

# Limiting Group Symmetry to Distinguish Non-toroidal, Ferrotoroidal, and Antiferrotoroidal Point Groups

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Physical properties are restricted by the point symmetry of the crystal. For example, the point groups which permit a net magnetization are subgroups of the limiting group  $\infty/m'm'$ . Likewise, the limiting group is  $\infty mm1'$  for ferroelectrics. All ferroic materials are characterized by a net alignment of moments. For ferromagnets, the magnetic spins are aligned along one crystallographic direction. For ferroelectrics, the dipole moments are aligned.

Ferrotoroidics are a novel class of ferroic ordering characterized by a net alignment of toroidal moments. In our review article we discussed several leading candidates for ferrotoroidic order, particularly LiCoPO<sub>4</sub> (Pnma', mmm') with the olivine structure type, and LiFeSi<sub>2</sub>O<sub>6</sub> (P21/c', 2/m') with the pyroxene structure type.[1]

In previous years at this conference I presented neutron diffraction and magnetization measurements studying the magnetic structure in LiMPO<sub>4</sub> (M = Co, Mn)[2], as well as members of the solid solution series LiM<sub>n</sub>xM<sub>1-x</sub>PO<sub>4</sub> (M = Co, Fe). All the studied solid solutions were found to exhibit the same order as LiCoPO<sub>4</sub>, where net toroidization is allowed by the point symmetry mmm'. This demonstrated that the entire series could be considered candidate ferrotoroidic materials. In contrast, net toroidization is forbidden in LiMnPO<sub>4</sub> (Pn'm'a') with the point group m'm'm'. I then presented models for understanding how the toroidal moments can be modeled in this system to rationalize their net ferrotoroidic order. In doing so, the configuration of toroidal moments in LiMnPO<sub>4</sub> was not found to be non-toroidic. Rather, it was best described as antiferrotoroidic.

As a conclusion to my doctoral work on this topic,[3] I continued to study the underlying -1' site symmetry which leads to the ferrotoroidic and antiferrotoroidic configurations. Saxena et al. have argued that the point groups which permit a net ferrotoroidic moment are subgroups of the limiting group  $\infty/m'mm$ . [4] By considering the group-subgroup relations in these point groups, I argue that actually ten of those point groups are ferrotoroidic, and seven more are antiferrotoroidic. This rationale helps explain how ferrotoroidal, anti-ferrotoroidal, and non-toroidal configurations would be classified in structural analogs. As an example, I demonstrate these orderings in the olivine and pyroxene structure type.

## References

[1] Gnewuch, S.; Rodriguez, E. J. *Solid State Chem.* 2019, 271, 175-190.

[2] Gnewuch, S.; Rodriguez, E. *Inorg. Chem.* 2020, 59, 5883-5895.

[3] Gnewuch, S. *Magnetic and Toroidal Symmetry of Lithium Transition Metal Phosphates*. Ph.D. Dissertation, University of Maryland, College Park, (expected 2022).

[4] Saxena, A. *Integr. Ferroelectr.* 2011, 1, 3-24.

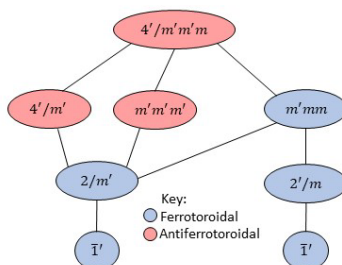


Figure 1