Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

On the difference between the pyroxenes $LiFeSi_2O_6$ and $LiFeGe_2O_6$ in their magnetic structures and spin orientations[1]

CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang University of Science and Technology, MYUNG-HWAN WHANGBO, North Carolina State University — The clinopyroxenes $LiFeSi_2O_6$ and $LiFeGe_2O_6$, crystallizing in a monoclinic space group $P2_1/c$, are isostructural and isoelectronic Their crystal structures are made up of zigzag chains of edge-sharing FeO_6 octahedra containing high-spin Fe3+ ions, which run along the c direction. Despite this structural similarity, the two have quite different magnetic structures and spin orientations. In $LiFeSi_2O_6$ the Fe spins have a ferromagnetic coupling within the zigzag chains along c and such FM chains have an antiferromagnetic coupling along a. In contrast, in $LiFeGe_2O_6$, the spins have an AFM coupling within the zigzag chains along c and such FM chains have an $\uparrow\uparrow\downarrow\downarrow$ coupling along a. In addition, the spin orientation is parallel to c in $LiFeSi_2O_6$, but is perpendicular to c in $LiFeGe_2O_6$. To explain these differences in the magnetic structure and spin orientation, we evaluated the spin exchange parameters by performing energy mapping analysis based on LDA+U and GGA+U calculations and also by evaluating the magnetocrystalline anisotropy energies in terms of GGA+U+SOC and LDA+U+SOC calculations. Our study show that the magnetic structures and spin orientations of $LiFeSi_2O_6$ and $LiFeGe_2O_6$ are better described by LDA+U and LDA+U+SOC calculations.

[1]This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(2013R1A1A2060341)

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Date submitted: 26 Dec 2013 Electronic form version 1.4