

## Neutron Diffraction and Mössbauer Studies of $\text{LiFePO}_4$

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The crystal structure of  $\text{LiFePO}_4$  has been determined to be orthorhombic ( $Pnma$ ) from neutron diffraction measurements. The temperature dependence of the magnetization was measured by using a SQUID magnetometer. The microscopic interaction was investigated with  $^{57}\text{Fe}$  Mössbauer spectroscopy. At temperatures below  $T_N = 51$  K,  $\text{LiFePO}_4$  exhibited an anti-ferromagnetic behavior while at temperatures below 23 K, we observed abrupt increases in the magnetization and the magnetic hyperfine field ( $H_{hf}$ ). The electric quadrupole splitting ( $\Delta E_Q$ ) reached its maximum value at 23 K and decreased steadily with decreasing temperature below 23 K. This indicated that the orbital angular momentum  $L$  was quenched by the strong crystalline field in the asymmetric octahedral structure at temperatures above 23 K.  $\Delta E_Q$  decreased due to spin-orbit coupling, and the orbital angular momentum contribution enhanced  $H_{hf}$  at temperatures below 23 K.

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