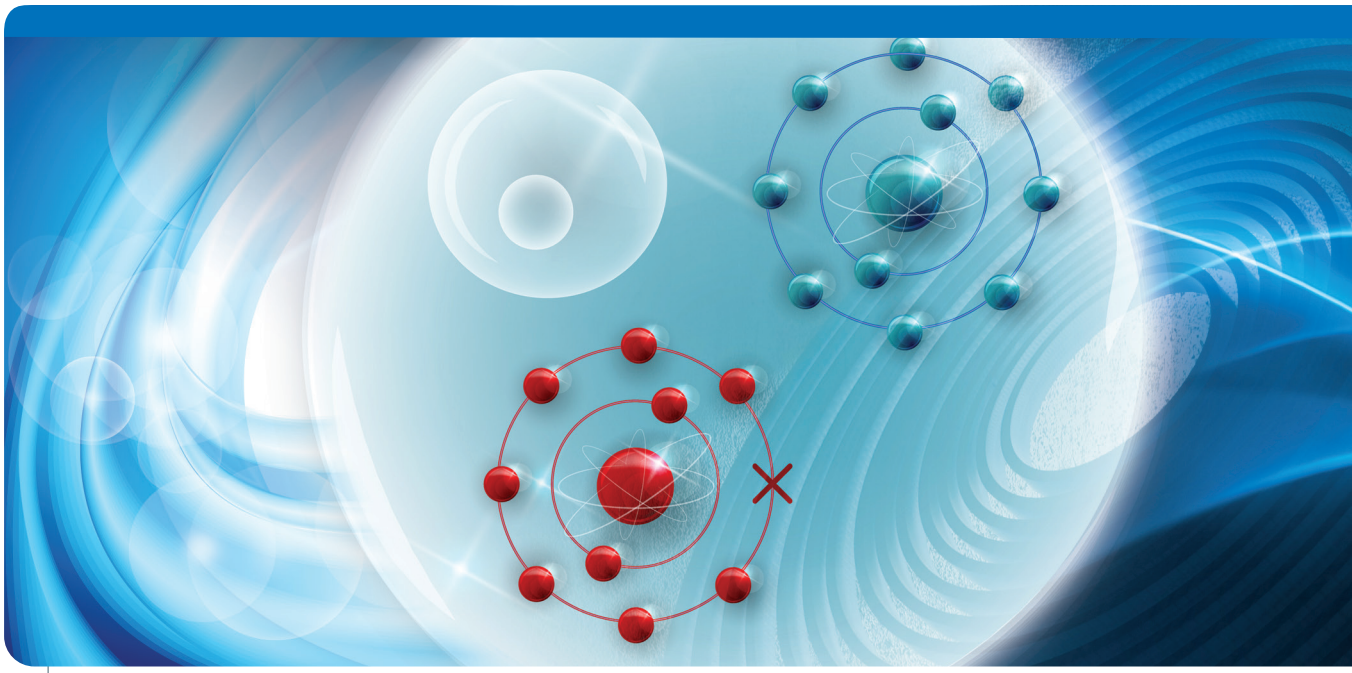


SpinFit

Identification and Characterization of EPR Species

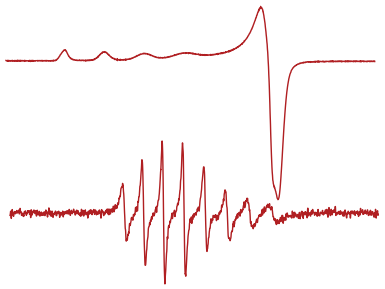
The identification of EPR active species (free radicals and transition metals) is a key step in understanding chemical reactions, biological processes and material properties. The EPR spectrum reflects the local and global environment of the unpaired electron: nearby nuclei, other unpaired electrons, solvent viscosity, molecular dynamics and concentration of species. Effects on the sample from external factors such as temperature, irradiation, and pressure can be followed through changes in the EPR spectrum. An approximate interpretation of the EPR spectrum can be done visually by measuring the prominent features with rough estimation of line positions, line splitting and line widths. A more in-depth analysis from simulation and fitting provides precise information on the local and global environment as well as changes triggered by external effects. Additionally, the measured spectrum can contain multiple species and the correct interpretation requires simulation and fitting.

SpinFit simulates and fits EPR signals to identify and characterize the EPR species. An arbitrary number of species can be easily separated into individual signals for characterization and quantification.

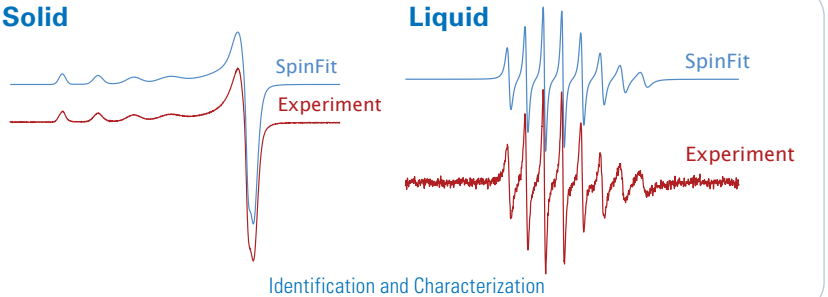
SpinFit

- Analyzes isotropic EPR signals of low-viscosity liquids
- Analyzes anisotropic EPR-signals of amorphous solid-state samples and frozen solutions
- SpinFit library: Comprises commonly encountered EPR-active species in both solid and liquid states as input to SpinFit
- SpinCount: Quantifies EPR species with high precision and reliability without additional user calibrations

CW-EPR Signal

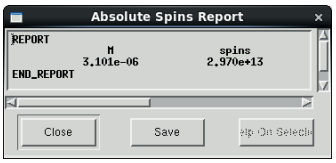


EPR Measurement



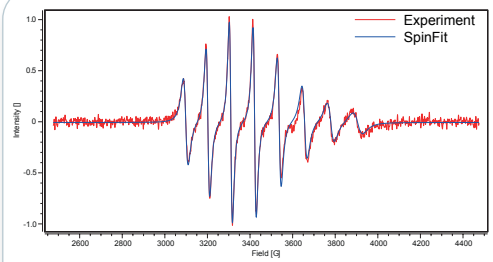
Identification and Characterization

Quantification

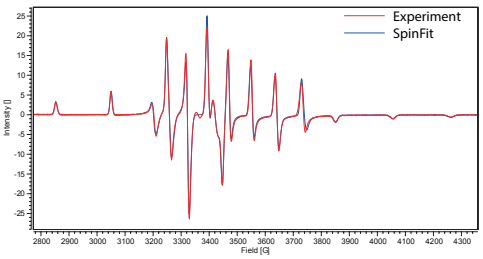


SpinCount

Correct Fit Regardless of Temperature



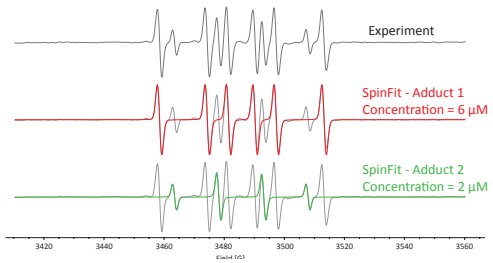
Isotropic EPR-signal at room temperature

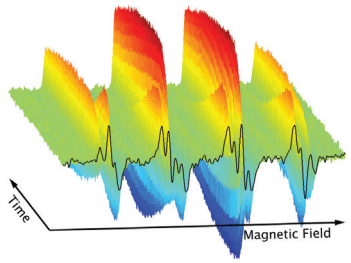


Anisotropic EPR-signal of frozen solution at 100 K

Simulation in both the liquid and solid state yields a complete picture of the EPR parameters and sheds light on the local coordination environment of the metal center of the vanadyl sulfate ($VOSO_4$).

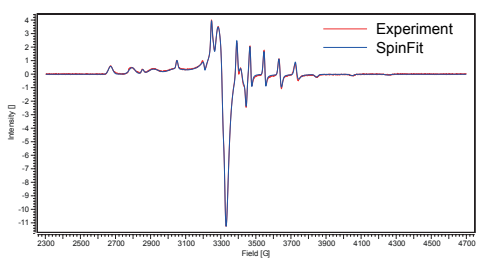
Multiple Component Identification and Quantification

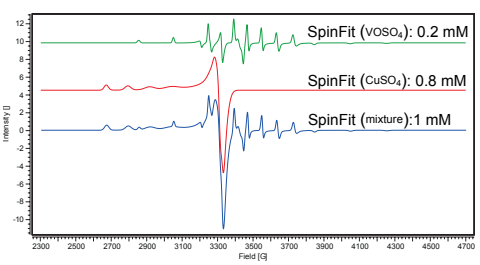




Individual components in time-dependent spin-trapping experiments

Two DMPO-radical adducts are identified and their concentrations are followed as a function of time to reveal the reaction kinetics of the system.





Individual components at any temperature

In this EPR spectrum at 100 K, a mixture of vanadium and copper signals is present. Fitting of the spectrum allows one to see the individual spectra and to determine their concentrations.

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