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Numerical Analysis of the EPR Spectrum of a Ni_4 Single-Molecule Magnet through Direct Diagonalization of the Four-Spin Hamiltonian ANTHONY WILSON, University of Florida, Department of Physics, STEVE HILL, University of Florida, Department of Physics — EPR studies have established the Giant Spin (GS) Hamiltonian parameters, D, B_4^0 and B_4^4, for members of the $[Ni(hmp)(ROH)X]_4$ (R = Me, Et, etc., and X = Cl and Br) family of single-molecule magnets.[1] Four $S = 1$ Ni^{II} ions, aligned on corners of a cubic core, couple ferromagnetically creating a spin $S = 4$ ground state. Experiments on an isostructural Ni/Zn alloy established single-ion d_i and e_i parameters, as well as the orientations of the local magnetic axes.[1] A numerical model utilizing matrix diagonalization has simulated EPR spectra for the coupled $S = 1$ Ni^{II} ions using parameters from the Ni/Zn studies. Fourth order anisotropy parameters in the giant spin model arise from the isotropic Heisenberg coupling, $JS_1.S_2$, and quadratic single-ion anisotropy in the four-spin Hamiltonian. Heisenberg coupling causes higher energy states to influence the $S = 4$ ground state addressed in the GS model. Matching the lowest nine energies of the four-spin model to those of the GS model allows direct spectroscopic determination of J. [1]E.-C. Yang et al., Inorg. Chem. **44**, 3827-3836 (2005).

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