

LiO Structure:

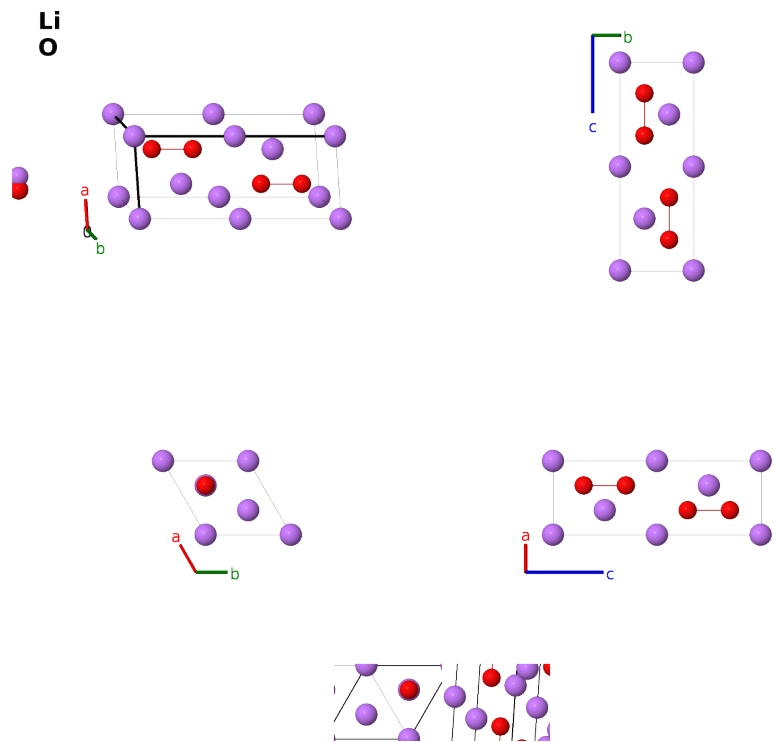
AB_hP8_194_ac_f-003

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<https://aflow.org/prototype-encyclopedia/JV7G>

https://aflow.org/prototype-encyclopedia/AB_hP8_194_ac_f-003



Prototype	LiO
AFLOW prototype label	AB_hP8_194_ac_f-003
ICSD	25530
CCDC	1601184
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB_hP8_194_ac_f-003 --params=a, c/a, z₃</code>

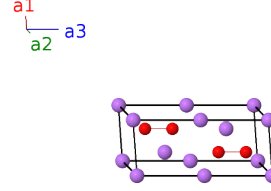
Other compounds with this structure

β -KTe, β -NaS, β -NaTe

- (Fehér, 1953) and (Föppl, 1957) presented competing structures for LiO, both in space group $P\bar{6}$ #174. First-principles calculation by (Cota, 2005) and (Chen, 2011) suggest that the Föppl structure is correct, but show that the proper space group is $P6_3/mmc$ #194. This is generally held to be the correct structure, *e.g.* (Jain, 2013). We use the symmetrization of Föppl’s original data made by (Cota, 2005).
- The ICSD entry is from Föppl, 1957), updated to make the space group $P6_3/mmc$.

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
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Li I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2a) 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) Li II
$\mathbf{B}_4$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c) Li II
$\mathbf{B}_5$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4f) O I
$\mathbf{B}_6$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_3 + \frac{1}{2})\hat{\mathbf{z}}$	(4f) O I
$\mathbf{B}_7$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4f) O I
$\mathbf{B}_8$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_3 - \frac{1}{2})\hat{\mathbf{z}}$	(4f) O I

References

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- [1] M. K. Y. Chan, E. L. Shirley, N. K. Karan, M. Balasubramanian, Y. Ren, J. P. Greeley, and T. T. Fister, *Structure of Lithium Peroxide*, J. Phys. Chem. Lett. **2**, 2483–2486 (2011), doi:10.1021/jz201072b.

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