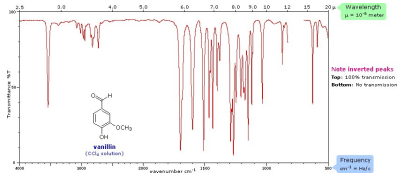
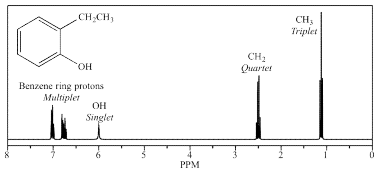
Biophysics

Ádám Orosz

Optical spectroscopic techniques, Radio spectroscopy methods



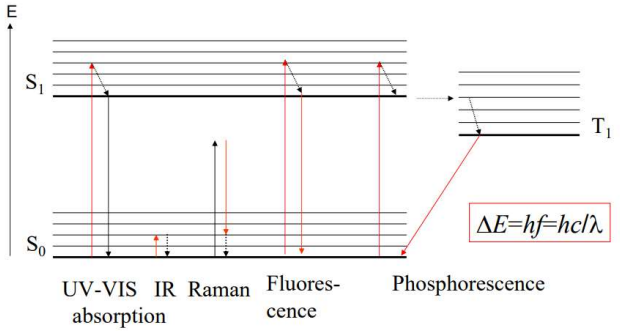


1. Optical spectroscopy - overview
2. Infrared spectroscopy
3. NMR spectroscopy

Lightabsoprtion and emission

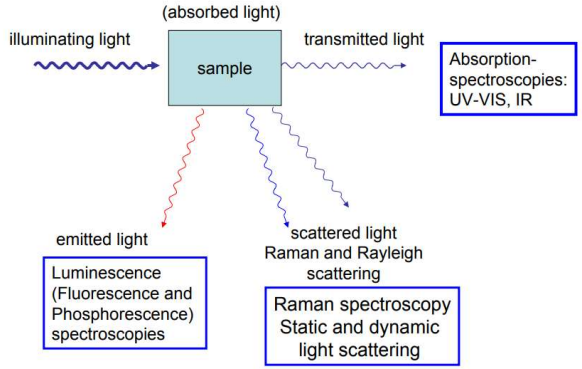
Why is light absorbed or emitted?

Jablonsky-diagram



Irradiation with EM waves

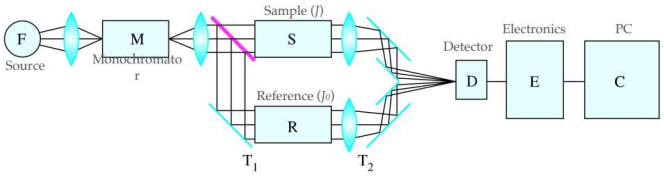
Which signals could be measured?

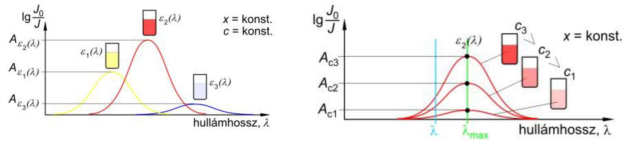


Absorption spectroscopy

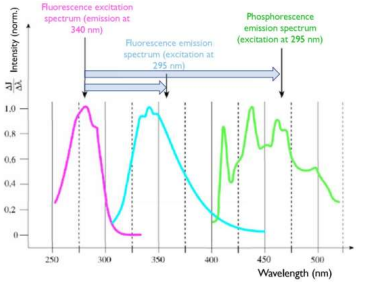
Qualitative and quantitave information

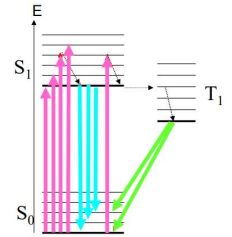
$$A = \lg\frac{J_0}{J} = \varepsilon(\lambda)cx \qquad A(\lambda)$$



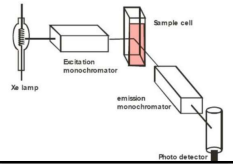


Emission spectroscopy





Fluorescence Phoshorescence



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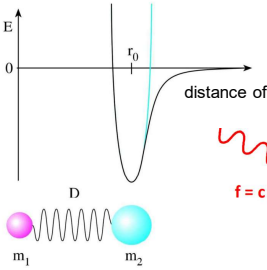
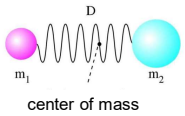
Infrared spectroscopy

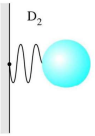
- Infrared light (IR): **λ= 800 nm – 1000 µm**
- Absoprtion spectroscopy
- Absorbed energy creates **molecular vivrations**
- Information on molecular structure

- Near infrared (NIR): λ= 800 nm – 2,5 µm
- **Middle infrared (MIR): λ= 2,5 µm – 50 µm**
- Far infrared (FIR): λ= 50 µm – 1000 µm





center of mass



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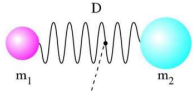
Wavelenght and wavenumber

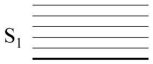
$$f = \frac{1}{2\pi}\sqrt{\frac{D}{m_{red}}} \qquad \lambda = \frac{c}{f} = 2\pi c\sqrt{\frac{m_{red}}{D}} \qquad \nu = \frac{1}{\lambda} = \frac{1}{2\pi c}\sqrt{\frac{D}{m_{red}}}$$

Classical physics picture

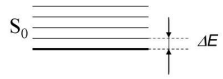


tömegközéppont

Quantum mechanical picture



$$f = \frac{1}{2\pi}\sqrt{\frac{D}{m_{red}}}$$



resonance with light of *f* frequency

$\Delta E = hf$

same!

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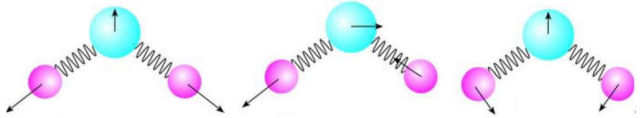
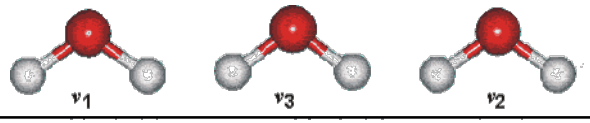
Normal vibrations

- Independent from eachother
- All atoms vibrate with the same frequency, but **different amplitudes** and **directions**.
- Example: normal vibrations of water



Symmetric stretch asymetric strech deformation



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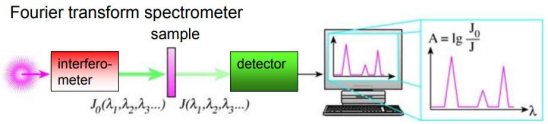
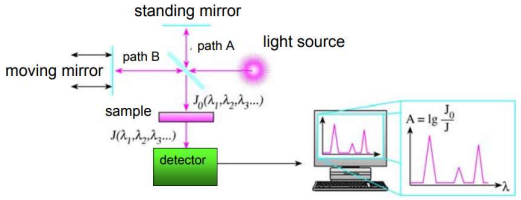
Measuring the IR spectrum





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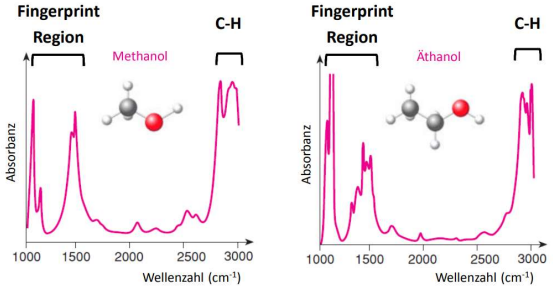
Identifying molecules, molecular structure



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Nuclear magnetic resonance (NMR)

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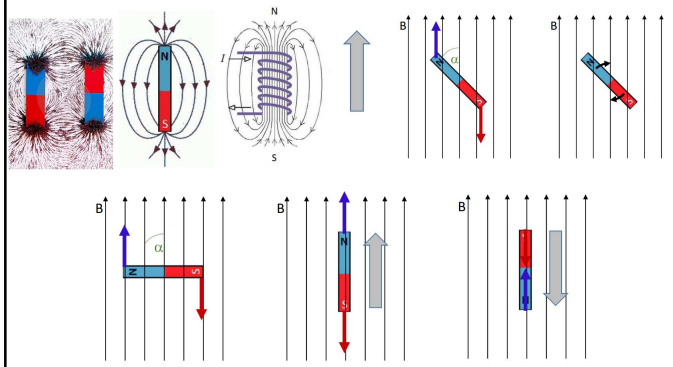
Magnetism



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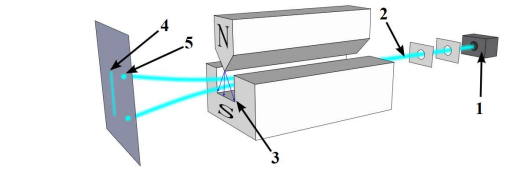
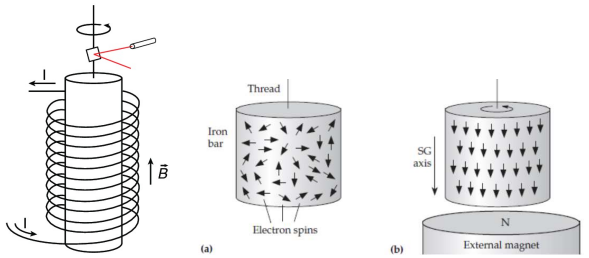
Magnetic momentum and spin





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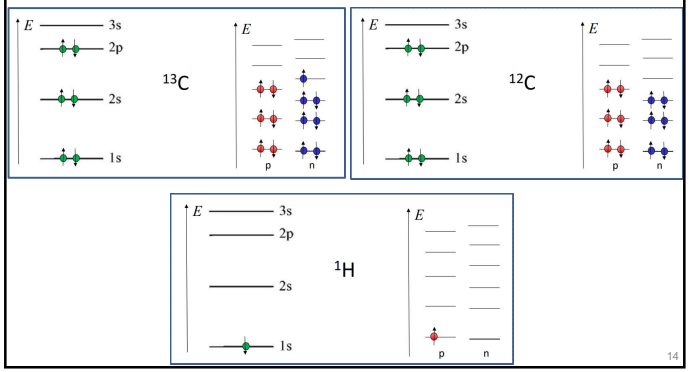
Nuclei which give NMR signal

^{1}H, ^{2}H, ^{3}H, ^{3}He, ~~^{4}He~~, ~~^{12}C~~, ^{13}C, ~~^{14}C~~, ^{14}N, ^{15}N ~~^{16}O~~
^{17}O, ^{19}F, ^{23}Na, ^{31}P...



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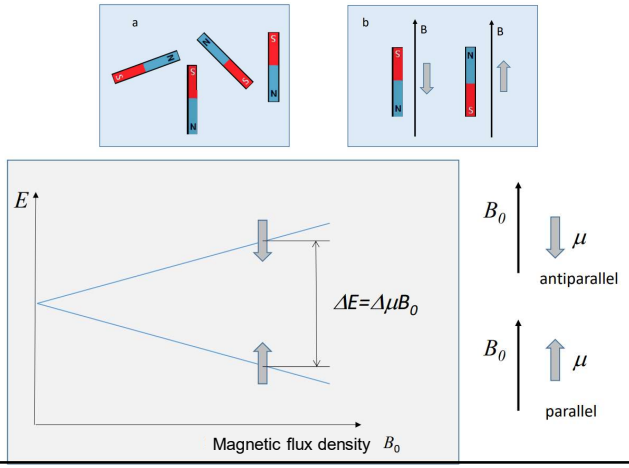
Zeeman effect



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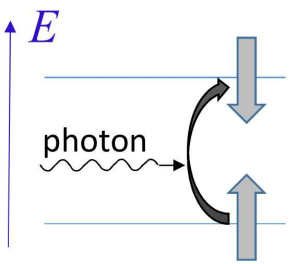
Resonance

$$\Delta E=\Delta\mu B_0=\gamma\hbar B_0$$

$$E_{photon}=hf=\Delta E$$

$$f=\frac{\gamma B_0}{2\pi}$$



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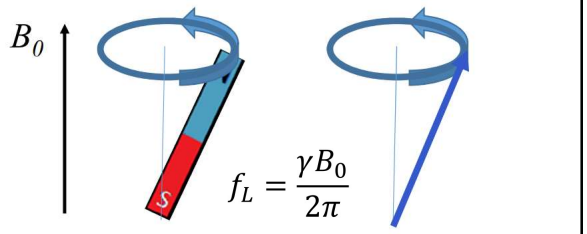
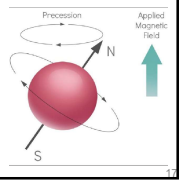
Spin (with magnetic momentum) in magnetic field
Precession





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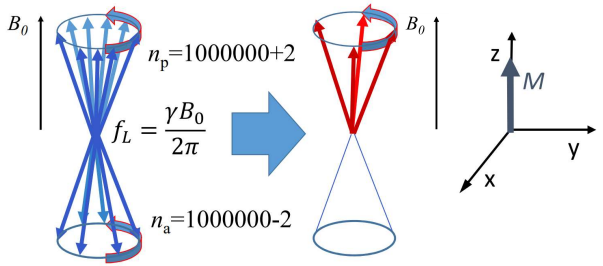
Resultant magnetisation



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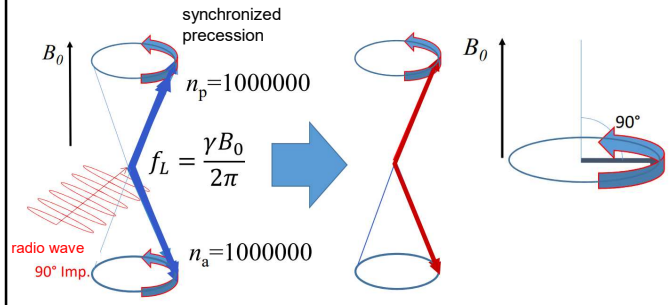
Excitation with RF-pulse
Measuring resonance frequency



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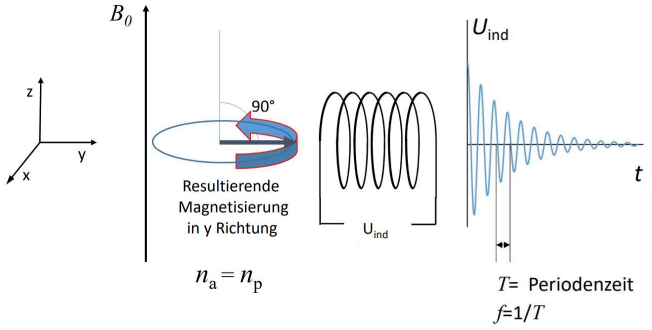
Free induction decay



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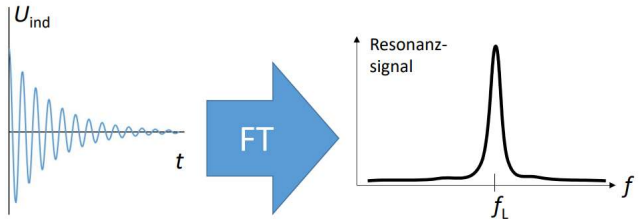
Spectrum from the FID signal



Fourier Transformation

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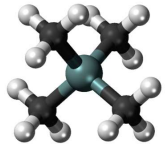
Chemical shift

- The chemical shift depends on the electron structure
- Gives information on the molecular structure
- Shielding effect – change in local magnetic field – Larmor frequency changes

$C_4H_{12}Si$

Tetramethylsilane (TMS):
reference compound
strong, sharp resonance line from its 12 protons,
with a chemical shift at low resonance frequency



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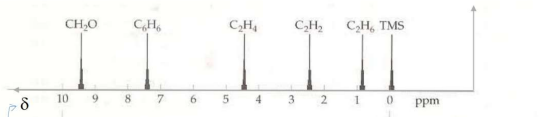
The NMR spectrum

signal intensity



60,0006 MHz — 60,0000 MHz — B_0 = 1,409248 T

1, 409234 T — 1,409248 T — f = 60 MHz

600 Hz — 0 Hz — chemical shift

chemical shift in ppm: $\delta = \frac{f_{H(Probe)} - f_{H(Standard)}}{f_{H(Standard)}} 10^6$

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