

Abstract Submitted
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Molecular Magnets based on Fe and TCNE (Tetracyanoethylene, $C_2(CN)_4$): structures from powder diffraction¹ JAE-HYUK HER, PETER STEPHENS, Stony Brook University, KONSTANTIN POKHODNYA, MICHAEL BONNER, JOEL MILLER, University of Utah — There are many interesting organic-based magnets for which understanding is limited because they are not available as single crystals. However, in many cases it has proved possible to determine complete crystal structures from high resolution powder diffraction data. We discuss two specific systems with Fe(II): $Fe[TCNE]_2$ (which is unexpectedly $Fe[TCNE][C_4(CN)_8]_{1/2}$), and $Fe[TCNE][MeCN]_2FeCl_4$. Both structures contain a previously unobserved configuration of $\mu_4-[TCNE]^-$ anion bonded to transition metal ions. High resolution powder diffraction patterns were collected at the X16C beamline, National Synchrotron Light Source, Brookhaven National Laboratory. Simulated annealing and direct methods programs (FOX, Topas-Academic, EXPO) were used to solve and refine the structures. One cannot hope to understand properties of systems such as molecular magnets without knowing their structures, and the present work demonstrates the utility of powder diffraction to obtain that information.

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