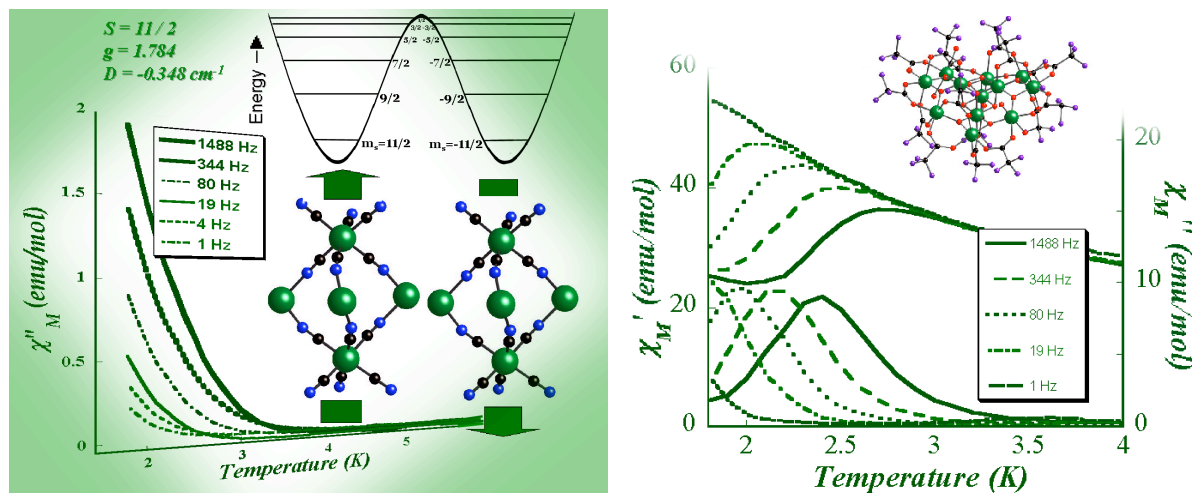


## NIRT Highlight

### Molecular Nanomagnets; DMR-0103455

The project is a study of the fundamental issues in the design of new Single Molecule Magnets (SMM), thin films and composite materials of SMM's. In addition, theoretical calculations on the interactions between single molecule magnets and their environment are being investigated. We have prepared the first incontrovertible example of a cyano-bridged SMM (Fig.1,Left) composed of manganese ions[1], and have been able to systematically prepare molecules of the same geometrical shape and nuclearity. A new SMM (Fig.1,Right) has also been prepared from the Mn<sub>12</sub> oxide family of compounds. This molecule is fully substituted with trifluoroacetate ligands and is suitable for deposition of thin films or adsorbed layers of SMM's.



**Figure 1. Left: [Mn<sup>III</sup>(CN)<sub>6</sub>]<sub>2</sub>[Mn<sup>II</sup>(tmphen)<sub>2</sub>]<sub>3</sub>, skeletal molecular structure and experimental data with potential energy diagrams, a New Cyano-Bridged SMM. Right: AC-susceptibility for the new SMM: [Mn<sub>12</sub>O<sub>12</sub>(CF<sub>3</sub>COO)<sub>16</sub>(H<sub>2</sub>O)<sub>4</sub>]**

The development of the cyanide-bridged SMM validates our proposed strategy for the synthesis of new magnetic clusters based on molecular architectures that have a unique axis of symmetry. The molecular shape is expected to profoundly affect the resulting magnetic properties of a given system, as high symmetry is expected to lead to cancellation of single-ion anisotropy. In addition to new SMM's with different symmetry, manipulation of the capping groups will be essential to efforts to control self-assembly of the SMM's into useful composite structures. Successful substitution of trifluoroacetate ligands on an SMM from the Mn<sub>12</sub> oxide family is a major step since it should be possible to use it to prepare numerous other derivatives of Mn<sub>12</sub> clusters.

This development of new SMM's as building blocks and the ability to selectively modify their peripheral components provides a potential basis for manipulation and assembly of SMM's into magnetic nanostructures whose interactions may be controlled by external magnetic fields and which may exhibit entirely new phenomena. Beyond the fundamental science of SMM's, the project will continue to pursue nanoscience applications vis-à-vis the manipulation and use of single molecules for such applications as high density magnetic data storage or quantum computing.

1. C. P. Berlinguette, D. Vaughn, J. R. Galan-Mascaros, K. R. Dunbar, *A Trigonal Bipyramidal Cyanide Cluster with Single-Molecule Magnet Behavior*, *Angewandte Chemie*, submitted.