EMR of high-spin Mn(III) ions in porphyrinic complexes

Krzysztof Tadyszak,[1] Czesław Rudowicz,[2,3] Hitoshi Ohta,[4,5] and Takahiro Sakurai[5]

[1] *NanoBioMedical Centre, AMU Poznań, Poland*
[2] *Faculty of Chemistry, AMU, Poznań, Poland*
[3] *Institute of Physics, West Pomeranian University of Technology Szczecin, Poland*
[4] *Graduate School of Science, Kobe University, Nada, Kobe, Japan*
[5] *Center for Supports to Research and Education Activities, Kobe University, Japan*

We have have performed semiempirical modeling of the spin Hamiltonian (SH) parameters aimed at the elucidation of the intrinsic magnetic nature of high-spin (S = 2) manganese (III) $3d^4$ ions at tetragonal symmetry sites in tetraphenyl - porphyrinato manganese (III) chloride (MnTPPCl) and related complexes. This modeling utilizes the microscopic spin Hamiltonians (MSH) approach developed for the $3d^4$ and $3d^6$ ions with spin S = 2 at orthorhombic and tetragonal symmetry sites in crystals, which exhibit an orbital singlet ground state arising from the ground ^{5}D multiplet.

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