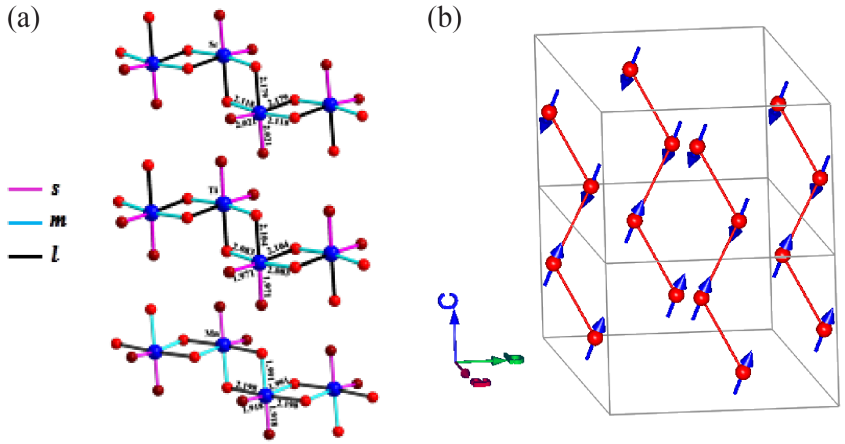
Neutron Study Reveals New Magnetic Structure in $NaMnGe_2O_6$ Pyroxene



(a) The schematic drawing of octahedra at the M site in the JT inactive $NaScGe_2O_6$, weak JT active $NaTiSi_2O_6$, and JT active $NaMnGe_2O_6$; (b) Magnetic structure of $NaMnGe_2O_6$ indicates the spin up-up-down-down intrachain ordering along the c-axis.

J. Cheng, W. Tian, J. Zhou, V. M. Lynch, H. Steinfink, A. Manthiram, A. F. May, V. O. Garlea, J. C. Neuefeind, and J. Yan, Journal of the American Chemical Society DOI: 10.1021/ja312038g **2013**.

Neutron diffraction work was performed at the ORNL Spallation Neutron Source's NOMAD and High Flux Isotope Reactor's HB-2A instruments.

Scientific Achievement

This work completes the study of the evolutionof magnetic properties of the alkali-metal pyroxenes as a function of the d-orbital occupancy from d^1 to d^5 and reveals a new magnetic structure in $NaMnGe_2O_6$

Significance and Impact

Neutron powder and single crystal x-ray diffraction reveals that the Jahn Teller (JT) distortion on Mn^{3+} is incompatible with the local structure distortion in pyroxene and addresses the long-lasting puzzle why high pressure is needed to synthesize Mn-pyroxene

Research Details

- $NaMnGe_2O_6$, a new pyroxene compound has been synthesized under high pressure and fully characterized
- Elastic neutron scattering experiments were performed (using a 50 mg sample for NOMAD and a 400 mg sample for HB-2A) to confirm the magnetic phase transition and determine the magnetic structure