Structural Investigation of Paramagnetic Transition Metal Complexes by EPR Spectroscopy

Schedule:

Week 1: Basic theory of EPR spectroscopy I – history, comparison with other spectroscopies, EPR-active substances, electron–Zeeman interaction, spectrometers at different frequencies, absorption for a molecule and macroscopic sample, spin relaxation, spectrometer structure, modulation technique, hyperfine interactions, line numbers and intensities.

Week 2: Basic theory of EPR spectroscopy II – hyperfine interaction (Fermi contact, dipole–dipole, spin polarization), Pascal triangle, interaction strength (McConnell equation).

Week 3: Paramagnetic metal complexes in solution – conditions for paramagnetism, electronic structure of paramagnetic metal ions, low/high-spin complexes, isotropic EPR spectra, line width descriptions, solution equilibria, stepwise deprotonation, pH-dependent spectra, temperature- and time-dependent spectra.

Week 4: Paramagnetic metal complexes in frozen solution I – anisotropy, g- and A-tensor orientation dependence, geometry of complexes, d-orbital splitting, spectra of Cu(II), VO(IV), Co(II), Fe(III), Ni(III), Ru(III) complexes.

Week 5: Paramagnetic metal complexes in frozen solution II – information from anisotropic spectra, detection of dimer complexes and coordination isomers, evaluation of pH-, time-, and temperature-dependent spectral series.

Week 6: Theory of pulsed EPR measurements – principles of ESEEM, ENDOR, HYSCORE, EDNMR; determination of coupling constants.

Week 7: EPR measurement practice – laboratory visit, introduction to the EPR instrument, measurement of pre-prepared samples.

Week 8: EPR measurement practice – recording pH-dependent room-temperature and low-temperature spectra; use of liquid nitrogen.

Week 9: EPR measurement practice – measurement of Cu(II) complex spectra at room temperature and 77 K; influence of parameters.

Week 10: EPR measurement practice – continued measurements; independent practice with samples.

Week 11: Spectrum simulation practice I – installation of DOSBox and 'epr' software; fitting of radical spectra; fitting of Cu(II) solution spectra; determination of isotropic parameters.

Week 12: Spectrum simulation practice II – decomposition of superimposed spectra; installation of '2d_epr'; evaluation of pH-dependent spectra.

Week 13: Spectrum simulation practice III – fitting anisotropic Cu(II) complex spectra using axial g-tensor models.

Week 14: Spectrum simulation practice IV – continued simulation tasks and evaluation.