EPR spectroscopy on metal ions and spin labels: Probing spectral features and local solvation effects

Melanie Heghmanns, Prof. Müge Kasanmascheff, TU Dortmund

Electron paramagnetic resonance (EPR) spectroscopy is a powerful tool for studying paramagnetic species, such as transition metal complexes, radicals, and metalloproteins. Paramagnetic metal ions, including Mn, Fe, Co, Ni, Cu and Mo, and radicals often exhibit characteristic spectral signatures, enabling their detection and identification in unknown compounds.

If the compound of interest is EPR inactive, a paramagnetic spin label can be attached at defined sites, allowing to probe, e.g., the local microenvironment of the label. One commonly used nitroxyl-based spin label is TEMPO.

We will use continuous wave (cw) EPR spectroscopy at X-band (9 GHz microwave frequency) to identify different metal ions and explore their spin states and hyperfine splittings. Moreover, we will investigate the spin label TEMPO in different solvents (H_2O/THF), mixtures and the rigid lattice. Using cw EPR at X- and Q-band (34 GHz) we enlighten the presence of a second species at higher frequency as a function of the used solvent. Simultaneous spectral simulations enable a straightforward analysis of the obtained spectra.

At the end of the day you know how to:

- record and analyze cw EPR spectra at room temperature and different frequencies
- simulate your spectra via Matlab
- differentiate between metal ions and radicals
- probe local solvent effects which influence the spectral line shape