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Simulation of AC Susceptibility and Electronic Structure of Mn-containing Molecular Magnets[1] MARK PALENIK, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — The family of Mn_{12}-Acetate molecular magnets has been recently enhanced by the synthesis of new members with S = 20/2 and S = 19/2 ground states. These closely related systems display similar but not identical AC susceptibility paterns which we have modelled in terms of their real (χ') and imaginary (χ'') components. The fits of AC data, as a function of frequency, show subtle differences between the parameters that control the spin dynamics in the S = 20/2 and S = 19/2 systems. To further understand the dynamic parameters we have performed electronic structure calculations based on spin density functional theory (SDFT) on both systems. Results from SDFT calculations, which describe the ground state and magnetic structures, have been correlated to the AC data to gain insight about the subtle differences in their magnetization dynamics.

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