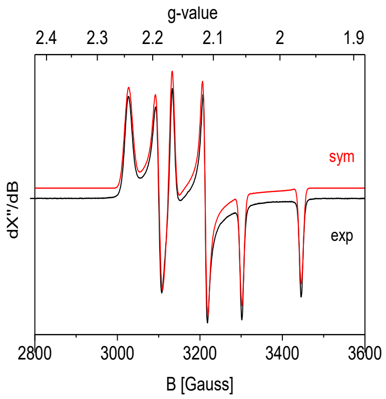
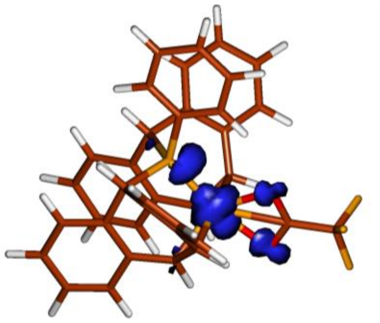
Physical Methods in Inorganic Chemistry 2025

Introduction to EPR spectroscopy

Prof. Dr. Bas de Bruin, University of Amsterdam (UvA)





<u>Expected knowledge</u>: Basic transition metal chemistry, basic knowledge of NMR, ligand field theory, and elementary quantum mechanics, some basic experience with MatLab.

<u>Content</u>: This 2-hour course presents an introduction to basic EPR spectroscopy. We focus mainly on (the interpretation of) EPR spectra of transition metal complexes containing one unpaired electron.

<u>Learning objectives</u>

Basic

Basic principles of (X-band) EPR measurements.
Understanding signal forms, spectrum symmetries and line shapes in EPR spectra.
Understanding which shapes can be expected in (frozen) solution or in the solid state.
Similarities/differences between EPR and NMR.

Interpretation of X-band EPR spectra of S = ½ systems

Which compounds do and which don't give a (measurable) X-band EPR spectrum.
Meaning of the g-value.
Information from (super)hyperfine couplings.
Correlation between EPR spectra and the electronic structure of a given compound.

Simulation of EPR spectra

Simple simulations of experimental EPR spectra with EasySpin/cwEPR.

You need to bring your own laptop with:

- Matlab R2024 installed
- EasySpin installed in Matlab (or at least downloaded: https://easyspin.org/)
- cwEPR 3.6.0 plugin for MatLab installed (or at least downloaded: https://nl.mathworks.com/matlabcentral/fileexchange/73292-cwepr)