

LiCoO ₂	<i>hP8</i>	(186) <i>P6₃mc</i> – b ³ a
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LiCoO₂ O2-type [1]

Structural features: Close-packed O layers in hc stacking; Co and Li in octahedral voids in alternating interlayers.

Carlier D. et al. (2001) [1]

Co_{0.94}LiO_{1.88}

$a = 0.28025$, $c = 0.95358$ nm, $c/a = 3.403$, $V = 0.0649$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Co1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.1081	0.94	octahedron O ₆
Li2	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.3671		octahedron O ₆
O3	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.7165	0.93	trigonal prism Co ₃ Li ₃
O4	<i>2a</i>	<i>3m.</i>	0	0	0.0	0.95	octahedron Co ₃ Li ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.8919

Experimental: powder, diffractometer, neutrons, R_B = 0.048, T = 300 K

References: [1] Carlier D., Saadoune I., Croguennec L., Menetrier M., Suard E., Delmas C. (2001), Solid State Ionics 144, 263-276.