

**Stony Brook University
The Graduate School**

Doctoral Defense Announcement

Abstract

Powder Diffraction Tells You What Your Sample Really Is: Case Studies

By

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Powder diffraction is a useful tool for examining a number of materials that do not form a single crystal for a variety of reasons. Unlike with single crystals, structure determination with powders is not a routine task. Two families of materials will be presented, coordination polymers containing pyrazine and HF_2^- and Prussian Blue analogs, that were investigated with powder diffraction.

The bifluoride ion, HF_2^- , contains a two-coordinate H-atom exhibiting the strongest known hydrogen bond. This was used to form materials of the form, $\text{Ni}(\text{HF}_2)(\text{pyz})_2\text{X}$ ($\text{X} = \text{PF}_6^-, \text{SbF}_6^-$). These materials are quasi-1D magnets, with magnetic pathways along the bifluoride ion. Two polymorphs of the PF_6^- version were found and have different magnetic behavior, directly related to the structure.

$\text{Cs}_2\text{Mn}^{\text{II}}[\text{Mn}^{\text{II}}(\text{CN})_6]$ has the archetypal *fcc* Prussian blue structure, with the cations in the cubic voids. Substitution with smaller alkali ions lead to structural distortions and a marked increase in ordering temperatures. On the other hand, substitution of larger cations, NMe_4^+ drives a rearrangement of the Mn-CN-Mn network and produce several previously unobserved Mn(II) coordination geometries and a unexpected structure.

Date: May 11, 2012

Time: 11:30 am

Place: Physics, B-131

Program: Physics

Dissertation Advisor: Peter W. Stephens