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Can large magnetic anisotropy and high spin really coexist?[1]
CLAUDIA LOOSE, Institute for theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany, ELISEO RUIZ, JORDI CIRERA, JOAN CANO, SANTIAGO ALVAREZ, Departament de Quimica Inorganica and Institut de Recerca de Quimica Teorica i Computacional, Universitat de Barcelona, Diagonal 647,08028, JENS KORTUS, Institute for theoretical Physics, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany — This theoretical study discusses the interplay of the magnetic anisotropy and magnetic exchange interaction of two Mn_6 complexes. Our results for two polynuclear Mn_6 complexes show a very strong dependence of the D value on the spin of the ground state while the energy barriers are practically constant. Thus, complex 2 with a large spin (S = 12) favoured by ferromagnetic interactions has a small D value, while the lower spin complex 1 (S = 4) has a large D value. Therefor we suggest, that a large magnetic anisotropy is not favoured by a high spin state of the ground state.
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