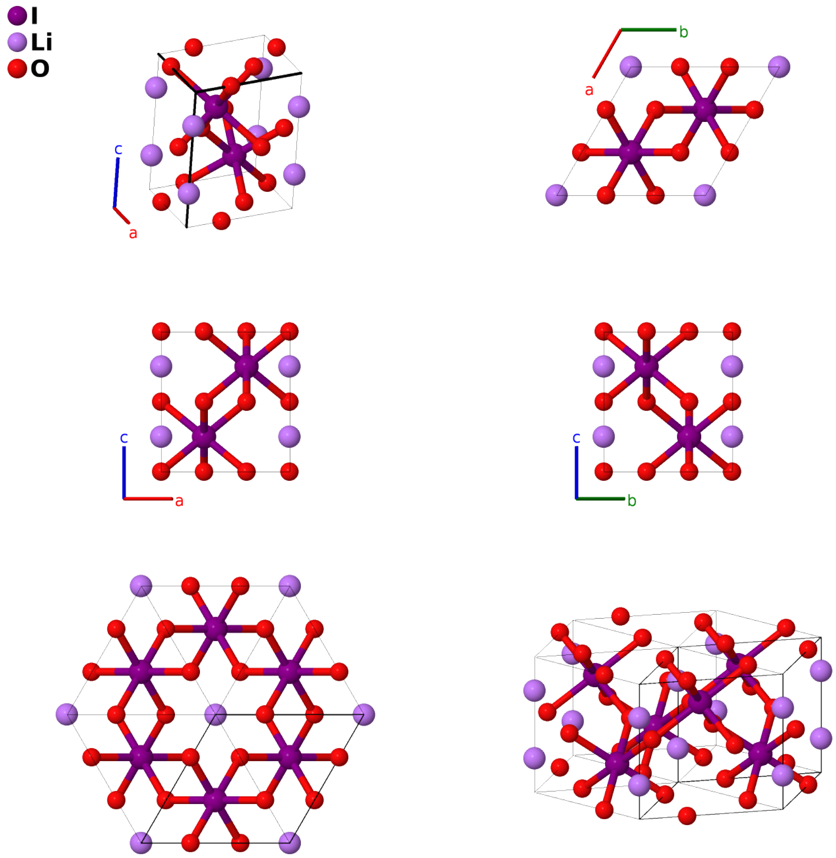
This structure originally had the label `ABC3_hP10_182_c_b_g`. Calls to that address will be redirected here.

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/6B26

https://aflow.org/p/ABC3_hP10_182_c_b_g-001

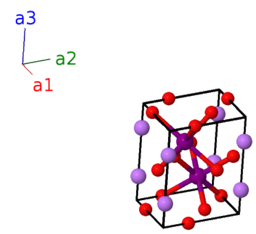


Prototype	$ILiO_3$
AFLOW prototype label	ABC3_hP10_182_c_b_g-001
***Strukturbericht* designation**	$E2_3$
ICSD	20012
Pearson symbol	hP10
Space group number	182
Space group symbol	$P6_322$
AFLOW prototype command	`aflow --proto=ABC3_hP10_182_c_b_g-001 --params=`$a, c/a, x_3$

- $LiIO_3$ 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* $E2_3$. (this structure)
  - (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.
- 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 is from (Butolin, 1975). If we can obtain a copy we will report on their research into this structure.

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Li I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Li I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	I I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6g)	O I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6g)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(6g)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	O I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	O I

References

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

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

[3] S. A. Butolin, L. F. Belova, R. N. Samoylova, O. M. Kotenko, I. M. Dokuchaeva, and N. M. Ivanova, *Optical and physico-chemical properties of* $\alpha LiIO_3$ *monocrystal*, Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy **11**, 862–865 (1975).

Found in

[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.