

Investigation of Microscopic Crystal Field in Co-Doped Lithium-Iron Phosphate

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We present the study on the structural and the magnetic properties of LiFePO_4 and $\text{LiFe}_{0.8}\text{Co}_{0.2}\text{PO}_4$. The crystal structure was determined to be orthorhombic with space group $Pnma$ by Rietveld refinement method. We have observed the increase in the lattice constants with Co^{2+} ion substituted. The Mössbauer spectra of olivine LiFePO_4 and $\text{LiFe}_{0.8}\text{Co}_{0.2}\text{PO}_4$ have shown distorted line broadening below T_N . In order to explain the observed line broadening, we have analyzed the Mössbauer spectra by considering the full Hamiltonian for the ^{57}Fe nucleus, and both the magnetic dipole and the electric quadrupole interactions. Also, we have observed the anomalous change in the electric quadrupole splitting near the T_N .

Index Terms—Crystal field, Mössbauer spectroscopy, olivine structure.