Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Exact Diagonalization studies of frustrated AFM Heisenberg polytopes IOANNIS ROUSOCHATZAKIS, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL), ANDREAS LAEUCHLI, Institut Romand de Recherche Numerique en Physique des Materiaux (IRRMA), EPFL, FREDERIC MILA, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL) — We explore the low energy physics of the AFM $s = 1/2$ Heisenberg model on a number of frustrated magnetic molecule systems using exact diagonalization (ED). Particular emphasis is given to molecules with spins occupying the vertices of symmetric polyhedra. To this end, we have extended the standard ED technique in order to exploit the full point group (permutation) symmetry, thus including higher than one-dimensional irreducible representations. Apart from classifying the energy spectra according to both spin and permutation symmetries, our method provides the exact level degeneracies. In particular, for large frustrated polytopes, we find the existence of an accordingly large number of low-lying singlets below the first triplet, similarly to the case of frustrated 2D magnets. We also study the properties of the local spectral density functions, in view of interpreting recent neutron scattering experiments in Fe_{30}, one of the biggest AFM frustrated molecule available (comprising 30 spins 5/2 mounted on the vertices of a icosidodecahedron).

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Date submitted: 17 Nov 2006 Electronic form version 1.4