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Structure refinement strategy of Li-based complex oxides using GSAS-EXPGUI software package

Abstract

This paper discussed refinement strategy that been used to reveal crystallographic properties of lithium-based complex oxides with layered rock salt structure. Rietveld analysis using XRD data was used to determine the amount of interlayer mixing and estimate oxygen contents. The structural model and refinement methodology was controlled and validated initially using a standard sample. Thus, this paper summarized structure refinement strategy that been used to quantify the degree of cation order associated with interlayer mixing and investigate the sensitivity of laboratory XRD data to oxygen non-stoichiometry that recently published elsewhere

Keywords

Layered rock salt structure; Oxygen non-stoichiometry; Rietveld refinement