

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Evaluation of the exchange interaction and crystal fields in a prototype Dy₂ SMM¹ QING ZHANG, MYRIAM SARACHIK, City College of New York, CUNY, MICHAEL BAKER, Stanford University, YIZHANG CHEN, ANDREW KENT, New York University, EUFEMIO PINEDA, ERIC MCINNES, The University of Manchester — In order to gain an understanding of the INS and magnetization data obtained for Dy₂, the simplest member of a newly synthesized family of dysprosium-based molecular magnets [1], we report on calculations of the magnetic behavior of a Dy₂ cluster with the formula [hqH₂][Dy₂(hq)₄(NO₃)₃]MeOH. The molecular complex contains one high symmetry Dy(III) ion and one low symmetry Dy(III) ion. Our calculations suggest that exchange coupling between the two ions controls the behavior of the magnetization at low temperature, while the crystal field of the low symmetry Dy(III) ion controls the behavior at higher temperature. A point charge electrostatic model, based on crystallographic coordinates, provides a starting point for the determination of the crystal field [2]. Parameters in these calculations are adjusted to provide best fits to inelastic neutron scattering data (INS) and low temperature magnetometry [3]: the INS measurements access crystal field energies and low temperature magnetization probes the Dy-Dy exchange interaction. [1] E. M. Pineda, et al. Nat. Commun. 5, 5243 (2014). [2] J.J. Baldov, et al J. Comput. Chem. 34 (22), 1961-1967, 2013. [3] N. F. Chilton, et al. J. Comput. Chem. 34, 1164-1175 (2013).

¹Work supported by ARO W911NF-13-1-1025 (CCNY) and NSF-DMR- 1309202 (NYU).

Qing Zhang
City College of New York, CUNY

Date submitted: 06 Nov 2015

Electronic form version 1.4