

LiCoO <sub>2</sub>	<i>hP10</i>	(186) <i>P6<sub>3</sub>mc</i> – b <sup>3</sup> a <sup>2</sup>
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**LiCoO<sub>2</sub> O2-type** [1]

Structural features: Close-packed O layers in hc stacking; Co and main part of Li in octahedral voids, additional Li in tetrahedral voids (displaced from the center).

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

Co<sub>0.94</sub>Li<sub>1.03</sub>O<sub>1.88</sub>

*a* = 0.28025, *c* = 0.95358 nm, *c/a* = 3.403, *V* = 0.0649 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Li1	2 <i>b</i>	3 <i>m.</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.019		
O2	2 <i>b</i>	3 <i>m.</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.3684	0.93	tricapped trigonal prism Co <sub>3</sub> Li <sub>6</sub>
Co3	2 <i>b</i>	3 <i>m.</i>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.76	0.94	octahedron O <sub>6</sub>
Li4	2 <i>a</i>	3 <i>m.</i>	0	0	0.0	0.03	
O5	2 <i>a</i>	3 <i>m.</i>	0	0	0.1519	0.95	

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.24

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.048, T = 300 K

Remarks: Metastable phase. Short interatomic distances for partly occupied site(s).

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