Abstract Submitted
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A Crystal Field Approach to Orbitally Degenerate SMMs: Beyond the Spin-Only Hamiltonian[1] LAKSHMI BHASKARAN, Department of Physics and NHMFL, Florida State University, Tallahassee, USA , KATIE MARRIOTT, MARK MURRIE, WestCHEM, School of Chemistry, University of Glasgow, Glasgow, UK , STEPHEN HILL, Department of Physics and NHMFL, Florida State University, Tallahassee, USA — Single-Molecule Magnets (SMMs) with large magnetization reversal barriers are promising candidates for high-density information storage. Recently, a large uniaxial magnetic anisotropy was observed for a mononuclear trigonal bipyramidal (TBP) [$Ni^{II}Cl_3$(Me-abco)$_2$] SMM [1]. High-field EPR studies analyzed on the basis of a spin-only Hamiltonian give D>400 cm^{-1}, which is close to the spin-orbit coupling parameter $\lambda = 668$ cm^{-1} for Ni^{II}, suggesting an orbitally degenerate ground state. The spin-only description is ineffective in this limit, necessitating the development of a model that includes the orbital moment. Here we describe a phenomenological approach that takes into account a full description of crystal field, electron-electron repulsion and spin-orbit coupling effects on the ground state of a Ni^{II} ion in a TBP coordination geometry. The model is in good agreement with the high-field EPR experiments, validating its use for spectroscopic studies of orbitally degenerate molecular nanomagnets. [1] K. E. Marriott et al., Chem Sci (published Online)

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