β-NMR in liquids

Opening new frontiers for biomolecular studies and nuclear physics

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Outline

• β-NMR for biology
• Principles of β-NMR
• Experimental setup
• Measurements & results
• Conclusion and outlook
β-NMR for biology
Advantage over conventional NMR

- 10 billion times more sensitive
- Use probe nuclei with complementary properties
- Real-time observation of chemical reactions

picture courtesy of B. Karg
Principles of β-NMR
Asymmetric $\beta$-decay from polarized nuclei
Detection of the resonance by $\beta$-decay asymmetry

$\beta$-NMR

- Asymmetric $\beta$-decay from polarized nuclei
- Detection of the resonance by $\beta$-decay asymmetry
Experimental setup
β-detectors & chamber

β-detectors with Si-PMT’s
M. Madurga, Tennessee

PCB shimming coils

Sample ladder

RF excitation coil

Stabilization probe
M. Baranowski, Poznań

Exchangeable collimator

$B_0$
B₀-field stabilization

- Compact vacuum-compatible pulsed NMR probe
- PID driven variable resistor

**From 100 ppm drift to ~1 ppm stability**
NMR in liquids

- Molecular tumbling leads to narrow peaks
Measurements & results
• Conventional NMR spectra always relative to a reference
  • (e.g. 0.1 M $^{23}$NaCl in D$_2$O)

• References needed for β-NMR
  • Indirect use of conventional NMR reference

\[
\frac{\nu ^{26}_{\text{Na}_{1.2T}}}{\nu ^{1}_{\text{H}_{1.2T}}} \sim \frac{\nu ^{23}_{\text{Na}_{7.05T}}}{\nu ^{1}_{\text{H}_{7.05T}}}
\]

• Use an absolute scale
  • (bare nucleus)
• ppm precise $^{23}\text{Na}/^{26}\text{Na}$ magnetic moment ratio

Indirect reference
Absolute scale: reference

- Accurate magnetic moments needed
  - Diamagnetic correction not accurate (up to 30% off)

<table>
<thead>
<tr>
<th>Method</th>
<th>Literature $^{23}$Na magnetic moment$^{[1]}$ ($\mu_n$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABMR</td>
<td>+2.217522(2)</td>
</tr>
<tr>
<td>NMR</td>
<td>+2.2176556(6)</td>
</tr>
</tbody>
</table>

- A difference of 134 ppm!

- New ab initio NMR shielding calculations save the day!

<table>
<thead>
<tr>
<th>Method</th>
<th>New $^{23}$Na magnetic moment$^{[2]}$ ($\mu_n$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABMR</td>
<td>+2.217495(2)</td>
</tr>
<tr>
<td>NMR</td>
<td>+2.217500(7)</td>
</tr>
</tbody>
</table>

- This gives us an accurate reference
  - Combined with ratios leads to accurate moments

Absolute scale: accurate $\mu_i$

- 100 times increase of precision of the magnetic moment of $^{26}\text{Na}$
- 10 times increase for $^{27-31}\text{Na}$ (from solid state $\beta$-NMR)\[^1\]

\[^1\] M. Keim et al. The European Physical Journal A 8, 31 (2000)
R.D. Harding et al. article in preparation
ppm precise magnetic moments

- set of beta-NMR isotopes with ppm precise magnetic moments allow for probing different chemical effects

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$I$</th>
<th>$T_{1/2}$ (ms)</th>
<th>$Q$(mb)$^{[1]}$</th>
<th>old $\mu_I$ ($\mu_N$)$^{[1]}$</th>
<th>new $\mu_I$ ($\mu_N$)$^{[2]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{23}$Na</td>
<td>$3/2$</td>
<td>stable</td>
<td>+105.6(12)</td>
<td>-</td>
<td>2.217500(7)$^a$</td>
</tr>
<tr>
<td>$^{26}$Na</td>
<td>3</td>
<td>1071</td>
<td>-5.3(2)</td>
<td>2.851(2)</td>
<td>2.849378(20)$^b$</td>
</tr>
<tr>
<td>$^{27}$Na</td>
<td>$5/2$</td>
<td>301</td>
<td>-7.2(3)</td>
<td>3.894(3)</td>
<td>3.89211(11)</td>
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<tr>
<td>$^{28}$Na</td>
<td>1</td>
<td>31</td>
<td>+39.5(12)</td>
<td>2.420(2)</td>
<td>2.41843(9)</td>
</tr>
<tr>
<td>$^{29}$Na</td>
<td>$3/2$</td>
<td>44</td>
<td>+86(3)</td>
<td>2.457(2)</td>
<td>2.45534(8)</td>
</tr>
<tr>
<td>$^{30}$Na</td>
<td>2</td>
<td>48</td>
<td></td>
<td>2.069(2)</td>
<td>2.06815(5)</td>
</tr>
<tr>
<td>$^{31}$Na</td>
<td>$3/2$</td>
<td>17</td>
<td></td>
<td>2.298(2)</td>
<td>2.29668(8)</td>
</tr>
</tbody>
</table>

$^a$ Corrected $\mu(^{23}$Na) based on NMR experiment
$^b$ Based on our improved ratio of the magnetic moments of $^{26}$Na to $^{23}$Na

- Applicable to:
  - Beta-NMR: Biomolecular studies, Material science & Nuclear Physics
  - Other fields

Summary

- β-NMR up to 10 billion times more sensitive
- Liquid state β-NMR 100 x increased resolution
  - referenced to conventional NMR
  - referenced to an absolute scale.
  - precise magnetic moments
- Interpretation of first biological measurements ongoing. See poster 18 – Kasia
Acknowledgements

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Nuclear Magnetic Resonance

- Nuclear spin ≠ 0
- B0 induces Zeeman effect
- Unequal distribution over magnetic substates (polarization)
- Spins flip due applied RF photons
- Detect emitted RF photon’s
Laser spin polarization

- Polarize atomic spins
- A laser accessible strong atomic transition (strong -> short T1/2)
- Circularly polarized light
- A closed “loop”

Nuclear polarization through hyperfine interaction
VITO Beamline

beam diagnostics
detection chamber
transitional field
optical pumping region
charge exchange chamber
5 degree deflector

electromagnet poles
Helmholtz coils for guiding field