SIMULATIONS OF THE THERMODYNAMIC PROPERTIES OF A DODECANUCLEAR NICKEL RING

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9.7 cm

The numerical exact diagonalization technique exploiting the point-group symmetry is worked out for the anisotropic Heisenberg spin Hamiltonian with the ring geometry. It is applied to the supramolecule $Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6$, in large-scale simulations, yielding the low-level energy spectra as a function of the single-ion anisotropy D and the thermodynamic functions. The constant D is analysed and estimated at $D/k_B = 1.5$ K. The results for the zero-field susceptibility and the field-dependent magnetization are presented and compared with experimental data.

13.4 cm

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