

Magnetic and Structural Properties of Thiophosphates $\text{Li}_2\text{MP}_2\text{S}_6$ where $\text{M} = \text{Fe}$ and Co

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Ferrotoroidics are a member of the ferroic materials family. Similar to the well-known types of ferroic orders (ferromagnetic, ferroelectric, and ferroelastic), ferrotoroidics undergo a spontaneous, physical change below a critical temperature. In this case, the change is a spontaneous alignment of toroidal moments. A toroidal moment is defined as the local moment that arises from a local vortex of magnetic moments [1]. Due to the potential applications in data storage and memory, the purpose of this research is to further support and expand the current understanding of ferrotoroidic materials. An example candidate for ferrotoroidic materials are lithium transition metal thiophosphates of the formula $\text{Li}_2\text{MP}_2\text{S}_6$, where $\text{M} = \text{Fe}, \text{Co}$. The thiophosphates were chosen because of their structural relations to LiCoPO_4 , which is arguably the most well studied ferrotoroidic [2]. Figure 1 depicts the layered honeycomb crystal structure of $\text{Li}_2\text{FeP}_2\text{S}_6$ found by Takada et al. using x-ray diffraction [3]. To the best of our knowledge, no magnetic properties of this material have been studied. In addition, neither the structural nor magnetic properties have been reported for the cobalt analog. Phase pure powders of both $\text{Li}_2\text{FeP}_2\text{S}_6$ and $\text{Li}_2\text{CoP}_2\text{S}_6$ have been synthesized via a solid-state method. Layered, black, metallic-like crystals have been synthesized, growing up to 6 mm long. The crystal structure of $\text{Li}_2\text{FeP}_2\text{S}_6$ reported by Takada et al. was confirmed using x-ray diffraction. The crystal structure of $\text{Li}_2\text{CoP}_2\text{S}_6$, which has not been published, was also determined using the single crystals that were grown. SQUID magnetometry demonstrated an antiferromagnetic to paramagnetic transition at 25 K for the iron sample, but demonstrated paramagnetic behavior for the cobalt sample down to 2 K. The magnetometry results suggest an antiferromagnetic ordering of the magnetic moments in the iron sample, while the cobalt sample suggests no sign of magnetic ordering. In order to further confirm or refute the magnetometry data, time-of-flight neutron powder diffraction was used to analyze each of these samples. The resultant neutron powder diffraction for the cobalt patterns were identical both above and below the transition temperature, suggesting that there is no magnetic ordering. This same result was observed for the iron sample. The purpose of this presentation is twofold: a) to discuss the novel structural and magnetic properties of the lithium transition metal thiophosphates, and b) to relate this data back to the overarching goal, ferrotoroidicity. References: 1) Schmid, H. *Ferroelectrics* 2001, 252, 41-50. 2) Zimmermann, A. S.; Meier, D.; Fiebig, M. *Nature Commun.* 2014, 5, 4796. 3) Takada, K.; Tabuchi, M. *Solid State Ion.* 2003, 159, 257-263. Acknowledgements: This work was funded by the U.S. DOE Office of Science (Grant#: DE-SC0016434). The authors would also like to acknowledge Oak Ridge National Laboratory for the use of their neutron powder diffractometer.

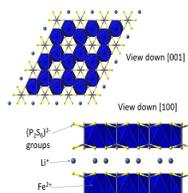


Figure 1