Magnetic Circular Dichroism Spectroscopy of Metalloporphyrins

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Many enzymes contain metalloporphyrins as prosthetic groups, which catalyse a vide variety of biologically important reactions. Hence, these species have been studied by a large number of spectroscopic techniques including Magnetic Circular Dichroism Spectroscopy (MCD). This method is especially useful to investigate the electronic structures and spectra of paramagnetic complexes [1]. However, detailed assignments of these MCD data are rare. To this end, we have performed MCD measurements on simple metalloporphyrin [M(TPP)(Cl)] model complexes. In correlation to TD-DFT and semiempirical calculations, this allows for a detailed assignment of the optical spectra of these systems, but also for a calibration of the theoretical methods. Here we present the low-temperature MCD spectra of [Fe(TPP)(Cl)] (hs: S = 5/2), [Mn(TPP)(Cl)] (hs: S = 2) and [Co(TPP)(Cl)] (ls: S = 0) in comparison. Figure 1 shows the absorption (top) and MCD (bottom) spectra of five-coordinate [Fe(TPP)(Cl)] as example. Due to the different selection rules, many additional electronic transitions are identified in the MCD compared to the absorption data again demonstrating the impact of this method.

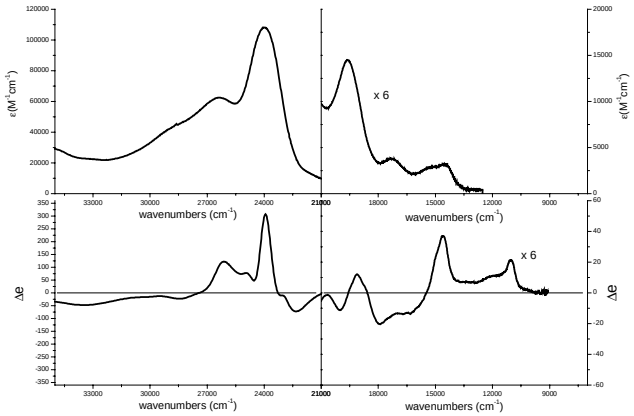

Figure 1. Absorption (top) and MCD spectrum (1.6 K and 3 T) of [Fe(TPP)(Cl)] (bottom).

[1] Solomon, E. I.; Pavel, E. G.; Loeb, K. E.; Campochiaro, C. *Coord. Chem. Rev.* **1995**, *144*, 369-460.