O2-$LiCoO_2$ Structure: ABC2_hP8_186_b_b_ab-001

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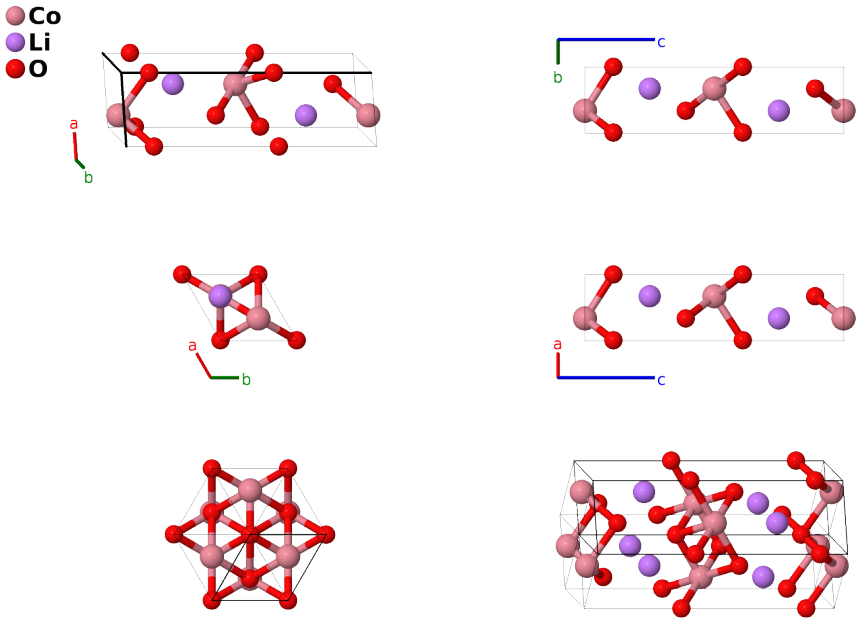
https://aflow.org/p/ABC2_hP8_186_b_b_ab-001



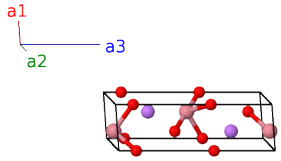
Prototype	$CoLiO_2$
AFLOW prototype label	ABC2_hP8_186_b_b_ab-001
ICSD	none
Pearson symbol	hP8
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=ABC2_hP8_186_b_b_ab-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

- $LiCoO_2$ structures are defined by the stacking arrangement of the edge-shared CoO_6 octahedra. In addition, the O3 and O4 structures may have stacking faults. (Yabuuchi, 2013) prepared all of these structures by treating "OP4"-$LiNaCo_2O_4$ using ion-exchange in aqueous media.
  - In O2-$LiCoO_2$ (this structure) the octahedra are stacked in an alternating cubic/hexagonal arrangement.
  - In O3-$LiCoO_3$ the octahedra are stacked in a cubic arrangement, taking on the α-$NaFeO_2$ structure.
  - In O4-$LiCoO_2$ the octahedra alternate between O2 and O4.
- (Delmas, 1982) give the composition of this sample as $Li_{0.93}CoO_{1.96}$. They state that the system is in space group $P3m1$ #156, but the coordinates they give imply that all of the lithium and cobalt atoms are in equivalent positions, and the space group becomes $P6_3mc$ #186.

- Space group $P6_3mc$ #186 does not specify the origin of the z-coordinate. We fix it here by setting $z_2 = 0$.

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)	O 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)	O 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)	Co 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)	Co I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Li I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Li 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)	O II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O II

References

[1] C. Delmas, J.-J. Braconnier, and P. Hagenmuller, *A new variety of $LiCoO_2$ with an unusual oxygen packing obtained by exchange reaction*, Mater. Res. Bull. **17**, 117–123 (1982), doi:10.1016/0025-5408(82)90192-1.

Found in

[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.