What is the medical importance of NMR?
(see lecture No. 13. in this semester!)

Physical bases, spins and nuclei

Spins and nuclei

Protons and neutrons (and also the electrons) are particles having a spin angular momentum of 1/2.

If the number of protons or neutrons is add in the nucleus, then the total nuclear spin will not be zero!

Properties of nuclear spin

Nucleus: proton and neutron

Two magnetic moments (spin) pointing in opposite directions \(\Rightarrow\) zero net magnetic moment!

Nuclei with even \(Z\) and even \(N\) have nuclear spin \(I=0\) (isotopes are important)

If there are unpaired protons or neutrons in a nucleus, then the net nuclear spin (the intrinsic nuclear magnetic momentum) differs from zero.
Atoms for NMR

\[ ^1H, ^2H, ^3H, ^4H, ^12C, ^13C, ^14C, ^15N, ^16N, ^17O, ^18O, ^19F, ^23Na, ^31P, \text{ etc.} \]

The most frequently applied nuclei: \[ ^1H, ^13C, ^15N, ^17O, ^19F, ^31P \]

Signal depends on:
- Magnitude of the magnetic moment
- Concentration of the isotope

The split of the energy states (Zeemann)

Spin states with the magnetic field aligned with the external field.
Spin states with the magnetic field aligned against the external field.

The energy difference between the spin states does depend on the strength of the external magnetic field.

Orientation and reorientation on the microscopic level

\[ H=0; \; M=0 \]
\[ H>0; \; M>0 \]

\( m: \) magnetic moment of the individual atom

Graphical representation

Remember, the energy is proportional to the frequency!

An example: \( CH_4 \)

We can probe the energy difference of the \( \alpha \) - and \( \beta \) - state of the protons by irradiating them with EM radiation of just the right energy. In a magnet of 7.05 Tesla, it takes EM radiation of about 300 MHz (radio waves). So, if we bombard the molecule with 300 MHz radio waves, the protons will absorb that energy and we can measure that absorption. In a magnet of 11.75 Tesla, it takes EM radiation of about 500 MHz (stronger magnet means greater energy difference between the \( \alpha \) - and \( \beta \) - state of the protons).

What is the problem with this concept?

It is difficult to compare the data from two instruments with different strengths of magnetic fields.

Let’s use the chemical shift!
Chemical shift or $\delta$

We need a reference sample to standardize our instruments!
1. Measure the absorbance frequency of the standard: $f_r$
2. Measure the frequency for your own sample: $f_s$
3. Let's calculate the difference between the two: $\Delta f = f_r - f_s$
4. Normalise the difference with the frequency of the reference: $\delta = \Delta f / f_r$

The $\delta$, i.e. the chemical shift will be characteristic for your sample, but will not depend on the parameters of the instrument used for the experiments!

Why? Let's take an example!

An example: chemical shift

Imagine that we have a magnet where our standard absorbs at 300,000,000 Hz (300 megahertz), and our sample absorbs at 300,000,300 Hz. The difference is 300 Hz, so we take $300/300,000,000 = 1/1,000,000$ and call that 1 part per million (or 1 PPM).

Now let's examine the same sample in a stronger magnetic field where the reference comes at 450,000,000 Hz, or 450 megahertz. The frequency of our sample will increase proportionally, and will come at 450,000,450 Hz. The difference is now 450 Hz, but we divide by $450,000,000 (450/450,000,000 = 1/1,000,000, = 1 PPM)$.

(We do not have to calculate all these, the NMR machine does it for us!)

NMR spectrum

The absorption is proportional to the concentration of the corresponding nuclei.

The NMR spectrum is the energy absorbed by the system as the function of the frequency ($f$) of the excitation energy ($\Delta E$) or the magnetic field ($H$, $B$).

Due to local effects and fields the excitation energy (and thus frequency) is different for different nuclei.

Applications of NMR

- Structure of organic molecules and substances;
- Interactions of organic molecules;
- Structure of macromolecules (proteins, nucleic acids);
- Biological and artificial membranes;
- MRI: Magnetic Resonance Imaging.

SUMMARY

Thank you!