EPR Spectroscopy and Imaging

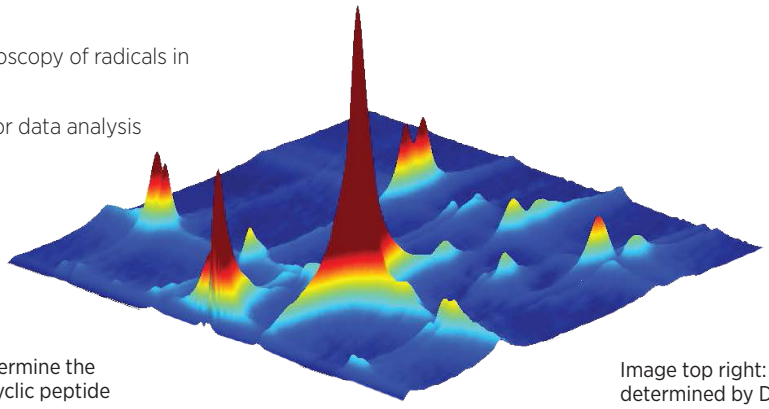
The University of Queensland's Centre for Advanced Imaging (CAI) contains a comprehensive range of Electron Paramagnetic Resonance (EPR) instruments. Samples for study must contain radicals (paramagnetic centres) and can be in the form of a powder, crystal, solution or solid with no limit on molecular size.

Access to the EPR facilities is available on a fee basis. Expert staff at CAI offer the following services:

- Experimental planning and optimisation
- Structural biology using spin probes and spin labels
- Continuous wave and pulse EPR spectroscopy for identification and structure determination of paramagnetic centres. Applications include inorganic and organic molecules, catalysts and active sites in enzymes.
- EPR imaging and spectroscopy of materials such as polymers
- EPR imaging and spectroscopy of radicals in small animals (mouse)
- Computation software for data analysis

Example applications include:

- Structural determination of soluble and membrane proteins, DNA and RNA using spin labels and paramagnetic probes
- Characterisation of catalytic centres
- Polymer characterisation
- Determine the type, amount and location of radicals in materials science using EPR imaging
- Measurement of tissue oxygen levels and detection of reactive oxygen species using *in vivo* EPR
- Quantification of antioxidant levels in food and beverage samples.



EPR spectroscopy is used to determine the structure of molecules like the cyclic peptide Cu(II) complex

Image top right: An example of a protein complex determined by DEER spectroscopy – a cytochrome P450 with its electron transfer partner

EPR spectroscopy detects radicals and determines their concentration, structure and chemical function.

EPR Spectroscopy

Bruker Elexsys E500 CW (X-, S-band) variable temperature (2 – 400 K) EPR Spectrometer

This spectrometer is equipped with N_2 heating and cooling in the range 100 – 400 K, or liquid helium cooling from 4 – 300 K.

We have specialised capabilities for:

- Quantitative EPR – spin (radical) counting
- Optical excitation of the sample
- Measurement in water / polar solvents at room temperature using dedicated resonators and sample holders (e.g. flat cells and capillaries)

Bruker Elexsys E580 Pulsed Q-band (33GHz) and X-band (9.6 GHz) Spectrometer with high power microwave amplifiers for EPR, ENDOR, ESEEM, DEER and ELDOR experiments in the temperature range 1.7-300 K

- Optical windows allow for sample illumination
- Field-sweep EPR in both continuous wave (CW) and pulse mode over the field range 0-1.4 T
- Electron nuclear double resonance (ENDOR) at both X-band and Q-band in the frequency range 0.1 – 200 MHz for measuring electron-nuclear couplings to magnetic nuclei including ^{1}H, ^{13}C, ^{14}N, ^{15}N, ^{17}O, ^{19}F, ^{31}P, ^{57}Fe
- Electron spin echo envelope modulation (ESEEM) experiments such as three-pulse ESEEM and HYSCORE, for measuring electron-nuclear couplings with high sensitivity at both X-band and Q-band due to the availability of high power traveling wave tube amplifiers
- Double electron electron resonance (DEER) or pulse electron double resonance (PELDOR) for the measurement of electron-electron distances in the range ca. 15-100 Å, typically for research on large biomolecules or polymers containing two or more spin labels. Sensitivity at Q-band is <20 µM with a sample size <10 µL. The spectrometer is suitable for paramagnetic spin labels based on organic radicals like the commonly used MTSSL or metal tags like ones based on Gd(III) ions. DEER at X-band in resonators accommodating either 2 mm, 3 mm, or 3.8 mm sample tubes offers a range of excitation bandwidths and sensitivities for experiments using organic spin labels or suitable centres intrinsic to the material under investigation
- ELDOR – electron double resonance capabilities employing two microwave sources. For example, ELDOR detected NMR for measuring electron-nuclear couplings

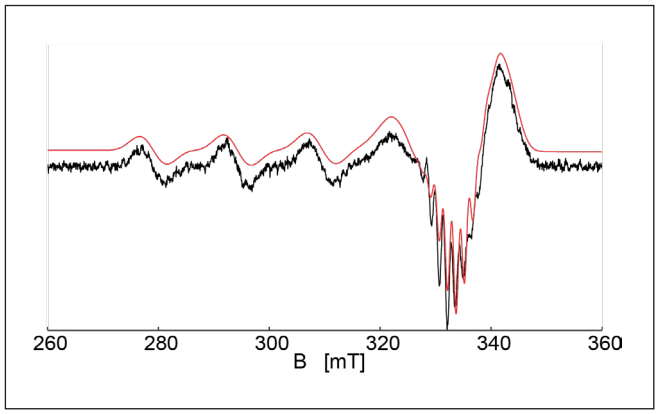
EPR Imaging

Non-invasive EPR imaging offers the capacity to spatially locate paramagnetic molecules in small animals and bulk materials.

Bruker Elexsys E540 (X-, L-band) Imaging Scanner

This technique enables identification of radicals in a sample using CW EPR spectroscopy and, spatial localisation of suitable spin probes or paramagnetic centres. Spatial resolution depends upon the spin probe, for narrow line radicals the resolution is around 500 µm. Example applications include the study of paramagnetic centres in materials such as polymers and *in vivo* imaging of small animals using introduced spin probes to measure for example oxygen concentration or spin traps to detect reactive oxygen species.

- Imaging at X-band offers high quality sensitivity and resolution for materials such as polymers, powders, or non-polar solutions at room temperature. For aqueous samples, e.g. cells or sections, measurement in flat cells and imaging in 2D is possible
- Imaging at L-band enables *in vivo* imaging of small objects up to the size of a mouse (active volume of 30 mm^3)



X-band (9.65 GHz) CW EPR spectrum (black) and its simulation using XSophe (red) which identifies a Cu^{2+} complex and its ligands

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