Hamiltonian of the Fe_4 SMM

This text is part of section 2 of Ref. [1].

The hamiltonian of the Fe_4 single-molecule magnet (SMM) in the presence of an external constant magnetic field with arbitrary direction is [2]

$$\mathbf{H}_S = \sum_{j=1}^{N} \mathbf{H}_j^{(S)}, \qquad j = 1, 2, \cdots, N, \tag{1a}$$

where

$$\mathbf{H}_j^{(S)} = -D_S (S_j^z)^2 + E_S[(S_j^x)^2 - (S_j^y)^2] - h_x S_j^x - h_y S_j^y - h_z S_j^z. \tag{1b}$$

The hamiltonian (1a) describes a Fe_4 SMM with N sites, in which h_x, h_y and h_z are the components of the constant external magnetic field. The set (S_j^x, S_j^y, S_j^z) corresponds to spin-5 operators at the jth-site.

The Fe_4 SMM has three isomers; for the AA isomer, the values of the parameters of hamiltonian (1b) are[3]

$$\frac{D_5}{k} \simeq 0.296K \quad \text{and} \quad \frac{E_5}{k} \simeq -0.0144K, \tag{2}$$

and k is the Boltzmann's constant.

References

[1] M.T. Thomaz, Onofre Rojas and E.V. Corrêa Silva, "*The specific heat and the magnetization of the Fe_4 and Fe_8 SMMs at $T \gtrsim 11K$*", submitted to publication.

[2] L. Cianchi *et al.*, Phys. Rev. B **65**, 064415 (2002).

[3] A. Bouwen *et al.*, J. Phys. Chem. B **105**, 2658 (2001).