Spin correlations in antiferromagnetic ferric wheels Fe_6 and Fe_{10}

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There are several mesoscopic clusters composed of transition-metal ions (Mn, Ni, Co etc.) bridged by oxo-groups. Antiferromagnetic ferric wheels Fe_n, $n = 6, 10, 18$, are profound examples of such molecules, when compensation of single-ion spins is complete, so the total spin $S = 0$. On the other hand these aggregates can be very well described as finite spin systems with dihedral symmetry group (D_n) and Hisenberg-like interactions between the nearest neighbours. The two first rings (Fe_6 and Fe_{10}) are investigated with application of group-theoretical and combinatorial methods followed by *exact* determination of states with given S and the total magnetization $M = 0$. The largest ferric wheel (Fe_{18}) is a subject of the so-called 'combinatorial explosion' (there are more than 10^{14} basic spin configurations) and left out in the present stage of calculations. It seems that we can perform some calculations for Fe_{14} ring (about $8 \cdot 10^{10}$ basic states), but synthesis of such a molecule has not been reported yet. Having determined eigenstates of a given Heisenberg Hamiltionan (for states with $M = 0$ and labelled by one-dimensional irreps of the symmetry group) we are able to investigate their properties such as spin correlations ω_r^z, for $1 \leq r \leq n/2$. It occurs that ω_1^z is very well approximated by linear function $aE + b$, where E is energy per spin, but the coefficients a, b depend on the total spin S: $a(S)$ is a linear function $\alpha S + \beta$ with $\alpha, \beta > 0$, whereas $b(S)$ is best fitted by the parabolic function $-\gamma S^2 + \delta S - \varepsilon$ with $\gamma, \delta, \varepsilon > 0$.

9.7 cm

13.4 cm

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