

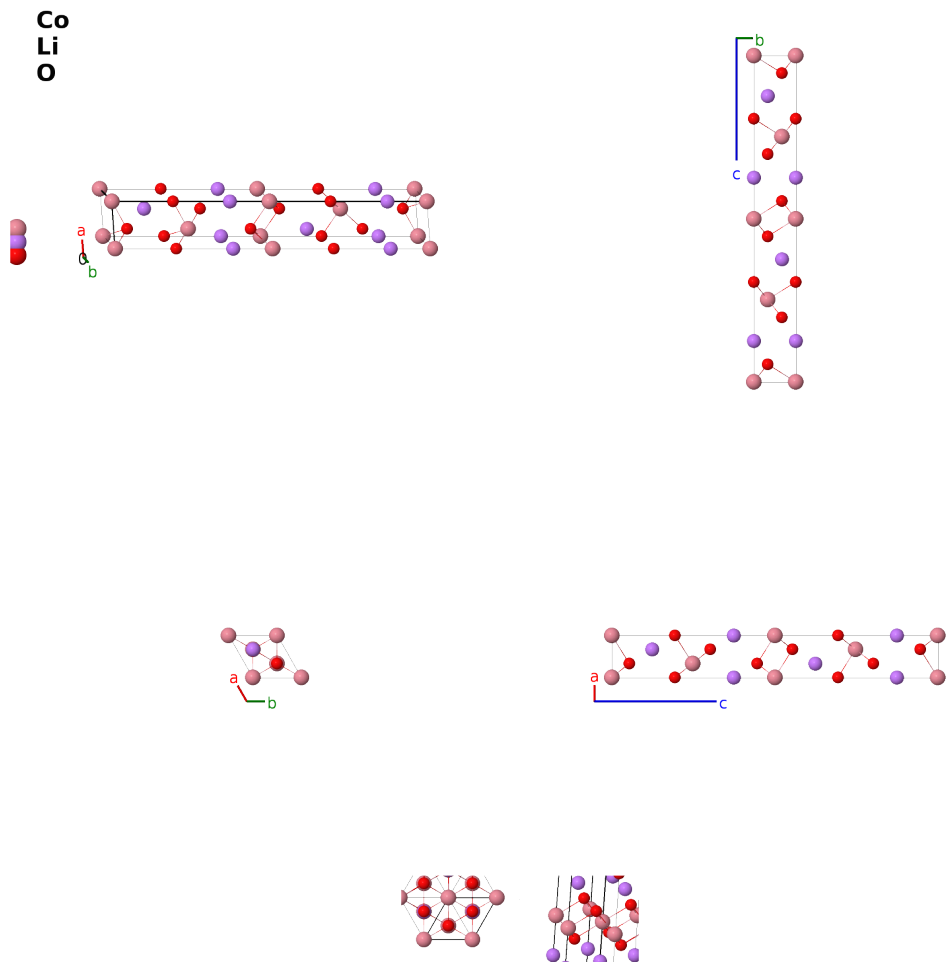
O4-LiCoO₂ Structure: ABC2_hP16_186_ab_ab_a3b-001

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<https://aflow.org/prototype-encyclopedia/3DYH>

https://aflow.org/prototype-encyclopedia/ABC2_hP16_186_ab_ab_a3b-001

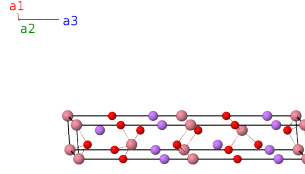


Prototype	CoLiO ₂
AFLOW prototype label	ABC2_hP16_186_ab_ab_a3b-001
Pearson symbol	hP16
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	<code>aflow --proto=ABC2_hP16_186_ab_ab_a3b-001</code> <code>--params=a, c/a, z₁, z₂, z₃, z₄, z₅, z₆, z₇, z₈</code>

- LiCoO₂ structures are defined by the stacking arrangement of the edge-shared CoO₆ octahedra. In addition, the O3 and O4 structures may have stacking faults. (Yabuuchi, 2013) prepared all of these structures by treating “OP4”-LiNaCo₂O₄ using ion-exchange in aqueous media.
 - In O2-LiCoO₂ the octahedra are stacked in an alternating cubic/hexagonal arrangement.
 - In O3-LiCoO₃ the octahedra are stacked in a cubic arrangement, taking on the α -NaFeO₂ structure.
 - In O4-LiCoO₂ (this structure) the octahedra alternate between O2 and O4.
- In this sample 10% of the lithium sites are vacant.
- Space group $P6_3mc$ #186 does not specify the origin of the z -coordinate. We fix it here by setting $z_1 = 0$.

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
$\mathbf{B}_1$	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_2$	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B}_3$	$z_2 \mathbf{a}_3$	=	$cz_2 \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_4$	$(z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_5$	$z_3 \mathbf{a}_3$	=	$cz_3 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_6$	$(z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_7$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B}_8$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Co II
$\mathbf{B}_9$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2b)	Li II
$\mathbf{B}_{10}$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Li II
$\mathbf{B}_{11}$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_{12}$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_{13}$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B}_{14}$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B}_{15}$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(2b)	O IV
$\mathbf{B}_{16}$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O IV

References

- [1] N. Yabuuchi, Y. Kawamoto, R. Hara, T. Ishigaki, A. Hoshikawa, M. Yonemura, T. Kamiyama, and S. Komaba, *A Comparative Study of LiCoO_2 Polymorphs: Structural and Electrochemical Characterization of O2-, O3-, and O4-type Phases*, Inorg. Chem. **52**, 9131–9142 (2013), doi:10.1021/ic4013922.

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