

High Field EPR: A powerful tool for the study of mononuclear Mn(II) sites

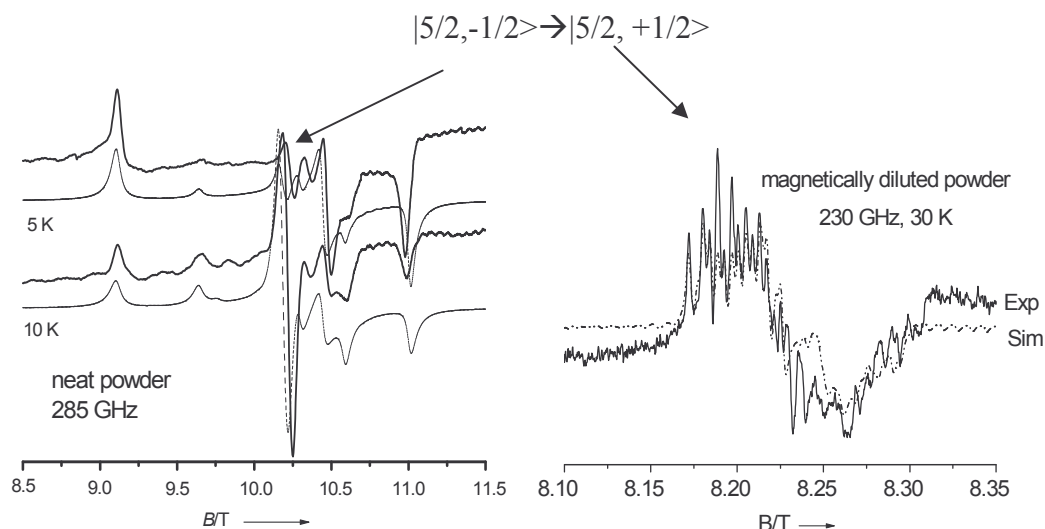
Carole Duboc,^a Jacques Pécaut,^b Claire Mantel,^{a,c} Thida Phoeung,^{a,c} Marie-Noëlle Collomb^c

^aHigh magnetic field laboratory of Grenoble-CNRS, France, ^bCEA Grenoble DSM/DRFMC/SCIB, France, ^cLEOPR - Joseph Fourier university Grenoble, France

Mononuclear Mn(II) complexes are present in several metalloproteins involved in various important biological processes. Since the manganese site is essential for their activity, a precise determination of the geometry and of the coordination shell of the metallic ion is required to understand the reactivity of these proteins.

EPR spectroscopy is one of the most powerful techniques for elucidating the electronic structure of a metallic center. However, in many cases (depending on the electronic parameters of the Mn(II) complex) the X-band EPR spectra are difficult or even impossible to interpret. We will illustrate here how high field EPR allows the study of *all* kinds of Mn(II) complexes and how the electronic parameters determined by EPR give important structural information (nature of the ligand, geometry, coordination number of the Mn(II)).

We will present studies performed both on synthetic mononuclear Mn(II) complexes and on metalloenzymes containing Mn(II). Since we have synthesized and characterized by X-ray crystallography and high field EPR several series of synthetic Mn(II) complexes, magneto-structural correlations will be reported. As an example, Figure 1 represents high field EPR spectra recorded on both neat and magnetically diluted powders of one complex ([Mn(tButerpy)(N₃)₂] with tButerpy = 4, 4', 4''-Tri-tert-butyl-2, 2':6',2''-terpyridine). The differences in the data from the two forms will also be discussed.



1. Mantel, C. ; Philouze, C. ; Collomb, M.-N. ; Duboc, C. *Eur. J. Inorg. Chem.* **2004**, 3880-3886.
2. Mantel, C.; Baffert, C.; Romero, I.; Deronzier, A.; Pécaut, J.; Collomb, M.-N.; Duboc, C. *Inorg. Chem.* **2004**, 43, 6455-6463.