RD-ZULF-NMR
Radiation detected Zero to ultralow-field Nuclear Magnetic Resonance

VITO – ISOLDE

Selim Zoorob

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A look into MRI Technology

MRI = Magnetic Resonance Imaging

NMR = Nuclear Magnetic Resonance

• While MRI is founded in NMR, both techniques relying on radiation data to identify unknown compounds.
• NMR uses radiofrequencies
• MRI based on radiation intensity

MRI technology can be improved

Brain MRI images [2]

MRI machine [10]

MRI machine prices [8]

MRI = Magnetic Resonance Imaging

NMR = Nuclear Magnetic Resonance

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Selim Zoorob | ZULF-RD-NMR
The future of MRI tech?
High-field NMR vs ZULF-NMR SETUP

The Earth's magnetic field intensity is roughly between 25 - 65 microT (.25 - .65 gauss)
Radiation detected NMR (β-NMR [9]):

• unstable probe nuclei
• spins polarized by external source = hyperpolarization (e.g. lasers)
• spins excited by radio-frequency pulses
• detection of anisotropy in emitted radiation

=> Spectra as in high-field NMR but stronger signal
Why RD-ZULF-NMR? [9]

β-NMR + ZULF-NMR = RD-ZULF-NMR

Characteristics:
- Use radioactive isotopes
- Hyperpolarized
- Spins excited by radio-frequency pulses
- Detection of anisotropy [3]

Combines β-NMR and ZULF-NMR advantages:
- Adaptive to specific applications
- ZULF-NMR:
  - Spin-spin interactions explored in different ways
  - Apparatus is cheap and transportable
  - No loss in spectral resolution associated with inhomogeneous samples
- β-NMR:
  - Extremely high sensitivity
  - Many more probe nuclei
RD-ZULF-NMR Setup

**pH\(_2\) setup**

- H\(_2\) gas
- Liquid N\(_2\)
- Catalyst

**Hyperpolarizing setup**

- 50% pH\(_2\)
- Liquid N\(_2\)
- B\(_0\)

**Parahydrogen**

**Orthohydrogen**

- Overall
- B\(_{w,core}\)
- B\(_{w,1}\)
- B\(_{w,2}\)

**Periodic Table**

- 13 N
- 7 8

**Chemical Composition**

- 9.965 m 1/2
- M 5345.48 (0.27)
- \(\beta^* = 100\%\)
Water cooled Helmholtz Coils

Up to 250 Gauss at 88 °C (with water cooling on)
Beta detectors

Two plastic scintillators + Two Silicon photomultipliers (SiPM) connected to a single board with separate preamplifiers.
Data Collection

DAQ = Data Acquisition System

Background noise peak at ~60mV

CAEN DAQ

With radioactive source (Strontium-90)

When removing radioactive source
• Approval of safety procedures
• Setup at Geneva Hospital
• Test of detectors in ZULF-NMR
• Polarization test at MAINZ University
Special thanks to:
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• Monika Piersa-Silkowska, PhD.
• Nikolay Azaryan, PhD.
• Marcus Jankowski, PhD Candidate.
References

Nuclear spin parameters specific to the system being studied:

- $J$-couplings ($J_{II}$ and $J_{IS}$),
- homonuclear chemical shift differences ($\delta_{I1} - \delta_{I2}$),
- heteronuclear gyromagnetic ratio differences ($\gamma_{I} - \gamma_{S}$),
- and characteristic spin relaxation times ($T_{relax}$).

[1]

**Example boundary values**

To get a sense of the real magnetic field values of the boundaries for a typical system, let us assume the following values for the molecule shown:

- $J_{II} = 10$ Hz
- $J_{IS} = 150$ Hz
- $\delta_{I1} - \delta_{I2} = 1$ ppm
- $T_{relax} = 1$ s for all spins

The gyromagnetic ratios for $^1H$ and $^{13}C$ are 42 MHz/T and 10.5 MHz/T, respectively.

This gives the following boundaries:

- a: Between 3.7 and 15 nT, depending on whether we are considering $^1H$ or $^{13}C$
- b: 750 nT
- c: 37 mT

For reference, Earth-field is around 50 µT.
\[ \vec{B}_o = 0 \]
Randomly oriented

\[ \vec{B}_o > 0 \]
Highly oriented

Radiofrequency: Change in orientation

\[ \Delta E \]
Mobile MRI System [12]

MRI machine dimensions [3]
<table>
<thead>
<tr>
<th></th>
<th>Standard NMR</th>
<th>ZULF-NMR</th>
<th>ZULF-RD-NMR</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Magnetic field</strong></td>
<td>Several - dozen Tesla</td>
<td>&lt; microTesla</td>
<td>0.5 – dozen Tesla</td>
</tr>
<tr>
<td><strong>Source of polarization</strong></td>
<td>Boltzmann distribution</td>
<td>hyperpolarization</td>
<td>In-situ or outside hyperpolarization</td>
</tr>
<tr>
<td><strong>Degree of polarization</strong></td>
<td>1e-5</td>
<td>1e-5 – dozens %</td>
<td>Several – dozens %</td>
</tr>
<tr>
<td><strong>Probe nuclei</strong></td>
<td>Stable</td>
<td>Stable (1H, 13C, …)</td>
<td>Unstable (ms to days t(^{1/2}))</td>
</tr>
<tr>
<td><strong>Signal detection</strong></td>
<td>Inductive (pick-up coil)</td>
<td>magnetometer</td>
<td>Anisotropy in emitted radiation</td>
</tr>
<tr>
<td><strong># nuclei to record signal</strong></td>
<td>1e16 – 1e17</td>
<td>…. - 1e16 – 1e17</td>
<td>1e6-1e8</td>
</tr>
</tbody>
</table>
β-NMR [4]

β-NMR explores the angular distribution ($w$) of beta-irradiation of polarized beta-active nuclei (beta-nuclei);

$$w(\theta, t) = 1 + ap(t)\cos\theta, \quad \cos\theta = pk/pk$$

to determine the evolution of nuclear polarization $p(t) = \langle I(t) \rangle$ by detection of β-particles.

Measurement of beta-decay asymmetry $\varepsilon$ :

$$\varepsilon = (N_+ - N_-)/(N_+ + N_-)$$

where $N_+$ and $N_-$ are numbers of decay electrons emitted along and against the nuclear polarization direction.

- $k$: translation momentum of the β-particles
- $I$: spin of beta-nucleus
- Angle brackets $\langle \rangle$: standard quantum statistical averaging
- $t$: time starting from the moment of creation of β-nucleus
- $a \sim 0.1$