Stony Brook University
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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, Ni(HF$_2$)(pyz)$_2$X (X = PF$_6^-$, SbF$_6^-$). These materials are quasi-1D magnets, with magnetic pathways along the biflouride ion. Two polymorphs of the PF$_6^-$ version were found and have different magnetic behavior, directly related to the structure.

Cs$_2$Mn$^{II}$[Mn$^{II}$($\text{CN}$)$_6$] 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 an unexpected structure.

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