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Mössbauer Studies of Olivine $Fe_{1-y}Mn_yPO_4$

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The olivine-structured $Fe_{1-y}Mn_yPO_4$ (y = 0.0, 0.1, and 0.3), a possible cathode material for lithium-ion secondary battery, has been studied by using x-ray diffraction (XRD) and Mössbauer spectroscopy. These $Fe_{1-y}Mn_yPO_4$ samples were prepared by using the chemical lithium deintercalation process from $LiFe_{1-y}Mn_yPO_4$. The crystal structures of the $Fe_{1-y}Mn_yPO_4$ samples were determined to be orthorhombic (space group *Pnma*) at room temperature by using the Rietveld refinement method. From the Mössbauer spectra at room temperature, the electric quadrupole splitting (ΔE_Q) and the isomer shift (δ) values of the $Fe_{1-y}Mn_yPO_4$ were determined to be ΔE_Q = 1.512 mm/s, and δ = 0.31 mm/s for y = 0.0, ΔE_Q = 1.502 mm/s, and δ = 0.31 mm/s for y = 0.1, and ΔE_Q = 1.382 mm/s, and δ = 0.31 mm/s for y = 0.3. The difference in the ΔE_Q values for $Fe_{1-y}Mn_yPO_4$ samples with varying Mn concentrations can be explained by the change in the exchange interaction due to the dependence of the asymmetry in the FeO_6 octahedral sites on the Mn concentration.

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