Large-scale simulations of the finite-temperature properties of the molecular assemblies Mn_6 and Ni_{12}

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9.7 cm

Assemblies of spins are interesting as objects providing the lower-size limit for magnetic nanoparticles. The spin aggregates are embedded as the cores in the macromolecules with well-defined size, shape and stoichiometry. They are separated from one another by shells of ligand molecules and can be synthesized in macroscopically large samples in regular structures. Here a numerical transfer-matrix approach, based on the Suzuki-Trotter formula and the checkerbord decomposition, as well as an exact diagonalization technique exploiting the point-group symmetry and the properties of the shift operator are worked out in the framework of quantum statistical mechanics. Both methods are applied, using the isotropic Heisenberg spin Hamiltonian and the large-scale simulations, to the title high nuclearity cyclic clusters $\mathrm{Mn_6}$ (i.e. $[\mathrm{Mn(hfac)_2NITPh}]_6$) and $\mathrm{Ni_{12}}$ (i.e. $\mathrm{Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6}$) in order to model quantitatively their magnetic properties. The mesoscopic parameters for both molecules ($J/k_B = 350 \pm 10K$ and $J/k_B = 8.5 \pm 0.5K, g = 2.23 \pm 0.01$) are obtained from a fit of the theoretical susceptibility curves to the experimental results.

13.4 cm

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