Structural and Magnetic Characterization of Mixed Oxides: A Study of Li-Ni-O and Li-Mn-O Systems

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The present paper details the way to determine the cation distribution in mixed oxides with transition ions from the diffraction and magnetic susceptibility data. This approach allows one to determine phase abundances and phase compositions by two combined procedures. By X-ray diffraction Rietveld profile refinement and magnetic susceptibility data analysis it is possible to estimate the ratio and the occupancy factor of paramagnetic ions in different oxidation states. A brief discussion of practical cases is reported. In the Li-Ni-O system the lithium cationic fraction of the ordered phase $Li_{2x}Ni_{2-2x}O_2$ increases monotonically with the total lithium fraction x_t for $0.31 \le x_t \le 0.46$. In the Li-Mn-O system for $0.36 \le x_t \le 0.53$ the Li_2MnO_3 fraction has been determined, and for the coexistent $Li[Li_yMn_{2-y}]O_4$ spinel phase the dependence of y on x_t has been evaluated.

Key words: X-ray Powder Diffraction; Magnetic Susceptibility; Lithium Nickel Oxides; Lithium Manganese Oxides; Lithium Manganese Spinel.