9.7 cm

Phenomenological modelling of molecular-based antiferromagnetic rings

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Two non-perturbative approaches: the direct exact diagonalization and quantum transfer matrix (QTM) techniques, applicable to Heisenberg spin systems modelling molecular rings, are described. The models include the single-ion anisotropy, alternating nearest-neighbour bilinear exchange coupling and the biquadratic term. Using these techniques and exploiting the Hamiltonian symmetry, we have performed calculations beyond the strong exchange limit for relatively large spin systems: (i) twelve spins s = 1 (Ni_{12}) and (ii) eight spins s = 3/2 (Cr_8). In both cases, the energy spectra in the presence of single-ion anisotropy, biquadratic exchange and magnetic field have been calculated using the direct exact diagonalization. The anisotropy-dependent splitting and spin-mixing as well as the field-dependent crossing of energy levels is presented and analysed. The efficiency and flexibility of QTM method is demonstrated for the spin s = 3/2 ring, including the exact magnetic torque calculations. The susceptibility and specific heat have been found to depend mainly on the mean value of the alternating couplings.

13.4 cm

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