Theoretical study of the exchange coupling in a Ni12 single-molecule magnet

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The exchange interactions in a Ni12 complex have been studied by using theoretical methods based on density functional theory. The calculated J values reproduce correctly the S = 12 ground state of this system found experimentally and indicate the presence of three different exchange interaction pathways, in agreement with previous inelastic neutron scattering experiments. The three interactions are ferromagnetic, one of them corresponding to a second-neighbor interaction through a syn-anti acetato ligand. A magnetostructural correlation was found for such coupling, confirming the ferromagnetic nature of such an interaction. Our results are in excellent agreement with two new fittings of the experimental magnetic susceptibility data. The spin density distribution of the Ni12 complex is also reported and discussed.