Magnetic Circular Dichroism Spectroscopy of Metalloporphyrins

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Many enzymes contain metalloporphyrins as prosthetic groups, which catalyse a wide 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.