



EPR

SpinFit Solids

Advanced EPR Simulation and Fitting Made Simple

Innovation with Integrity

Introduction

Electron Paramagnetic Resonance (EPR) spectroscopy is a vital technique for characterizing paramagnetic molecules and centers with unpaired electrons. In samples like powders, frozen solutions, or glasses, species are often anisotropic and randomly oriented. In such cases, computer simulation is typically the only reliable way to extract spin-Hamiltonian parameters needed for structural analysis.

SpinFit Solids (SFS) offers advanced simulation capabilities tailored for these challenges. It supports full matrix diagonalization for accurate modeling of isolated or coupled paramagnetic centers, enabling precise determination of energy levels and transition probabilities. Additionally, SFS optimizes lineshapes, linewidths, and amplitudes using experimental data, ensuring robust and reproducible results across diverse sample types.

Part of Neon's suite of processing and analytical tools, SpinFit Solids complements features like peak picking, polynomial baseline correction, and smoothing filters to enhance your data analysis capabilities.

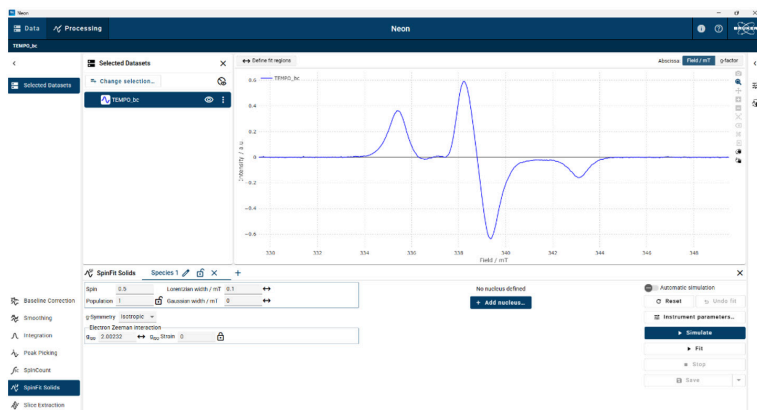
Features

- Easy-to-use interface
- A variety of fit parameters
- Simulation and fitting of 1D datasets
- Regional fitting, parameter locking and constraints
- Fitting of multiple species
- Fitting of data at various frequencies
- Full matrix diagonalization
- Supported file formats - *.xml of ESRStudio and BES³T of Xepr and Xenon software

Requires: Windows 11 operating system

I. SpinFit Solids Workflow

Data Upload in Two Clicks



Data can be easily uploaded in SFS using one of two ways:

- Browse files or folders
- Drag and drop files directly

Figure 1: SpinFit Solids user interface - uploading a spectrum of TEMPO at 120 K

Fitting Made Simple



Quick and intuitive simulation setup:

- User-friendly interface – navigating the parameter settings for g- and A-matrices is straightforward
- Streamlined workflow – set up preliminary simulation parameters in just a few clicks, no steep learning curve required
- Real-time feedback – instantly visualize how changes of the g-, A- and linewidth values affect your spectra
- Flexible input options – enter values manually or import from existing datasets with ease

Figure 2: Selecting nucleus for hyperfine splittings (HFS)

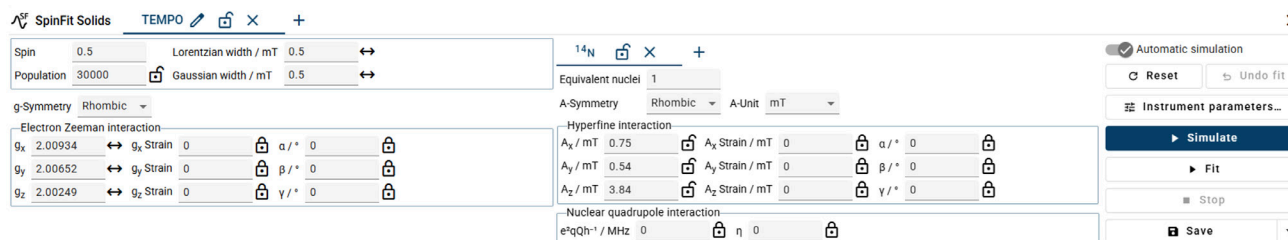


Figure 3: Choosing initial parameters for simulation



Figure 4: The superposition of the fitted and experimental dataset

- Start the fit - click the Fit button to begin the simulation fitting process
- Flexible timing - fitting duration may vary depending on the number of parameters introduced (e.g., g-values, A-values, constraints)
- Control at your fingertips - use the Stop button anytime to interrupt the fitting process
- Evaluate fit quality - check the R² coefficient in the bottom-right corner to assess how well the simulation matches your data
- Comprehensive reporting - a detailed report containing all simulation parameters can be exported as *.CSV file – perfect for sharing or further analysis

II. Accurate Simulation of g- and A-Strains



Figure 5: Fitted spectrum of CuSO₄ with g- and A-strain parameters

SpinFit Solids excels at modeling linewidth anisotropy caused by variations in spin Hamiltonian parameters across individual radicals or transition metal complexes. The software allows users to simulate distributions in magnetic properties, including g- and A-values, commonly referred to as strain, providing realistic and detailed spectral outputs. These capabilities make SpinFit Solids an indispensable tool for researchers aiming to interpret complex EPR spectra with greater precision and confidence.

III. High Spin Systems with Zero-Field Splitting (ZFS)

High-spin systems such as Cr³⁺-doped cesium aluminum sulfate, where zero-field splitting dominates the spectrum, can be effectively modeled using SFS. Leveraging axial symmetry and a nearly isotropic g-matrix, the software enables precise refinement of D and E parameters for accurate simulation. This example highlights the tool's ability to achieve excellent fit quality (R² = 0.9599) by incorporating zero-field splitting into the analysis.

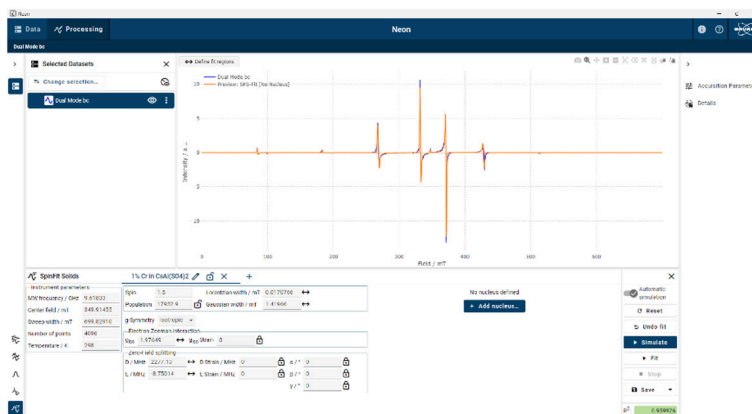


Figure 6: Spectrum of CsAl(SO₄)₂·12H₂O doped with 1% ⁵²Cr³⁺ (S = 3/2)

IV. Multicomponent Simulations

SpinFit Solids enables precise simulation of multicomponent EPR spectra, which often arise from varying spin states or chemical environments. In the reaction of myoglobin with azide, both high-spin and low-spin Fe^{3+} species coexist shortly after the reaction begins. SFS accurately models these overlapping components, helping researchers extract meaningful parameters and achieve strong alignment with experimental data.

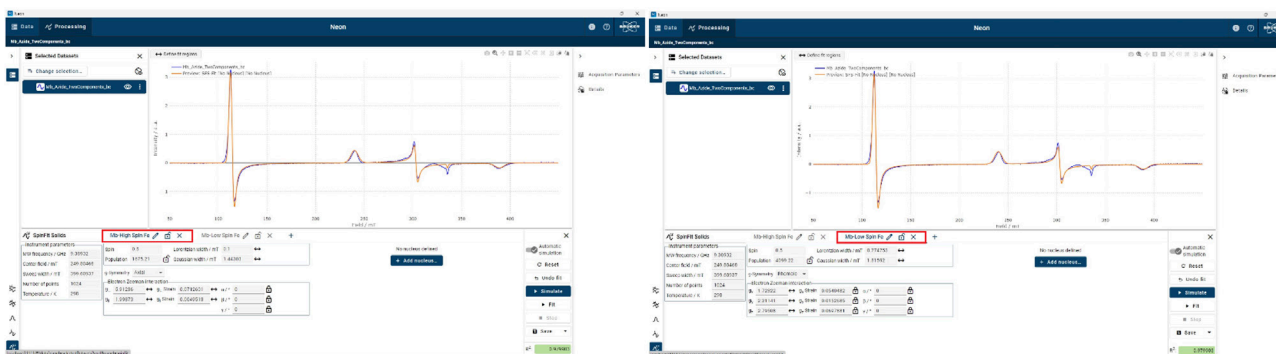


Figure 7: The two-component fit for the freeze-quench of the reaction mixture of myoglobin with azide

Conclusion

Designed for modern EPR spectroscopy, this powerful and intuitive simulation tool enables comprehensive spectral analysis - from g- and A-tensor modeling to zero-field splitting, nuclear quadrupole interactions, Euler angles, and multicomponent spectra. With a user-friendly interface, real-time visualization, and robust fitting capabilities, including strain effects and complex spin systems, it provides researchers with a reliable and efficient solution for spectral analysis. Whether working with transition metal complexes, free radicals, or high-spin systems, users benefit from precision, flexibility, and ease of use.

Bruker BioSpin is continually improving its products and reserves the right to change specifications without notice.
© BS-100112 10/2025 Bruker BioSpin.

Bruker BioSpin
info@bruker.com

bruker.com

Customer Support
<https://www.bruker.com/en/services/support.html>

EPR Simulation and Fitting Suite
Product Page

