MULTI-FREQUENCY EPR OF HETEROMETALLIC TRANSITION METAL CLUSTERS

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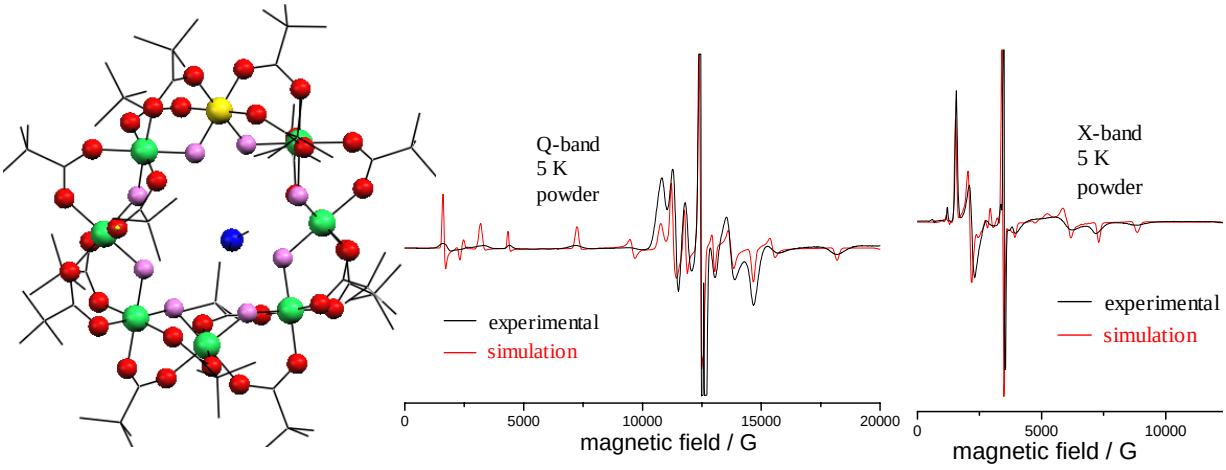
The results of multi-frequency c.w. EPR studies on the family of antiferromagnetically coupled heterometallic "wheels" $(R_2NH_2)[Cr^{III}_7M^{II}F_8(Me_3CCO_2)_{16}]$ (M = Mn, Fe, Co, Ni, Cu, Zn, Cd) [1] will be presented, where the ground state spin can be tuned by choice of M. Such clusters have attracted interest for potential applications as diverse as quantum computing and magnetic refrigeration [2,3] - these phenomena require a detailed understanding of the electronic structure. Single-crystal and powder, variable temperature (4 – 30 K), 9 – 95 GHz EPR give complex spectra which can be modelled (i) as super-positions of the isolated cluster ground and low-lying excited *S* states (giving *S*, *g*, *D*, *E* of these states), but also (ii) via full interaction spin-Hamiltonians incorporating single-ion and exchange terms, giving insight into the origin of the cluster spin-Hamiltonian parameters. However, for the full spin systems this would involve diagonalisation of huge matrices (up to 4^7x6^1 for M = Mn) - beyond our computational resources. Therefore, we will detail an approach based on smaller polymetallic fragments reflecting the chemical composition and magnetic structure of the full system.



1. F.K. Larsen, E.J.L. McInnes, H. El Mkami, J. Overgaard, S. Piligkos, G. Rajaraman, E. Rentschler, A.A. Smith, G.M. Smith, V. Boote, M. Jennings, G.A. Timco, R.E.P. Winpenny, *Angew. Chem. Int. Ed.* 2003, **42**, 101.
2. F. Troiani, A. Ghirri, M. Affronte, S. Carretta, P. Santini, G. Amoretti, S. Piligkos, G. Timco and R.E.P. Winpenny, Preprint Archive, *Condensed Matter* 2004, 1-5, arXiv:cond-mat/0405507.
3. M. Affronte, A. Ghirri, S. Carretta, G. Amoretti, S. Piligkos, G. A. Timco and R. E. P. Winpenny, *Appl. Phys. Lett.* 2004, **84**, 3468.