

Temperature dependent valence states and magnetic properties of lithium delithiated $\text{Li}_{0.59}\text{FePO}_4$

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Polycrystalline samples of $\text{Li}_{0.59}\text{FePO}_4$ were prepared by oxidation reaction of pure LiFePO_4 , and temperature dependent valence states and magnetic properties were studied. X-ray diffraction patterns showed a biphasic olivine-type orthorhombic structure (space group: $Pnma$) where triphylite (LiFePO_4) and heterosite (FePO_4) coexisted. Also, we have observed the biphasic antiferromagnetic ordering of triphylite and heterosite with different antiferromagnetic to paramagnetic ordering transition temperatures. Mössbauer spectra of $\text{Li}_{0.59}\text{FePO}_4$ showed a two-phase asymmetrical eight line pattern due to the different electric quadrupole interactions in triphylite and heterosite. The iron ions of triphylite and heterosite are at Fe^{2+} ($3d^6$) and the Fe^{3+} ($3d^5$) valence state. Also the large value of ΔE_Q for the triphylite phase was originated from the asymmetric charge distribution of FeO_6 . These results indicate that the charge distributions around the Fe nucleus in the triphylite are more asymmetric because of the contribution from the crystal field and the ion valence state. © 2010 American Institute of Physics. [doi:10.1063/1.3337680]