Poster Presentation

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The Transition-Metal Citrate Cubane as a Synthon for a Large Family of SMM's

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The transition-metal citrate cubane is a symmetrical, anionic molecular fragment that possesses twelve partially negatively charged oxygen atoms around its periphery. The cobalt variants have proved to be single molecule magnets (SMM), as demonstrated in studies by Murrie and by others.[1] All of the negatively charged points on the surface of the fragment are potential linkage positions for metal atoms, and extended products of from zero- to three dimensions have been synthesized and characterized.[2] In this presentation we describe products with five different combinations of linkage points for cobalt or manganese. A one-dimensional Co-containing cubane polymer has been found to undergo reversible cross-linking in the crystal to produce a two-dimensional polymer. A second Co-containg product, a discrete molecular solid with SMM behavior, undergoes reversible reaction in the crystal to produce an unsymmetrical product, also with SMM behavior -- a switchable SMM pair. A third product, a symmetrical two-dimensional Co-containing polymer, is an SMM with two blocking processes. A one-dimensional polymer of manganese citrate cubanes has been demonstrated to conduct protons via the Grotthuss mechanism.[3] All of these products have different patterns of peripheral metal-atom linkage to the twelve surface-resident oxygen atoms of the cubane fragment. A systematic naming scheme for the citrate cubane topology is used to provide simple descriptions of the diverse linkage geometries found to date.

[1] *M. Murrie, S. J. Teat, H. Stoeckli-Evans, et al., Angewandte Chemie-International Edition 2003, 42, 4653-4656.,* ***[2]*** *T. A. Hudson, K. J. Berry, B. Moubaraki, et al., Inorganic Chemistry 2006, 45, 3549-3556.,* ***[3]*** *J. Campo, L. R. Falvello, I. Mayoral, et al., Journal of the American Chemical Society 2008, 130, 2932-2933.*

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