

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

The Effect of Ligands on the Unoccupied Density of States in Mn12 Acetate Molecular Magnets: An X-ray Absorption Near-Edge Study NADIA LEYAROVSKA, XSD, Advanced Photon Source, Argonne National Laboratory, MONICA SOLER, Michigan State University, GEORGE CHRISTOU, University of Florida, CARLO SEGRE, JEFF TERRY, Illinois Institute of Technology — Mn K-edge x-ray absorption spectra have been collected from three different samples of the Mn Acetate family of Single Molecule Magnets (SMM). The XANES region of the spectra shows large differences due to the presence of Mn ions of different oxidation state (II, III, IV) and different ligand environment. Self-consistent calculation of the local density of states (LDOS) and the x-ray absorption coefficient of the above samples were performed and compared to experimentally measured near edge absorption spectra (XANES). The good agreement between the calculated and measured absorption coefficient in the preedge and near edge regions for the three compounds with different ligand environment gives an opportunity for systematic correlation between the electronic and magnetic properties of this rapidly developing class of nanomagnets.

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Date submitted: 02 Jan 2007

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