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Modeling the organic magnet Fe[TCNE]$_2$ J. MORENO, M.A. MAJIDI, University of North Dakota, K.I. POKHODNYA, North Dakota State University — Recent experiments have revealed the crystal structure of Fe[TCNE]$_2$, (TCNE = tetracyanoethylene), an organic-based magnet with a transition temperature around 100 K and a saturation magnetization corresponding to an effective spin of 3/2 per formula unit. Its structure consists of undulating layers of TCNE anion-radicals bound to four Fe(II) ions, where Fe ions between adjacent layers coupled via diamagnetic σ-dimerized TCNE.[1] Since the angular momentum of Fe(II) is almost quenched due to the asymmetric crystal field, we model the system using a Heisenberg Hamiltonian with antiferromagnetic in-plane coupling between the Fe(II) S=2 spins and the near-neighbor (TCNE) S = 1/2 spins and also antiferromagnetic superexchange coupling between the Fe(II) spins at adjacent planes. By comparing our results with magnetization measurements as function of temperature and field, we extract the values of the inter- and intra-plane antiferromagnetic couplings. We discuss how to extend our approach to other TCNE-based magnets, such as the amorphous semiconducting V[TCNE]$_x$, a room temperature ferrimagnet and promising candidate for multifunctional spintronic applications.

[1] J.-H. Her, P. W. Stephens, K. I. Pokhodnya, M. Bonner and J. S. Miller, An gew. Chem. Int. Ed. 2007, 46, 1521

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