Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The Effect of Uniaxial Pressure on the Spin Hamiltonian of Mn12-Ac Single-Molecule Magnet[1] JAMES ATKINSON[2], JONATHAN FRIEDMAN, Department of Physics, Amherst College, Amherst, Massachusetts 01002, C. BEEDLE, D. HENDRICKSON, Department of Chemistry & Biochemistry, UCSD, La Jolla, California 92093, Y. MYASOEDOV, E. ZELDOV, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel, K. PARK, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061 — We study the effect of uniaxial pressure on the magnetic hysteresis loops of the single-molecule magnet Mn12-Ac. We find that the application of pressure along the easy axis increases the fields at which quantum tunneling of magnetization occurs. Density functional theory (DFT) calculations yield the pressure dependence of the energy barrier for spin reversal that is consistent with the experimental results. The observations, when constrained by the DFT calculations, indicate that the pressure induces changes in both the second-order anisotropy constant D and the fourth-order anisotropy constant A.

[1]Work supported by NSF grants DMR-0449516 and DMR-1006519.
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Date submitted: 19 Nov 2011 Electronic form version 1.4