# O4-$LiCoO_2$ Structure: ABC2_hP16_186_ab_ab_a3b-001

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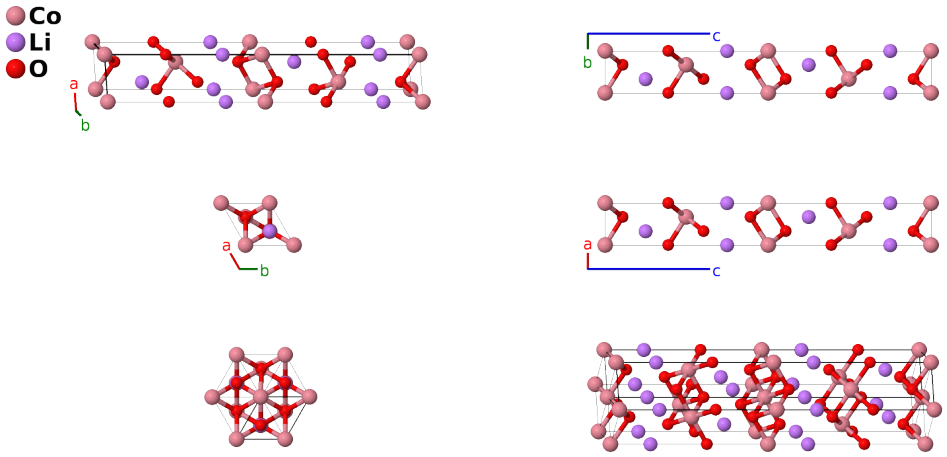
https://aflow.org/p/3DYH

https://aflow.org/p/ABC2_hP16_186_ab_ab_a3b-001

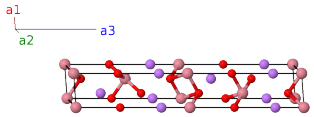



| | |
|---|---|
| **Prototype** | $CoLiO_2$ |
| **AFLOW prototype label** | ABC2_hP16_186_ab_ab_a3b-001 |
| **ICSD** | none |
| **Pearson symbol** | hP16 |
| **Space group number** | 186 |
| **Space group symbol** | $P6_3mc$ |
| **AFLOW prototype command** | `aflow --proto=ABC2_hP16_186_ab_ab_a3b-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8$ |

- $LiCoO_2$ 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-$LiCoO_2$ 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 $\alpha$-$NaFeO_2$ structure.
  - In O4-$LiCoO_2$ (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

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (2a) | Co 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) | Co I |
| $\mathbf{B_3}$ | = | $z_2\,\mathbf{a}_3$ | = | $cz_2\,\hat{\mathbf{z}}$ | (2a) | Li I |
| $\mathbf{B_4}$ | = | $\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2a) | Li I |
| $\mathbf{B_5}$ | = | $z_3\,\mathbf{a}_3$ | = | $cz_3\,\hat{\mathbf{z}}$ | (2a) | O I |
| $\mathbf{B_6}$ | = | $\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_8}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2b) | 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 |
| $\mathbf{B_{10}}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{12}}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{14}}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_{16}}$ | = | $\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (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.