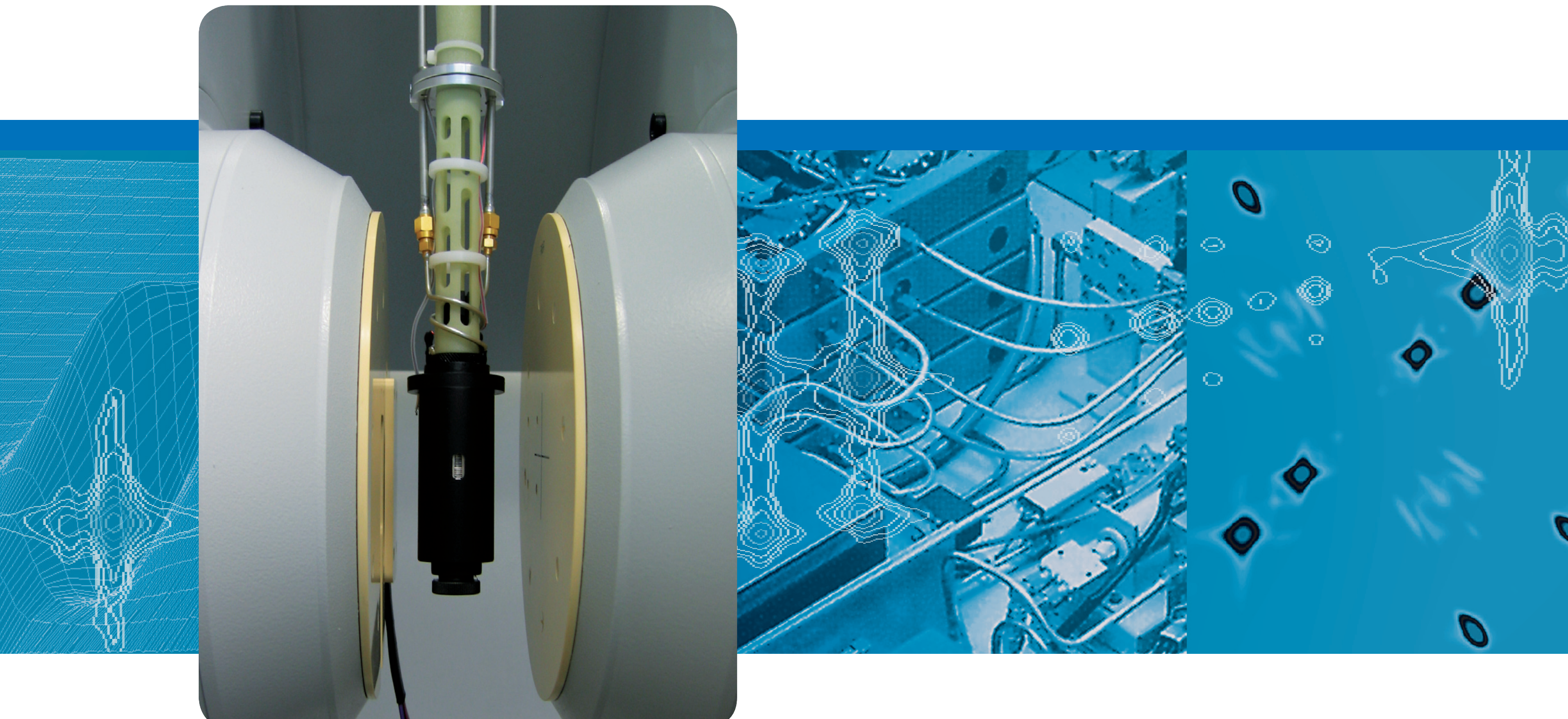
BRUKER



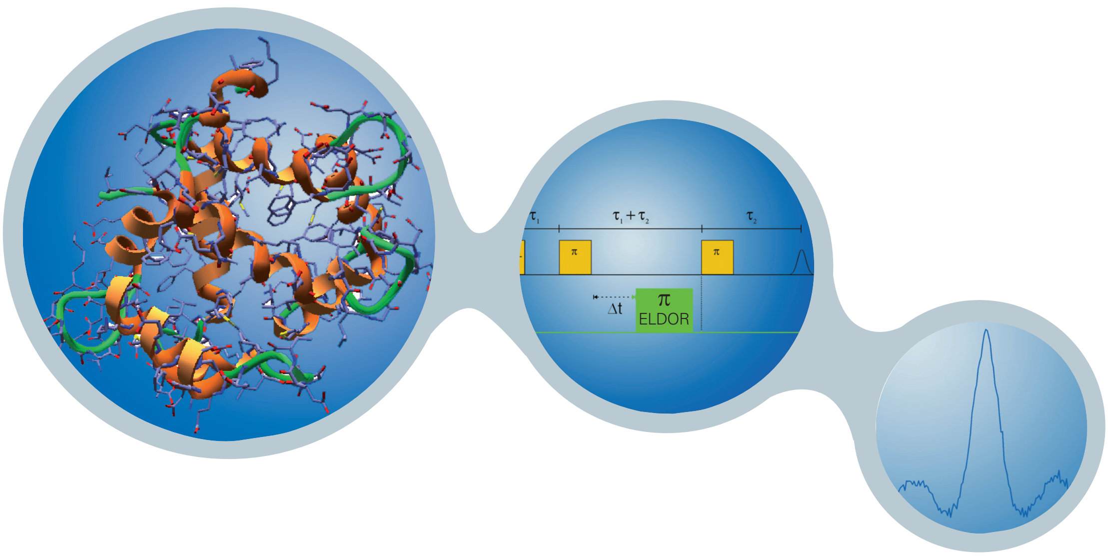
ELEXSYS E 580

- The ultimate EPR System for Life Science, Materials Science and Quantum Computing

Pulse-EPR

Innovation with Integrity

E 580 FT/CW EPR Spectrometer



The ELEXSYS™ E 580, a masterpiece for Electron Spin Echo spectroscopy, ESEEM, 2D spectroscopy, Pulse-ENDOR, Pulse-ELDOR (DEER), Transient EPR and Multi-frequency EPR in Life science, Material science and Quantum computing.

With the introduction of the ESP 380 CW/FT EPR spectrometer in 1987 Bruker started the era of commercial pulse-EPR. A breakthrough in sensitivity was achieved with the second generation, the ELEXSYS™ E 580. The digital units PatternJet™ and SpecJet™, developed for the needs of pulse-EPR, allowed for the first time to average FIDs and echoes in the sample T_1 limit and eliminated the previous time consuming bottleneck in averaging.
Over the last 20 years the basic X-Band spectrometer was continuously extended to multifrequency applications.
Based on the Bruker Intermediate Frequency (IF) concept the full range of EPR frequencies from L-Band to W-Band is now available for pulse-EPR spectroscopy.
The multifrequency platform is complemented by multi resonance accessories for Pulse-ENDOR and Pulse-ELDOR (DEER).
Our continuing development has now culminated in the second generation of the E 580 series featuring PatternJet-II and SpecJet-II both with a 1 GHz clock.
In addition to the unparalleled capabilities of the E 580 in the world of pulse-EPR it has the full functionality of the E 500 CW-EPR spectrometer as well.

Microwave Bridge & IF

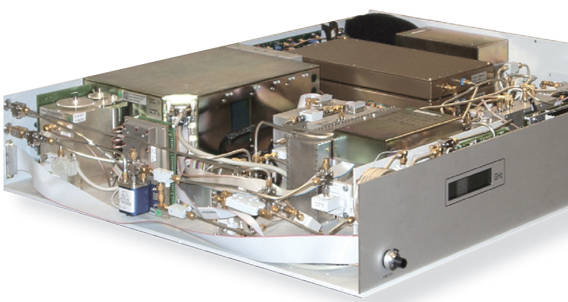
The heart of every Pulse EPR Spectrometer is the microwave bridge. From shaping of pulses to amplification of the signal, the versatility and performance of the SuperX-FT/CW MW bridge is unparalleled. The modular design ensures the flexibility required for a research instrument.

SuperX-FT

- CW and Pulse operation
- SPFU for pulse shaping
- Low power pulse monitor (TM)
- High power pulse monitor (RM)
- Quadrature detection: 100 dB gain, ± 200 MHz bandwidth

ELDOR Unit (option)

The ELDOR unit (E 580-400) generates a second MW excitation frequency with an 800 MHz range for Electron-Electron Double Resonance experiments, applicable at all microwave bands (L, S, X, Q, and W).
An upgrade for the ELDOR unit is the Coherent ELDOR Option, which allows phase coherence between the detection system and the ELDOR source.



SuperX-FT bridge

MPFU (option)

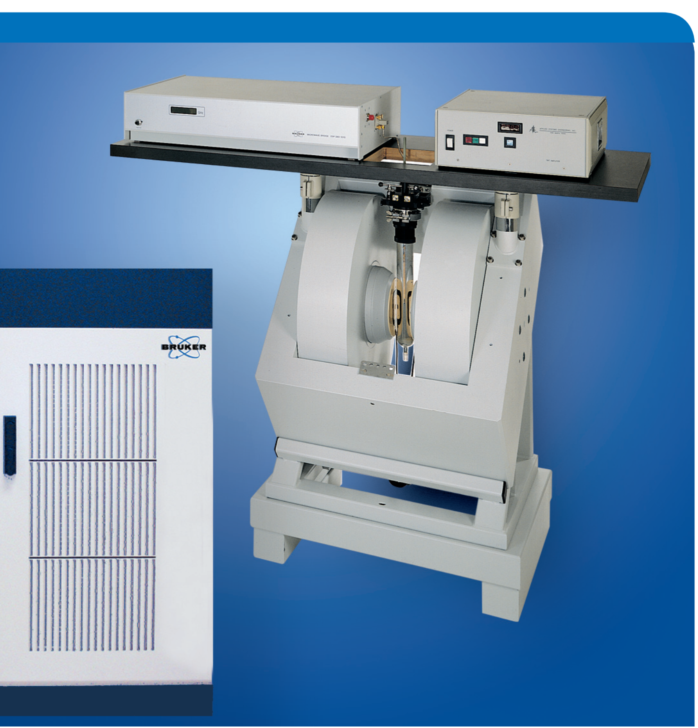
The MPFU allows the freedom of choice in pulse phase and amplitude setting. It supports experiments combining soft and hard pulses or generating composite pulses with an arbitrary phase relation. Up to 4 additional microwave channels can be included.

Low Power CW Detection (option)

With the LCW path, it is possible to generate hard pulse, low power CW excitation sequences for CW detected saturation recovery experiments or Coherent Raman Beat experiments. The digital DC-AFC provides the long term stability required for these experiments.

Intermediate Frequency (IF) Path (option)

For EPR at different frequency bands (L, S, Q, and W), the IF path is used to direct the X-band frequencies (excitation and detection) to and from the additional band. All features of the X-band bridge are retained at the new operating frequency.



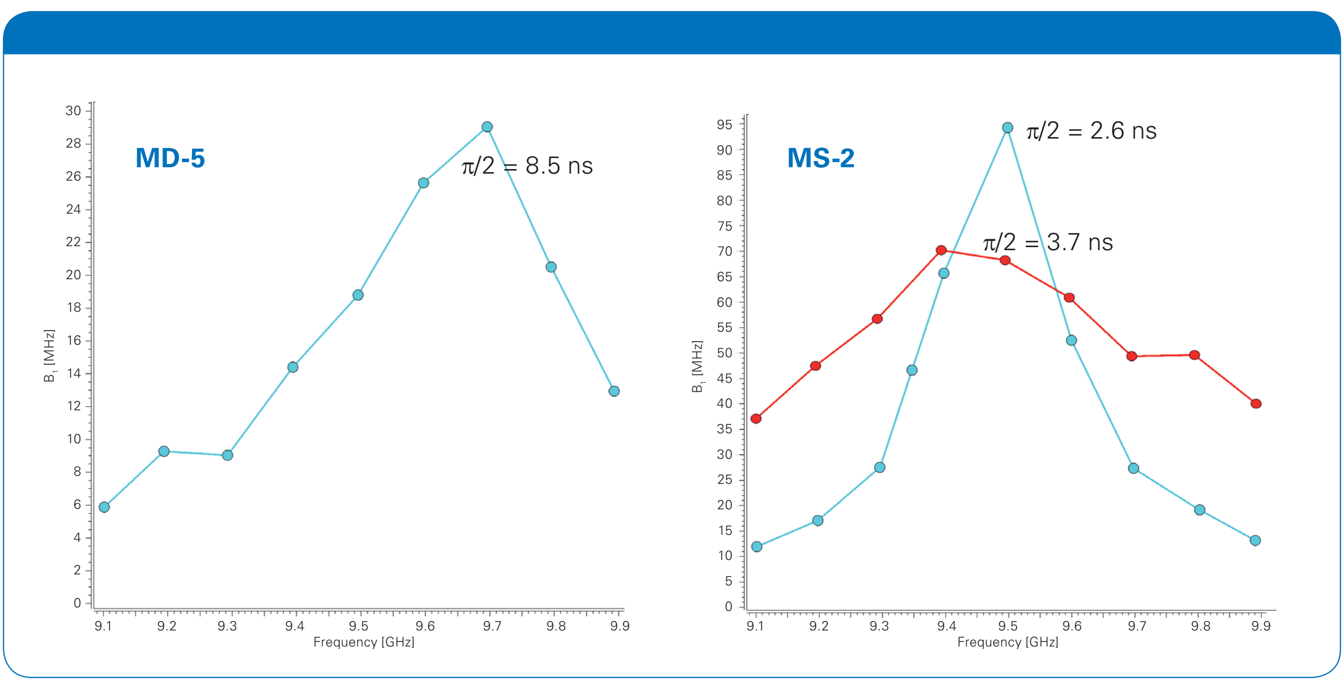
Standard Pulse Former Unit (SPFU)

- Four independent pulse channels: +X, +Y, -X, & -Y.
- Programmable pulse position and length in each channel
- Common phase and amplitude for pulses within a channel
- No restriction on delay between pulses in different channels, even crossing and overlapping

Probes & Cryogenics

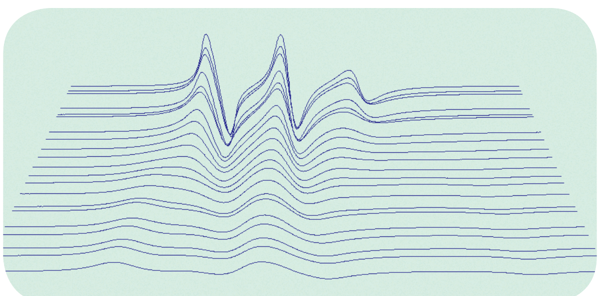
Flexline
Pulse-ENDOR
resonator
EN 4118X-MD4

The resonator is a central part of the spectrometer. It has to provide a high microwave field strength to generate short pulses and it governs to a large extent the system sensitivity. With the Flexline™ series of dielectric and split-ring resonators Bruker offers universal and dedicated probes which combine high performance and ease of use.
The universal ER 4118X-MD5 probe accommodates the largest sample volume and thus has the highest sensitivity if sample quantity is not a limiting factor. The split-ring series of Flexline probes is designed for high time resolution in transient experiments and for highest B_1 at lowest Q for ELDOR measurements. The 2 mm split-ring resonator offers the highest sensitivity for point samples.



High B_1 and large bandwidth: Flexline bandwidth and B_1 at various coupling strengths (1 kW TWT)

Helium Cryostat ER 4118CF



Cryogenics

The sample temperature is a key parameter in many EPR experiments. It is used to investigate the temperature dependence of a certain sample property or to establish a desired sample condition.

The universal ER 4118X-MD5 Flexline probe

- Variable Q from 5000 to 20
- Up to 5 mm sample tubes
- Up to 255 µl sample volume
- High B_1 at low Q
- Low dead-time
- CW-EPR (critical coupling, modulation coils)
- Variable temperature 2 – 300 K
- Quick sample change
- Easy handling
- Optional Pulse-ENDOR version
- Optional optical window

The split-ring Flexline series ER4118X-MS

- Dedicated probes for transient EPR, saturation recovery EPR and ELDOR
- Versions with 5, 3 and 2 mm sample access
- Up to 1 GHz bandwidth (Q = 10)
- Extremely high B_1 at very low Q
- High time resolution at critical coupling

Flexline cryostats compatible with the Nitrogen or Helium based temperature control system:

- ER 4118CF for 2 – 300 K
- ER 4118CV for 100 – 300 K

PatternJet™ & SpecJet™

Matched excitation and detection for Pulse EPR: The PatternJet-II delivers high time resolution with up to 1 ns resolution for pulse length, position, and evolution. The SpecJet-II delivers high speed acquisition with 1 ns time resolution and on-board digital signal processing.

The PatternJet-II pulse programmer continues to provide the EPR community with the flexibility and precision required for the ever evolving field of pulse EPR. The combination of high speed evolution, fast repetition, and precision positioning are indispensable for high quality pulse EPR spectroscopy.

Enhanced Execution

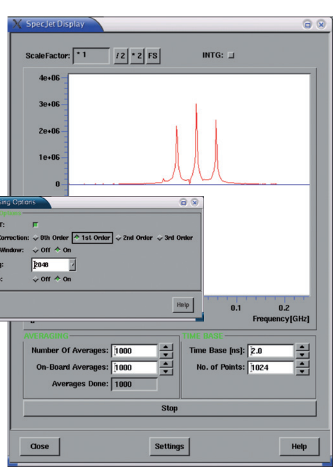
With the PatternJet-II, execution time is reduced for experiments with phase-cycles and/or multidimensional time evolutions, e.g. a HYSCORE experiment of 256x256 points with a 4-step phase cycle can be completed without any reprogramming overhead.

Enhanced Opportunity

The PatternJet-II features extended memory on each pulse channel opening up more experimental possibilities, e.g. a pulse sequence with 512 pulses can employ up to 1024 different time evolutions.

PatternJet-II

- 1 or 2 ns resolution regardless of pulse length
- Dynamic range of 10^9
- Multidimensional time evolution without reloading
- Pulse evolution from shot to shot without delay
- Zero dead-time between shots and loops
- Same edge placement resolution for any number of pulses



SpecJet-II real-time FFT display

Real-Time Optimization

The high speed acquisition of up to 10^6 signals per second permits an unprecedented level of signal optimization prior to experiment execution. The addition of on board digital signal processing (DSP) to the SpecJet-II extends this optimization into the frequency domain by providing a real-time FT of the time domain signal.

Matched Resolution

With a maximum detection resolution of 1 ns, the SpecJet-II provides a natural counter part to the PatternJet-II with an excitation resolution of 1 ns. This matching permits the excitation and detection of signals up to 1 GHz.

SpecJet-II

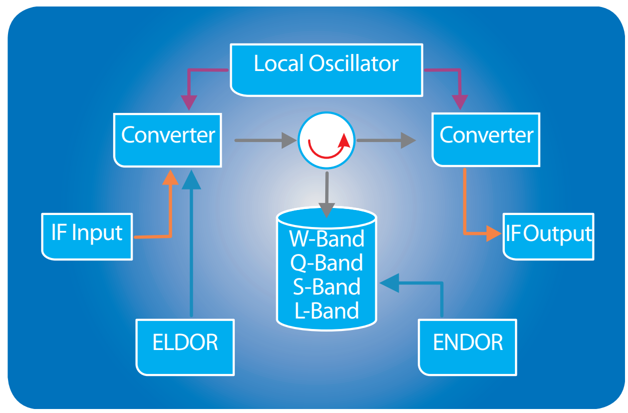
- Real-time FT or Time display
- Up to 65,536 averages on-board
- Variable time base from 1 ns to 10 ms
- Record length from 32 to 65,536 points
- Up to 1 million transients per second
- Internal, external and level trigger
- 1 GHz 8-bit digitizer

Multi-Frequency

Although traditional EPR experiments have been carried out at X-band (9-10 GHz), there are several advantages to working at higher and lower MW frequencies. With the Bruker IF concept pulse EPR is transformed from X-Band to all other common EPR frequencies.

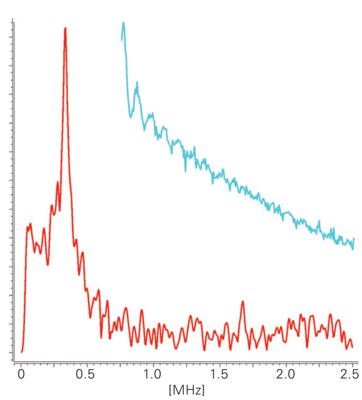
Intermediate Frequency (IF)

The IF concept utilizes the high quality and performance available from the SuperX-FT bridge for both excitation and detection. The X-band frequency is transformed to the desired operating frequency. All of the features of the SuperX-FT bridge are retained at the new MW frequency.



SuperL-FT (L-Band)

- Highest penetration depth into aqueous media
- Deepest ESEEM modulation depth
- Accommodate large samples (e.g. small animals).

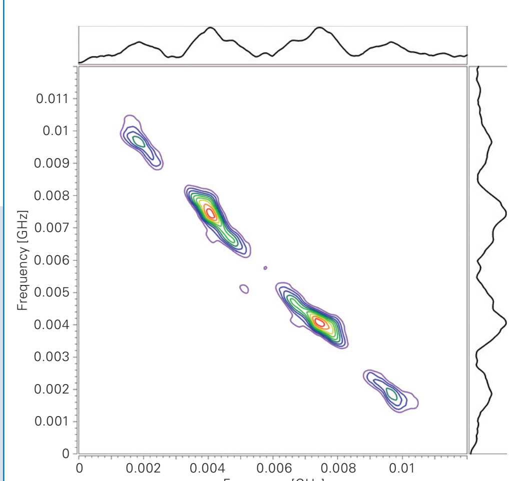


L-Band ^{29}Si –ESEEM. Increased modulation depth allows fewer averages for detection when compared to X-band.

SuperS-FT (S-Band)

- Increased modulation depth in ESEEM experiments
- Increased penetration in lossy samples
- Increase hyperfine resolution
- Reduced g-factor dispersion

The SuperL-FT and SuperS-FT microwave bridges are available as upgrade modules for the SuperX-FT bridge forming a multi band system. Variable temperature Flexline probes with 5 mm sample access complete the set-up.



S-Band ^{1}H –HYSCORE of BDPA

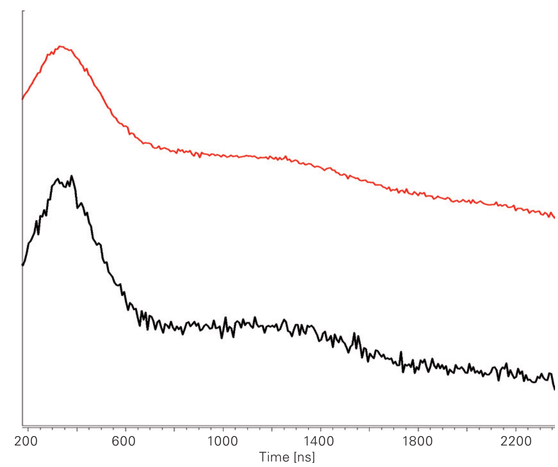
SuperQ-FT

Q-band is the most popular frequency for pulse and CW EPR after X-band. The increase in g-value resolution and the increased nuclear frequency resolution in ENDOR, ESEEM and HYSCORE experiments are significant benefits for structure determinations.

Q-Band

- Improved sensitivity
- Improved sensitivity in DEER measurements
- ESEEM experiments with high resolution
- Improved ENDOR resolution

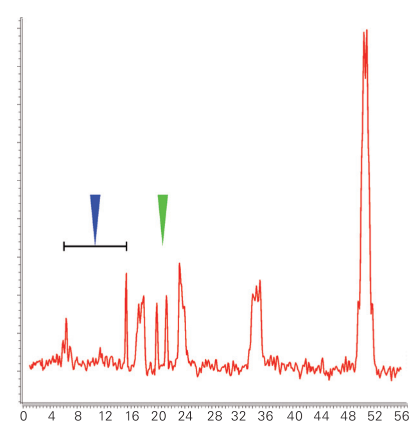
Q-Band resonator EN 5107D2



The superior S:N achieved at Q-band in the 4-pulse DEER experiment improves the reliability and accuracy of distances and distance distributions: Optimized sample amounts of spin labeled Ubiquitine, 10 µl at Q-band (red) and 150 µl at X-band (black).

The SuperQ-FT bridge is available as a stand-alone unit or as an upgrade for the SuperX-FT for dual band operation.

The set-up is complemented by the high performance EN 5107D2 resonator (EPR and ENDOR version) for variable temperature work.



Nuclear resolution enhancement in this Davies ENDOR spectrum of a Cu-Pt complex facilitates assignment of nuclear couplings for the ^{31}P and ^{195}Pt

High-Frequency / Field EPR

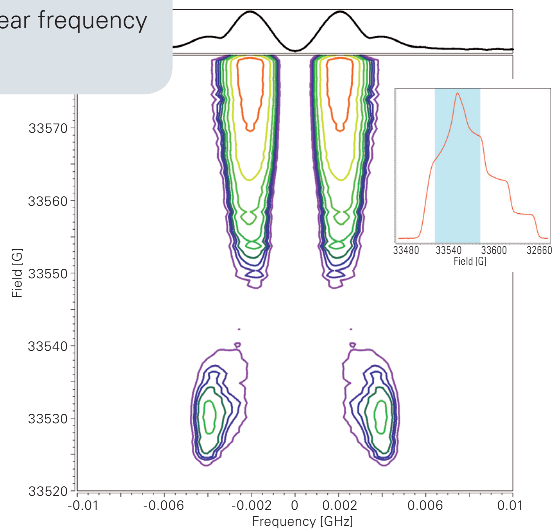
High-frequency EPR at W-band (94 GHz) provides an increased absolute sensitivity and increased resolution in g-values and nuclear frequencies. The ELEXSYS E 680 W-Band spectrometer is available as a stand-alone version or as an X-W dual frequency instrument.

W-Band

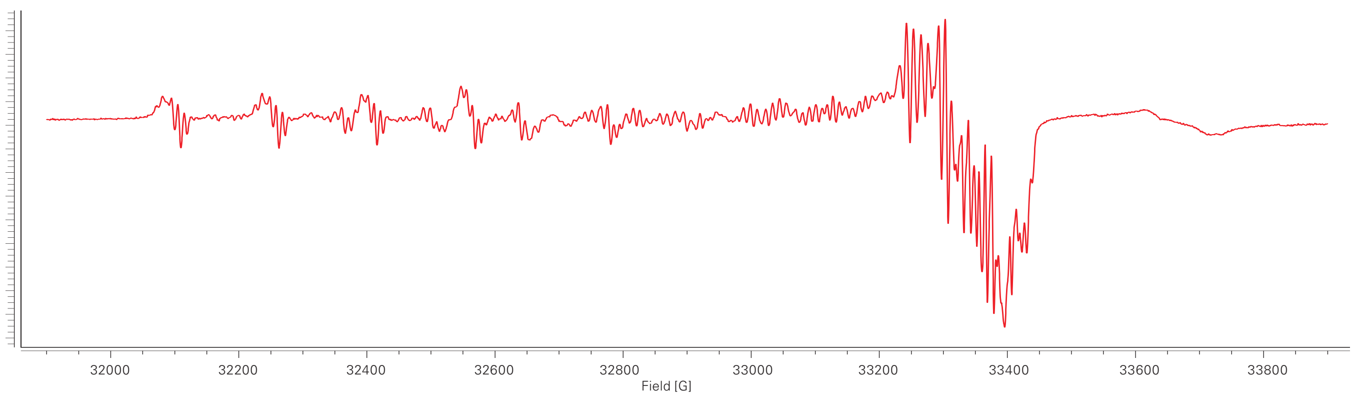
- High sensitivity for limited sample size
- High g-value resolution
- High nuclear frequency resolution

Super Conducting Magnet for EPR

From the very beginning, EPR performance was the drive behind design of the 6T EPR SC magnet. The main coils provide a 0-6 Tesla sweep in 30 min, while the high-resolution sweep coils have a 2000 G range. Full software control allows easy switching between main and sweep coil operation.



The higher g-value resolution at W-band provides the greater opportunities for orientation selective pulse experiments: 2D 4-pulse DEER experiment showing the parallel component of the dipolar spectrum with the pump pulse in the g_x region and the probe pulse in the g_y region.



With the 2000 G sweep coil range of the 6T EPR SC, many EPR species are accessible for pulse and CW EPR experiments without changing the persistent field of the magnet.

Xepr™ & MoSophe

Xepr is a comprehensive software package of the ELEXSYS series, accommodating the needs of every user with highly developed acquisition and processing tools. MoSophe solves the challenge of data interpretation by placing high powered simulation routines in an innovative environment.

Control

Xepr harnesses all of the features of the ELEXSYS spectrometer series providing a centralized system for monitoring and controlling the complete instrument. Xepr keeps the user informed of current states and provides a focused environment for experiment definiton.

Execution

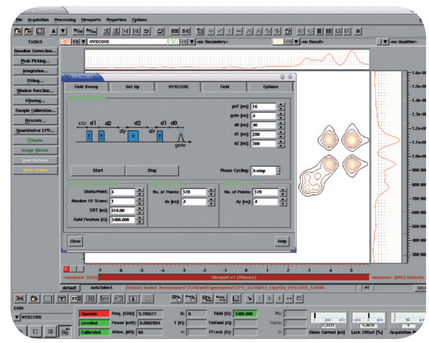
Xepr presents three contexts for Pulse EPR experiment definition: Assisted Pulse EPR, Pulse Tables, and PulseSPEL. Each environment is designed to meet the degree of control desired by the researcher.

Processing

Xepr implements a wide range of data processing techniques covering popular methods while providing an environment for the non-conventional.

Instrument Monitor

- Sample orientation
- Resonator temperature
- Resonator Q
- Field Position
- Teslameter Field
- Microwave Frequency
- Microwave Power



Data Processing

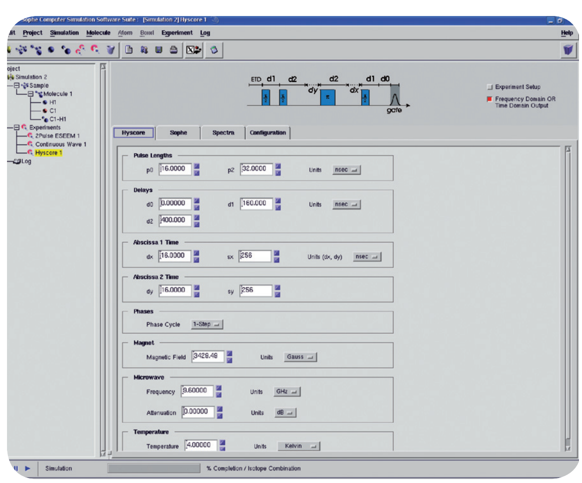
- Peak Analysis
- Fitting
- Deadtime Reconstruction
- FFT & Cross Term Averaging
- Convolution & Deconvolution
- User defined Macro processing
- And many more ...

Assisted pulse-EPR

- FT-EPR
- 2-pulse ESEEM
- 3-pulse ESEEM
- HYSCORE
- Pulsed ENDOR
- Pulsed ELDOR
- Saturation Recovery

Simulation & Interpretation

The optional simulation program Molecular Sophe bridges the gap between data collection and interpretation with an intuitive graphical user interface. A spin-system is built from atoms and bonds where magnetic interactions are easily defined and activated. Virtual experiments are then defined and configured as in real experiments with the E580.
With the inclusion of pulse sequence effects, e.g. tau-suppression and pulse selectivity, MoSophe simulations provide an added level of accuracy to aide researchers in data interpretation and experiment design.



Fourier Transform and Field Sweep Spectra

Acquiring the EPR Spectrum is the first step in probing the sample. In addition to providing the g-value and hyperfine structure, the EPR spectrum is the starting point for advanced studies of nuclear couplings, molecular motions and spin properties. Both FT and FS techniques provide selectivity that is not available via CW-EPR.

Sensitivity

When the spectral range is small (≤ 200 MHz), Fourier Transform (FT) techniques provide the EPR spectrum with superior sensitivity. Since the averaging of the signal is only limited by the electron relaxation (T_1), which is on the order of tens of microseconds, an incredible number of spectra can be recorded in a very short time.

Selectivity

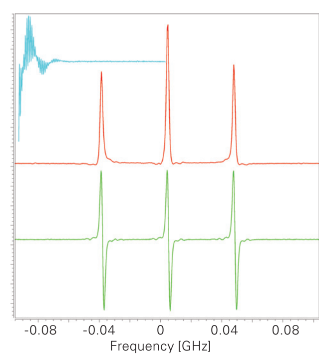
For large spectral ranges, Field Sweep (FS) techniques are required to record the EPR spectrum. Any pulse sequence which generates an ESE or FID, can be used to acquire the EPR spectrum. Numerous opportunities for filtering the spectrum are possible, e.g. exploiting differences in T_1 to record the individual EPR spectrum of species in overlapping spectra.

Interaction Isolation

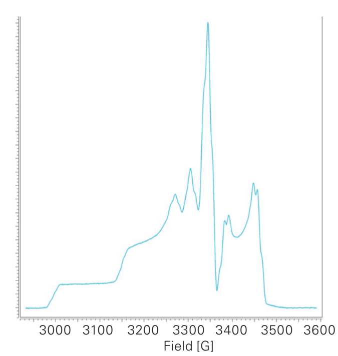
The 2D-SECSY (spin echo correlation spectroscopy) experiment records the T_2 variation across the EPR spectrum, either by FT technique or by a field sweep. The SECSY spectrum separates the homogeneous and inhomogeneous broadening contributions to the EPR spectrum.
The 2D-EXSY (exchange spectroscopy) experiment probes the magnetization transfer between different hyperfine lines or EPR species and thus offers a view of intra- and intermolecular processes in the system.

Resolution

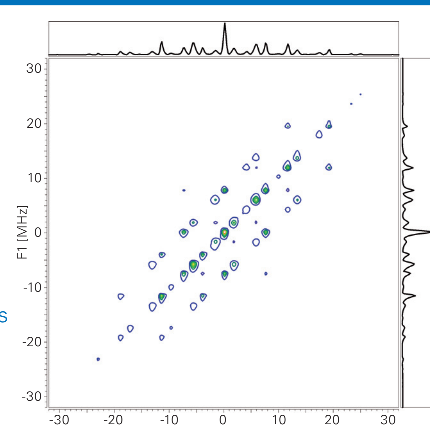
FT-EPR techniques are valuable for the study of short lived radical species such as those generated by optical excitation. The time between species generation and detection can be varied to monitor species growth/decay with a time resolution of a few nanoseconds.



FT-EPR (red) spectrum 400 000 averages in 10 s. CW-EPR (green) spectrum 1 scan in 10 s.



Field Sweep Echo Detected EPR Spectrum of Cu-Pt Complex



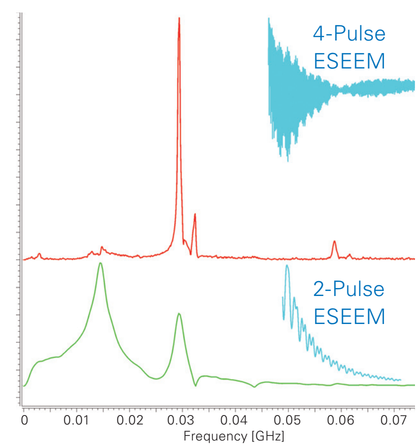
In the 2D-FT-EXSY spectrum, cross peaks occur when dynamic processes such as molecular reorientations (rotations), chemical reactions, or spin-exchange are present.

ESEEM & ENDOR

ESEEM and ENDOR techniques are invaluable tools for probing the microscopic environment of the paramagnetic centers. Both techniques record the nuclear hyperfine spectrum providing the identity, the geometry and number of nuclei present. Analysis of the couplings provides the spin density distribution and a picture of the molecular orbitals.

Electron Spin Echo Envelope Modulation - ESEEM

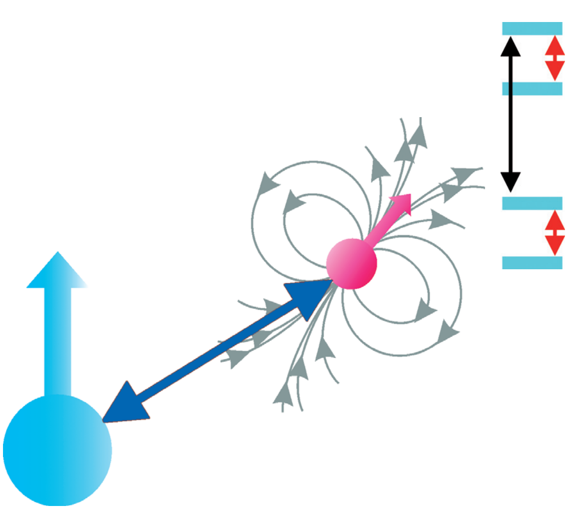
ESEEM experiments are time-domain microwave techniques that offer high sensitivity for small electron-nuclear couplings at low frequencies. Direct analysis of the time domain spectrum provides the number of interacting nuclei while analysis of the frequency domain spectrum shows the identity, coupling, and positioning of the nuclei.

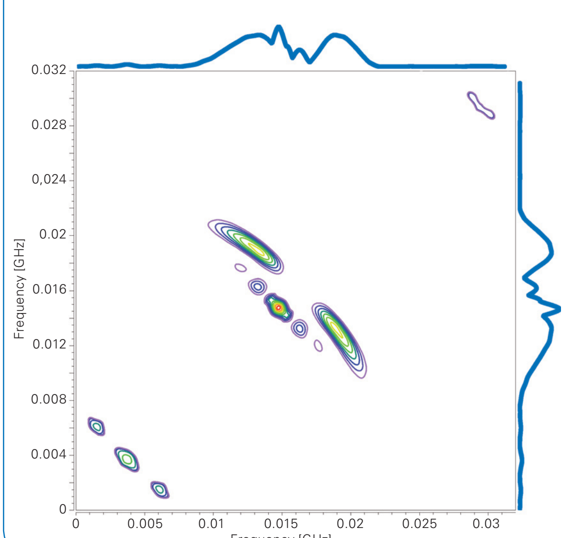


Numerous ESEEM sequences are available for increased sensitivity and resolution: 4-pulse (top) vs. the 2-pulse (bottom) ESEEM spectrum of powder spin label.

Hyperfine Sublevel Correlation-HYSCORE

The most popular ESEEM technique for the study of disordered systems is the 2D-HYSCORE experiment. The added spectrum dimension increases the sensitivity for the detection of nuclei with large anisotropic couplings, which are often missing from other ESEEM techniques.





HYSCORE experiments are ideal for the detection of broad ESEEM lines with high resolution: ^{1}H and ^{13}C HYSCORE of powdered spin label.

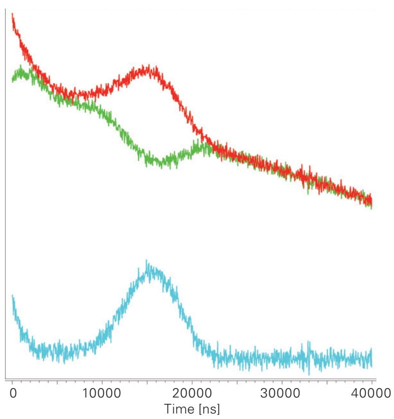
The E 560 DICE Unit

Electron Nuclear Double Resonance - ENDOR

Combining both MW and RF pulses, Pulse-ENDOR experiments are a versatile set of multi-resonance techniques to probe weak and strong electron-nuclear couplings selectively.
The Mims and Davies ENDOR sequences are here the most prominent techniques but the capabilities of the DICE unit go far beyond. Combined with the legendary Flexline pulse-ENDOR resonator numerous advanced sequences are executed at the highest level of performance.

- Pulse-TRIPLE
- HYEND
- Hyperfine selective ENDOR
- Pulse-ENDOR induced EPR
- Nuclear spin FID/echo detection
- Multiple quantum ENDOR
- Nuclear spin nutation
- Stochastic excitation

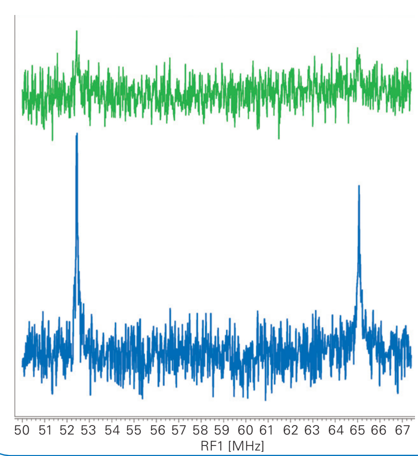
Nuclear Spin FID and Echo



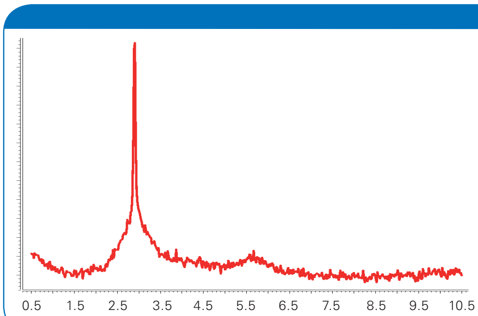
Nuclear spin FID and echo detection gives access to the nuclear spin relaxation times and provides additional filters for the ENDOR spectrum.
RF phase cycling is required to eliminate unwanted signal contributions.

Stochastic ENDOR

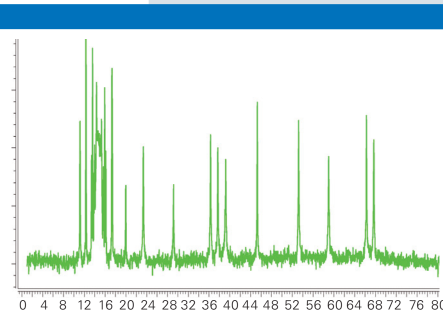
In a conventional ENDOR experiment the RF is swept in a linear way while in stochastic ENDOR the excitation frequencies are chosen randomly.
A considerable improvement in baseline stability and a reduction of the relaxation bottleneck greatly improves the ENDOR spectrum.



Linear sweep (top) and stochastic excitation (bottom) of ^{31}P nuclear spins in silicon at 10 K



Davies ENDOR of natural abundant ^{29}Si in quartz showing an excellent sensitivity at very low frequencies.



Davies ENDOR of ^{1}H in a succinic acid single crystal showing an excellent sensitivity over a large frequency range.

ELDOR & Relaxation

The global structure of molecules, long range distances and motional dynamics are readily probed using ELDOR techniques and relaxation measurements. Distances up to 80 Å can be measured by 4p-DEER. Internal vibrations, external collisions, and global tumbling can be assessed via relaxation measurements of T_1 and T_2.

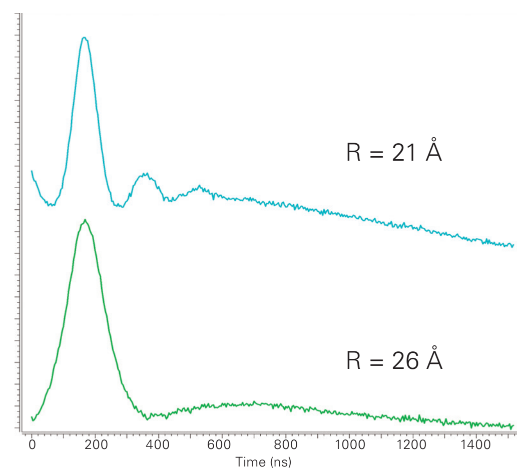
Long Range Distances

Pulse DEER techniques combined with site directed spin labeling are invaluable in the structural study of large molecules, such as proteins and polymers. Utilizing two microwave sources, DEER experiments are routinely used to probe distances between unpaired electrons from 15 Å to 80 Å.

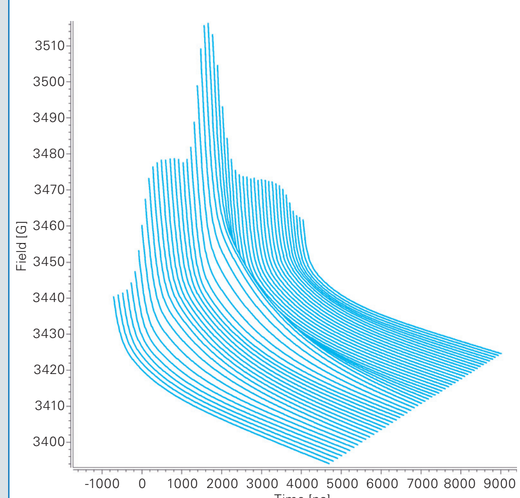
Distribution of Distances

A major advancement in distance measurements was the introduction of the dead-time-free DEER sequence. In addition to the average distance between EPR species, the 4-pulse DEER experiment allows the determination of the distance distribution as well.

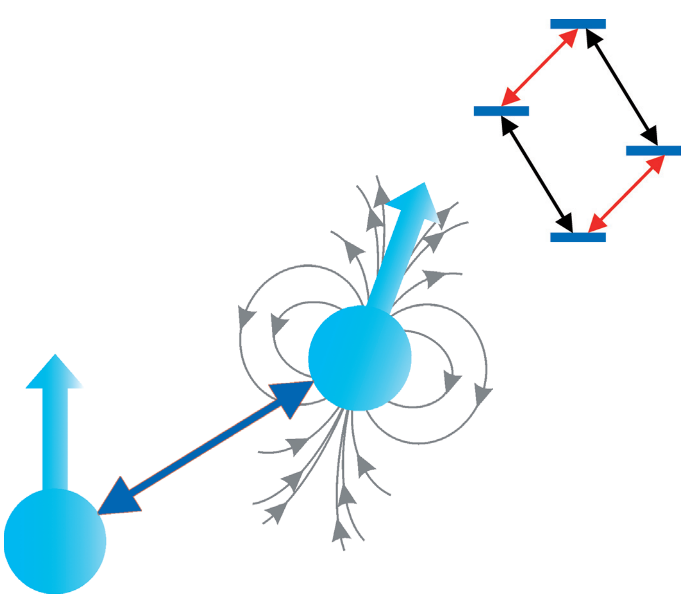
4-pulse DEER measured with the E 580-400 ELDOR unit



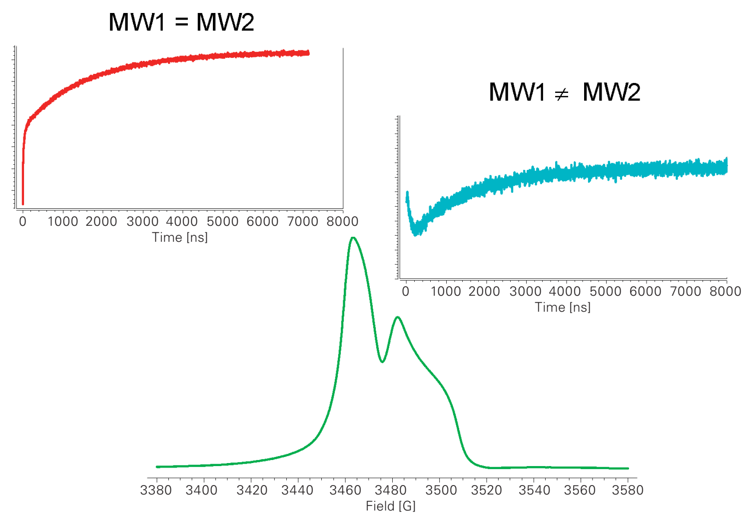
DEER techniques access long range distances as well as the distribution of distances in the system: 4p-DEER spectra of spin labeled Lysozyme.
Data courtesy W. Hubbell



2D relaxation times reflect the system dynamics as related to the molecular structure: Echo decay (T_2) vs Field of spin label encapsulated in Li-X.



SR-ELDOR measured with the LCW channel and E 580-400 ELDOR unit



Relaxation process connecting different parts of the EPR spectrum provide insight into structural dynamics: Saturation Recovery EPR and ELDOR of ^{15}N spin labeled Hemoglobin.
Data courtesy P. Fajer.

Internal Relaxation

Investigating how different parts of the EPR spectrum communicate via cross relaxation and nuclear relaxation pathways provides valuable information towards understanding dynamic processes and the structure of the system. A variation of the Saturation Recovery experiment to measure these influences is the SR-ELDOR experiment where two microwave frequencies are used to measure the saturation recovery.

Structure and Dynamics

Through the electronic relaxation times, T_1 and T_2, a wealth of information about dynamics and structure are available.

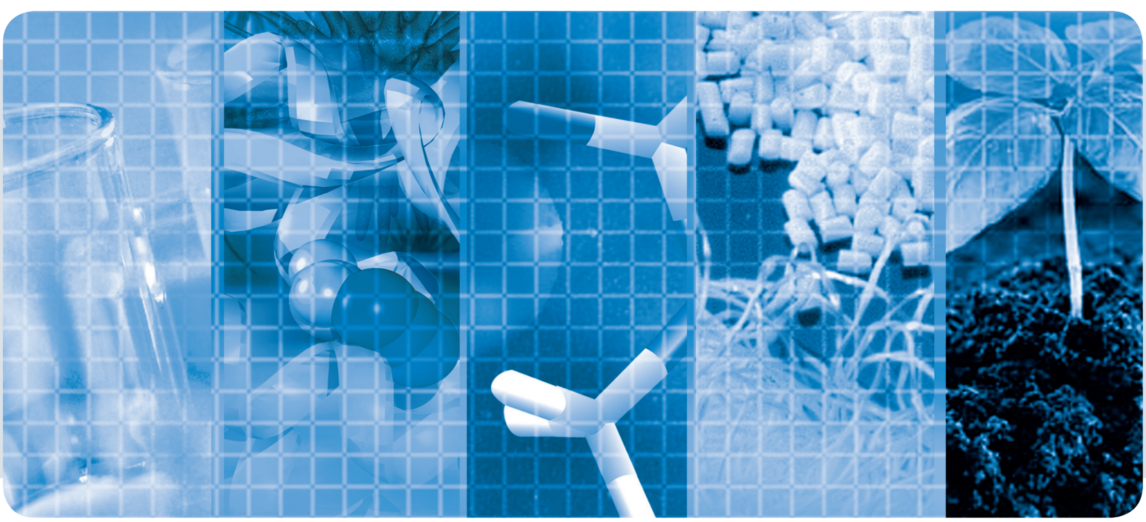
Spin Lattice Relaxation, T_1	Spin-Spin Relaxation, T_2
• Molecular collisions	• Molecular tumbling
• Excited state coupling	• Internal rotation
• Lattice vibrations	• Dipolar interactions

Bruker BioSpin, your Solution Partner

Bruker BioSpin provides a world class, market-leading range of analytical solutions for your life and materials science needs.

Our ongoing efforts and considerable investment in research and development illustrates our long-term commitment to technological innovation on behalf of our customers. With more than 40 years of experience meeting the professional scientific sector's needs across a range of disciplines, Bruker BioSpin has built an enviable rapport with the scientific community and various specialist fields through understanding specific demand, and providing attentive and responsive service.

Our solution-oriented approach enables us to work closely with you to further establish your specific needs and determine the relevant solution package from our comprehensive range of instruments, or even collaborate with you on new developments.



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