

## Temperature dependent magnetic structure of lithium delithiated $\text{Li}_x\text{FeSO}_4\text{F}$ ( $x = 0, 1$ ) by Mössbauer spectroscopy

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Recently, lithium iron sulfate compounds have been highly considered for a positive electrode material for lithium ion batteries. In this work,  $\text{LiFeSO}_4\text{F}$  and the fully delithiated  $\text{FeSO}_4\text{F}$  were prepared by the ionothermal process and chemical oxidation reaction method. The  $\text{Li}_x\text{FeSO}_4\text{F}$  ( $x = 0, 1$ ) samples show the triclinic structure with  $P-1$  space group. In the case of delithiated  $\text{FeSO}_4\text{F}$ , changes in lattice parameters were observed due to the disappearance of the Li site while maintaining the triclinic structure. Temperature-dependent magnetic susceptibility curves show the antiferromagnetic (AFM) structure with the ordering temperature of 28 K for  $\text{LiFeSO}_4\text{F}$  and 99 K for  $\text{FeSO}_4\text{F}$ . Also, temperature-dependent Mössbauer spectra of  $\text{LiFeSO}_4\text{F}$  below  $T_N$  were fitted with two-sets of eight Lorentzian indicating the existence of two different types of  $\text{Fe}^{2+}$  ions due to the different hyperfine and electric quadrupole interactions. With the lithium delithiated, the  $\text{Fe}^{3+}$  iron ions in  $\text{FeSO}_4\text{F}$  exhibit two-sets of six-line patterns due to the electron transfer in  $\text{FeO}_4\text{F}_2$  site by lithium delithiation. These suggest that the different AFM ordering in  $\text{Li}_x\text{FeSO}_4\text{F}$  can be originated from the  $\text{Fe}^{2+}/\text{Fe}^{3+}$  magnetic ions with different charge distributions and spin contributions. © 2012 American Institute of Physics. [doi:10.1063/1.3677865]