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Determination of interlayer mixing and oxygen non-stoichiometry in LiNi0.8Mn0.1Co0.1O2-δ using powder diffraction data

Abstract

The effect of preparation conditions, temperature and atmosphere, on oxygen stoichiometry and interlayer cation mixing in the layered rock salt material LiNi0.8Mn0.1Co0.1O2-δ has been investigated using X-Ray powder diffraction, including Rietveld refinement. Interlayer mixing occurs as a direct consequence of oxygen deficiency; samples with least oxygen deficiency and most cation order were obtained on firing in O2 at ~ 900 - 950°C

Keywords

Interlayer mixing; Layered rock salt; Lithium ion batteries; Oxygen non-stoichiometry; Rietveld refinement