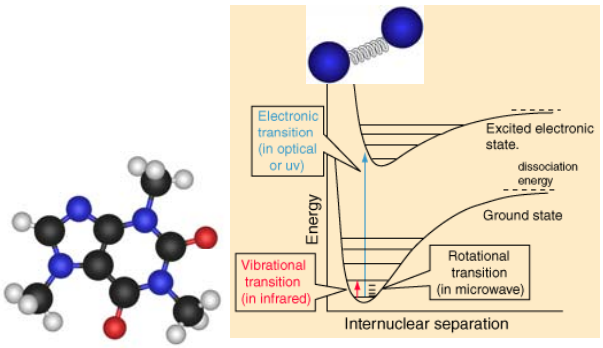
Babeș-Bolyai University Cluj-Napoca
Biomolecular Physics Department - BPD

Bio-medical applications of IR and Raman spectroscopy

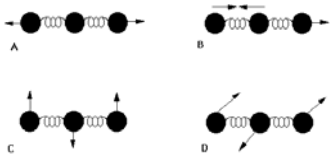
Energy levels in diatomic molecule

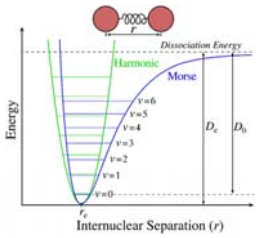


Vibrational modes

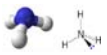
Degrees of freedom	linear	non-linear
Translational	3	3
Rotational	2	3
Vibrational	3*N*–5	3*N*–6
Total	3*N*	3*N*

N = number of atoms in molecule



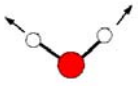


How many vibr. modes for ammonia?

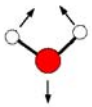


Vibration types

- There are two different types of vibrational modes:
- Vibrations can either involve a change in bond length (stretching) or bond angle (bending)



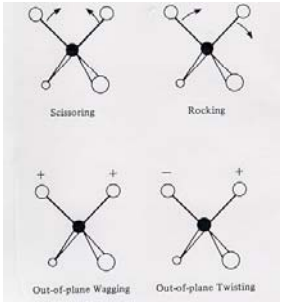
Stretching



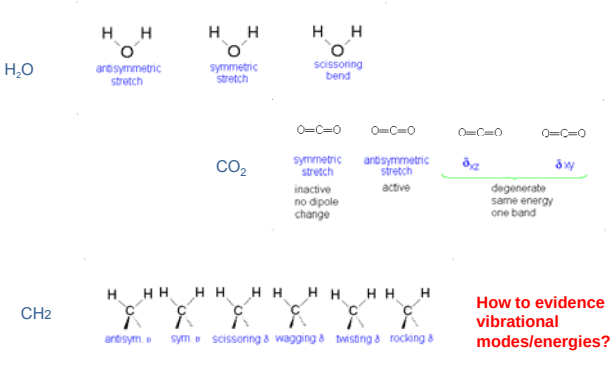
Bending

Vibration types

- The bending vibrations are often subdivided into ***scissoring, rocking, wagging, and twisting.***

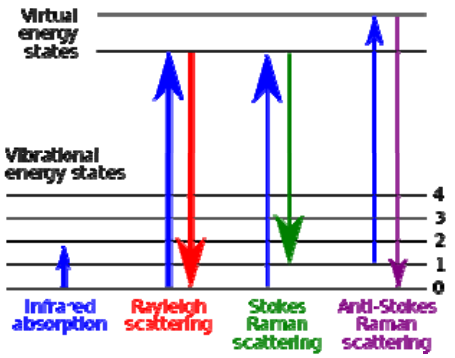


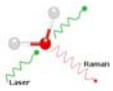
Vibration types



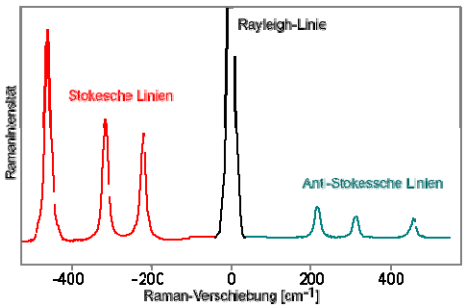
How to evidence vibrational modes/energies?

Interaction of photons and vibrational energy excitation



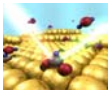


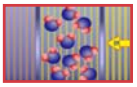
Stokes/Anti-Stokes Raman scattering



Vibrational spectroscopic methods

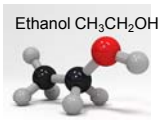
- Raman spectroscopy
  - FT-Raman, Raman microscopy, Resonance Raman (RR), surface-enhanced Raman scattering (SERS)
  - Uses monochromatic light / laser light
  - Scattering effect
- IR spectroscopy
  - FTIR, ATR-FTIR, FTIR microscopy, SEIRA, NIR
  - Uses polychromatic light in the IR spectral region
  - Absorption effect





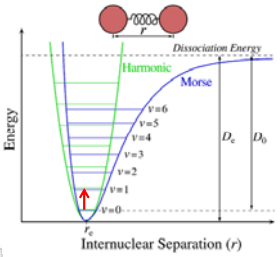
IR absorption spectroscopy (FTIR)

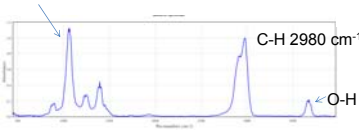
Ethanol CH_3CH_2OH



$$E = \frac{hc}{\lambda}$$

v(C-O) 1055 cm^{-1}=0.13 eV

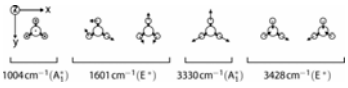


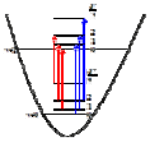


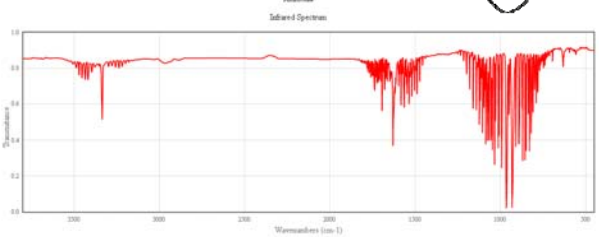
C-H 2980 cm^{-1}=0.37 eV

O-H 3390 cm^{-1}=0.42 eV

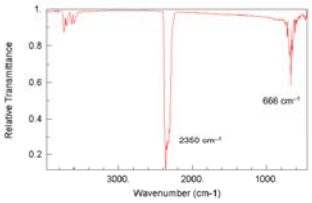
Rotational-Vibrational IR spectrum



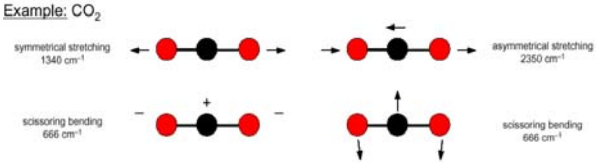




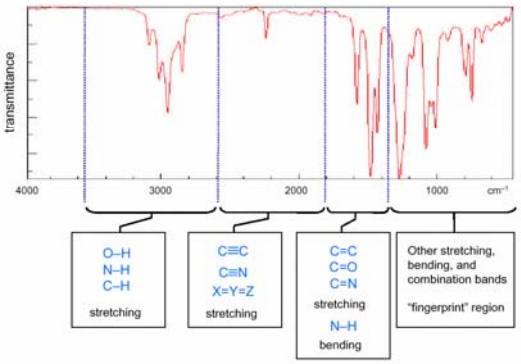
Infrared Spectrum of Carbon Dioxide



Example: CO_2



Absorption Regions



Fingerprint region

- Bands in the **fingerprint region** are characteristic of the molecule as a whole. This region finds widespread use for identification purpose by comparison with library spectra.

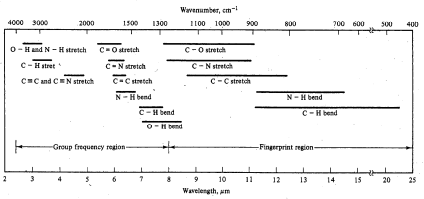


FIGURE 14-3 Frequencies of various group vibrations in the group frequency region and in the fingerprint region.

Absorbance ~ concentration

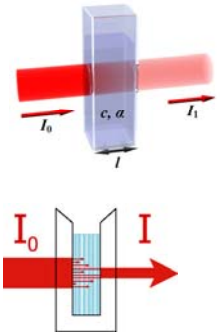
- Beer-Lambert's law

$$T = \frac{I_1}{I_0} = 10^{-A} = 10^{-\alpha l c}$$

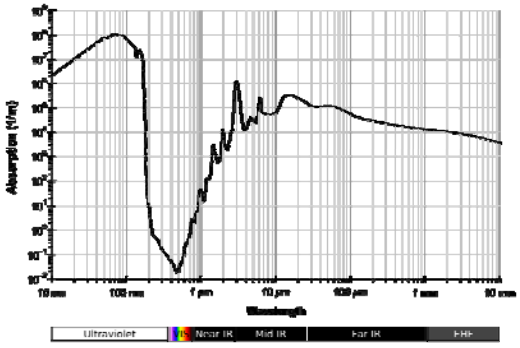
$$A = \log_{10}\left(\frac{I_0}{I_1}\right)$$

$$A = \alpha\, l\, c$$

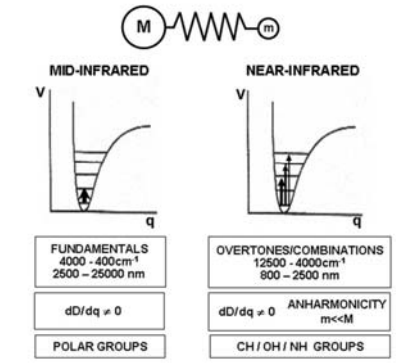
$$\alpha = \frac{4\pi k}{\lambda}$$



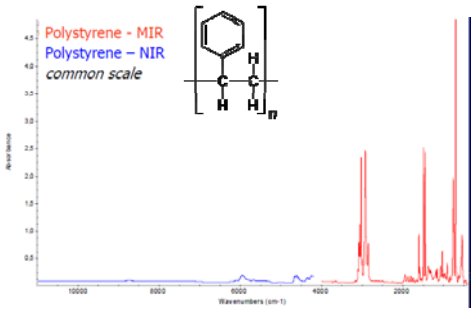
Absorption spectrum of water



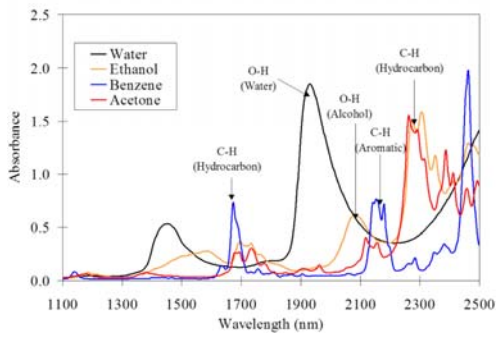
Mid-Infrared and Near-Infrared Spectroscopy



MIR vs NIR intensity



Common Chemical Groups Easily Measured
O-H, C-H and Others in the NIR spectral region



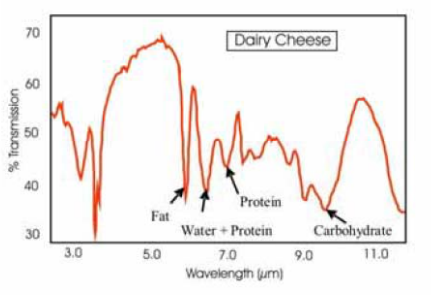
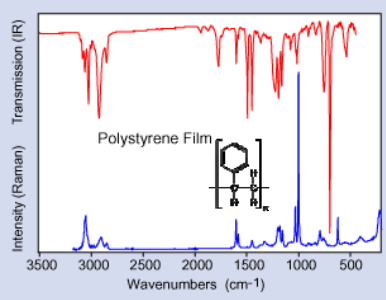


Figure 2. Typical near and mid spectra of food stuff.

Application, mainly in food and pharma industry

Raman vs FTIR



advantage/
disadvantage
-optics
-detection
-water
-sensitivity

Literatură referate

- https://docs.google.com/document/d/1SzI3HGcoioszvcmpnExtFzMrKq4fUZwbgjBeofeIJR8/edit

Homework

Prof. Ioan Notingher
http://www.biophotonics-nottingham-nanoscience.net/

Prof. Jürgen Popp
http://www.agpopp.uni-jena.de/Research.htm

Renishawdiagnostics
http://www.renishawdiagnostics.com/en/9944.aspx

EU-project
http://www.photosens.eu/PHOTOSENS/Home.html