The EPR Lab at the School of Chemical Sciences University of Illinois

- Electron Paramagnetic Resonance

- Also called ESR (Electron Spin Resonance) or EMR (Electron Magnetic Resonance)

- Uses permanent electromagnets (therefore can be turned on/off on a regular basis), as opposed to superconducting magnets in NMR
The Electron Paramagnetic Resonance Lab is a service facility supported by user fees and by the School of Chemical Sciences.

This facility provides the University of Illinois as well as other members of the scientific community with EPR (also called ESR, electron spin resonance, or EMR, electron magnetic resonance), ENDOR, and ESEEM facilities and expertise. Additionally, the facility is involved in collaborative research and works with scientists worldwide who are interested in EPR techniques. We encourage scientists of all disciplines to visit our center and undertake collaborative or other work. Where feasible, samples can be sent in for spectral examination by laboratory personnel. Prospective users should contact the Lab Manager, Dr. Mark Nilges, to discuss the scientific problem and make the necessary arrangements.
Electron Paramagnetic Resonance Lab Staff

Mark Nilges, Ph.D.
Lab Manager
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List of publications

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NMR/EPR Lab Director
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Mark's Hours of Operation:
Monday: 9 am - 5 pm
Wednesday: 1 pm - 5 pm
Friday: 1 pm - 5 pm

Andre's Hours of Operation:
Monday-Friday 9 am - 5 pm
Instruments are located in the basement of the Medical Sciences Building (across from Noyes)
EPR Spectrometers

14D Medical Sciences Building

**VarianXBand**
- E-12” CW EPR
- X-band (8-10 GHz)
- 320 mT at g=2

Available for Use

**VarianQBand**
- E-15” CW EPR
- Q-band (35 GHz)

Not Yet Available

**Elexsys2**
- E-12” FT EPR (E560 series)
- Pulse/CW mode

Not Yet Available
Self-service Instrument Use

SCS EPR Lab Financial Authorization Form - This form must be filled out, printed and then signed by both the user and their faculty advisor.

1. All users must have a signed authorization form with a valid account number on file. Contact Tracie Hubert with questions (thubert@illinois.edu). The signed form must be dropped off in 146 RAL.
2. Users operating instruments by themselves must have training and approval prior to use.
3. All users are responsible for supplies such as liquid helium and EPR tubes.
4. Food and Beverages are not allowed in the instrument labs.
5. Safety glasses must be worn when handling samples at cryogenic temperatures.
6. No open-toe shoes.
7. If you will not use the instrument after signing up, please cancel as soon as possible. Persons who do not cancel by 9:00 a.m. the day that they run or do not show up will be charged a $25 fee.

SCS EPR Rates
Effective Starting 1 Dec 2016

<table>
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<tr>
<th>EPR Spectrometer</th>
<th>Internal Rate ($/hour)</th>
<th>Non-UI Academic Rate ($/hour)</th>
<th>External Rate ($/hour)</th>
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<tbody>
<tr>
<td>Varian XBand</td>
<td>20.00</td>
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<td>EPR Staff Service</td>
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<td>Data Analysis</td>
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Supplies

<table>
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<th>Supplies</th>
<th>Cost</th>
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<tr>
<td>Liquid Helium</td>
<td>$14.00/Liter</td>
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<tr>
<td>Helium Dewar Rental</td>
<td>$5.00/Day</td>
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<tr>
<td>Liquid Nitrogen</td>
<td>$0.50/Liter</td>
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<tr>
<td>Tech Grade Quartz EPR Tubes</td>
<td>$5.00 Each</td>
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What EPR Can Do For You

Similar to NMR (nuclei), except in EPR we are detecting unpaired electrons’ transitions

- detect any species that have unpaired electrons, including free radicals, transition metal ions (Cu$^{2+}$; Co$^{2+}$, Mn$^{2+}$, etc.) and defects in materials

- unambiguously detect unpaired electrons / paramagnetic species
- sensitive to local environments, insight to molecular structure
- line shape changes, investigate dynamic process

Other methods include ENDOR (EPR + NMR) and ESEEM

- They are extremely powerful techniques for probing the structure of “active sites” in metalloproteins

- **ENDOR** = Electron-Nuclear **DOuble Resonance**; it is an EPR-detected NMR technique
  - monitor EPR signal coming from induced NMR transitions
  - significantly increased spectral resolution (hyperfine couplings)
  - measure the interactions of the electron with the surrounding nuclei

- **ESEEM** = Electron **Spin Echo Envelope Modulation**
  - induced by nuclei hyperfine-coupled to the unpaired electron spin
Detection of Cu(II) species in metalloprotein

Gennis and Lu group

Figure 2. (a) Crystal structure of Cu(II)-Nmar1307 (PDB ID: 5FC9). (b) Zoom-in of the copper binding site with nearby amino acids shown in black ball-and-stick representation. The coordinating water is shown as a red sphere, the primary ligands as cyan sticks, and the Cu ion as cyan sphere.

Detection of Co(II) species in inorganic complex

Fout group

Also to $^{35}$Cl and $^{37}$Cl (2b, bottom left)
Detection of Ni(I) and Fe(II) species

Both Ni and Fe species

Hyperfine coupling to $^{31}\text{P}$

Rauchfuss group