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Computational Analysis of Magnetic Molecules JARED SINGLETON, LARRY ENGELHARDT, Francis Marion University — A "magnetic molecule" is a cluster of both magnetic and non-magnetic atoms, where the non-magnetic atoms serve to isolate the magnetic core of a magnetic molecule from any neighboring molecules. This makes the intermolecular interactions between the magnetic sites negligible, such that the analysis of a macroscopic collection of these molecules can yield properties about a single magnetic molecule. For my analysis, the parameters of two magnetic molecules, Cr8Gd8 and Ni21Gd20, were determined by matching predictions of theoretical models to experimentally measured data. To simulate the molecules in a magnetic field, the Heisenberg model was used. The results were obtained through computations using a quantum Monte Carlo algorithm from the ALPS library. Multiple thermodynamic properties were analyzed to determine the strength of the intramolecular bonds, the gyromagnetic ratio, and the anisotropy. The thermodynamic properties that were used included the magnetic susceptibility, magnetization, and heat capacity, where the heat capacity was integrated over the temperature range to determine the change in entropy.

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