

Determination of magnetic structure in $\text{LiFe}_{1-x}\text{Mn}_x\text{PO}_4$ by neutron powder diffraction

Zakiah Mohamed^{a,c}, Chris D. Ling^a, Maxim Avdeev^b,

^a School of Chemistry, The University of Sydney, NSW 2006, Australia.

^b Bragg Institute, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia.

^c Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Malaysia.

Lithium orthophosphates $\text{LiFe}_{1-x}\text{Mn}_x\text{PO}_4$ ($x=0, 0.2, 0.4, 0.6, 0.8, 1$) were successfully synthesized using a solid state reaction method and characterized by X-ray powder diffraction, neutron powder diffraction and magnetic susceptibility measurement. Structure refinements against powder diffraction data were carried out in the orthorhombic space group $Pnma$. Magnetic susceptibility measurements showed all samples undergo AFM ordering at low temperature. Mn^{2+} doped in Fe-site resulted the below Néel temperature T_N decreased from 52 K ($x=0$) to 38 K ($x=1$). The magnetic structures from neutron powder diffraction data confirmed the AFM ordering with magnetic space group $Pnma'$ for LiFePO_4 and all intermediate compounds, with a propagation vector $k = (0\ 0\ 0)$. Only the pure LiMnPO_4 sample behaves differently showing an AFM ordering with magnetic space group $Pn'm'a'$. A weak ferromagnetic component in the c-direction also observed in LiMnPO_4 .

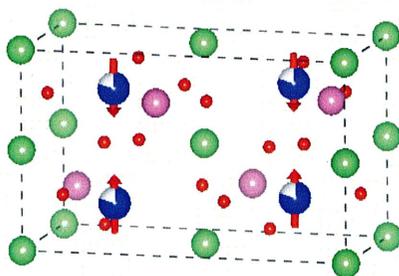


Fig. 1: Magnetic structure of $\text{LiFe}_{0.8}\text{Mn}_{0.2}\text{PO}_4$ at 3 K

[1] C. M. Julien, A. Mauger, K. Zaghbi, R. Veillette and H. Groult, *Ionics* 2012, 18, 625-633.

[2] S. Y. Chung, J. T. Bloking and Y. M. Chiang, *Nat Mater* 2002, 1, 123-128.