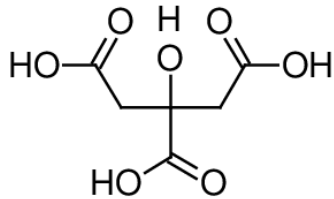
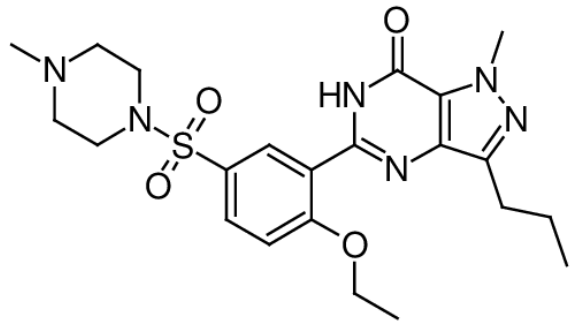


Homework 1



Calculate sildenafil's (Viagra) M, elemental composition, DBE!
What kind of isomers can it have other than constitutional, draw one example!

Tautomers

DBE: S with 6 valences, therefore formula and structure does not provide the same answer!

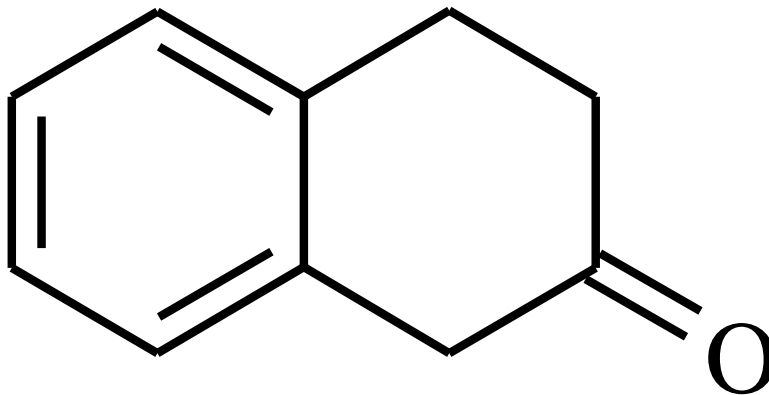
M=1 449; C 54,7 %, H 5,22 %, Cl 4,89 %, N 8,7 %, O 26,5 %

Calculate the compound's molecular formula and DBE!

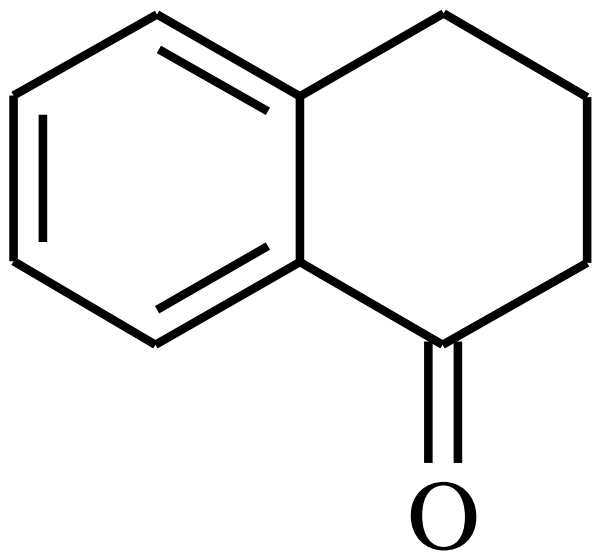
m(H)=75.6, N(H) =76 not true, have to divide with 1.01!!!

DBE cannot be half for „normal” molecules

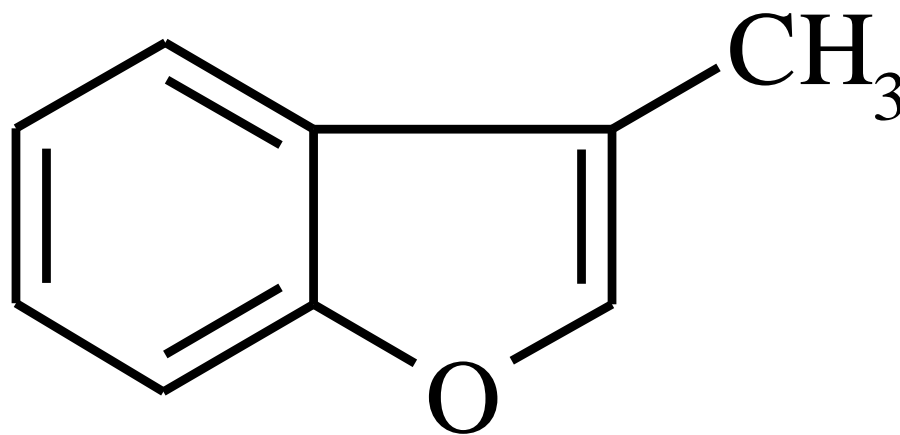
Homework 2



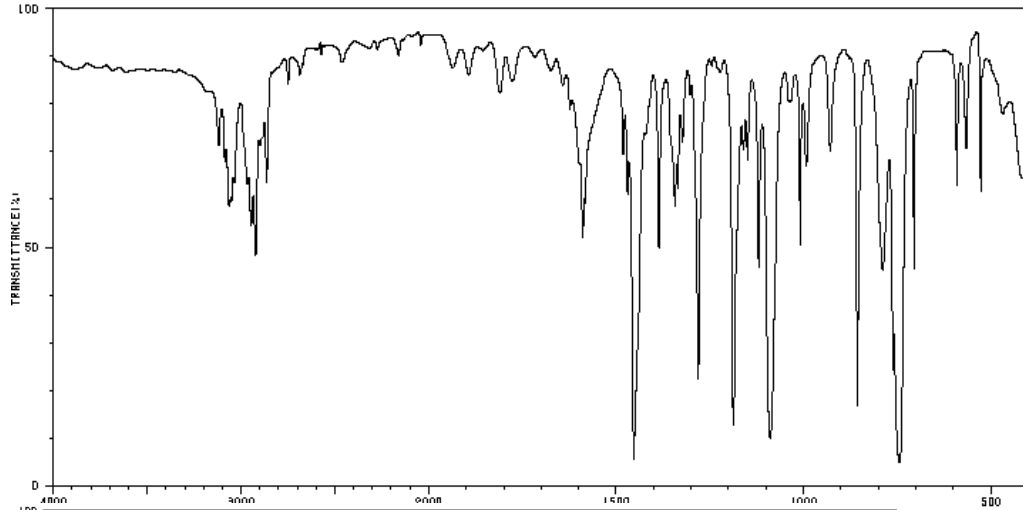
2-tetralone



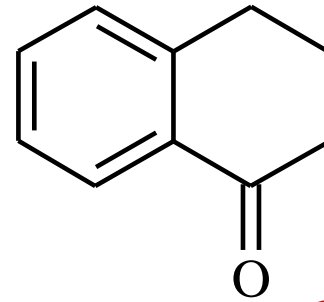
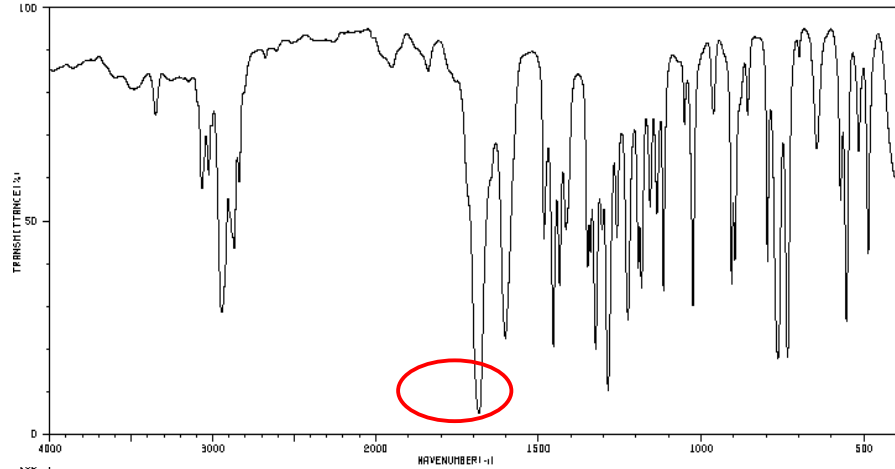
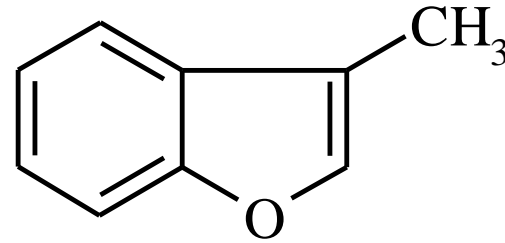
1-tetralone



3-methyl-benzofurane

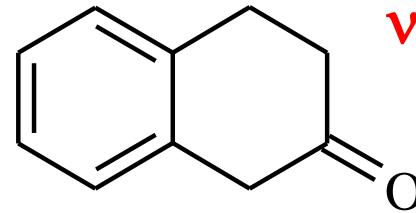
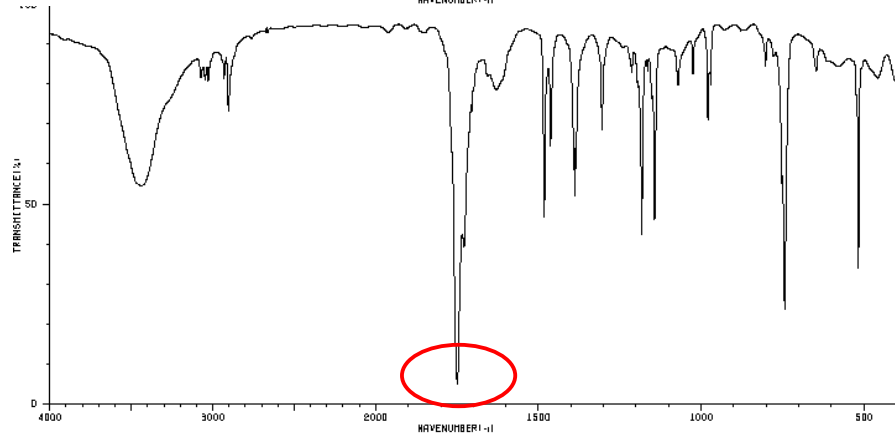


$\nu_{C=O} = ?$



Conjugation decreases
C=O bond order!

$\nu_{C=O} = 1683 \text{ cm}^{-1}$

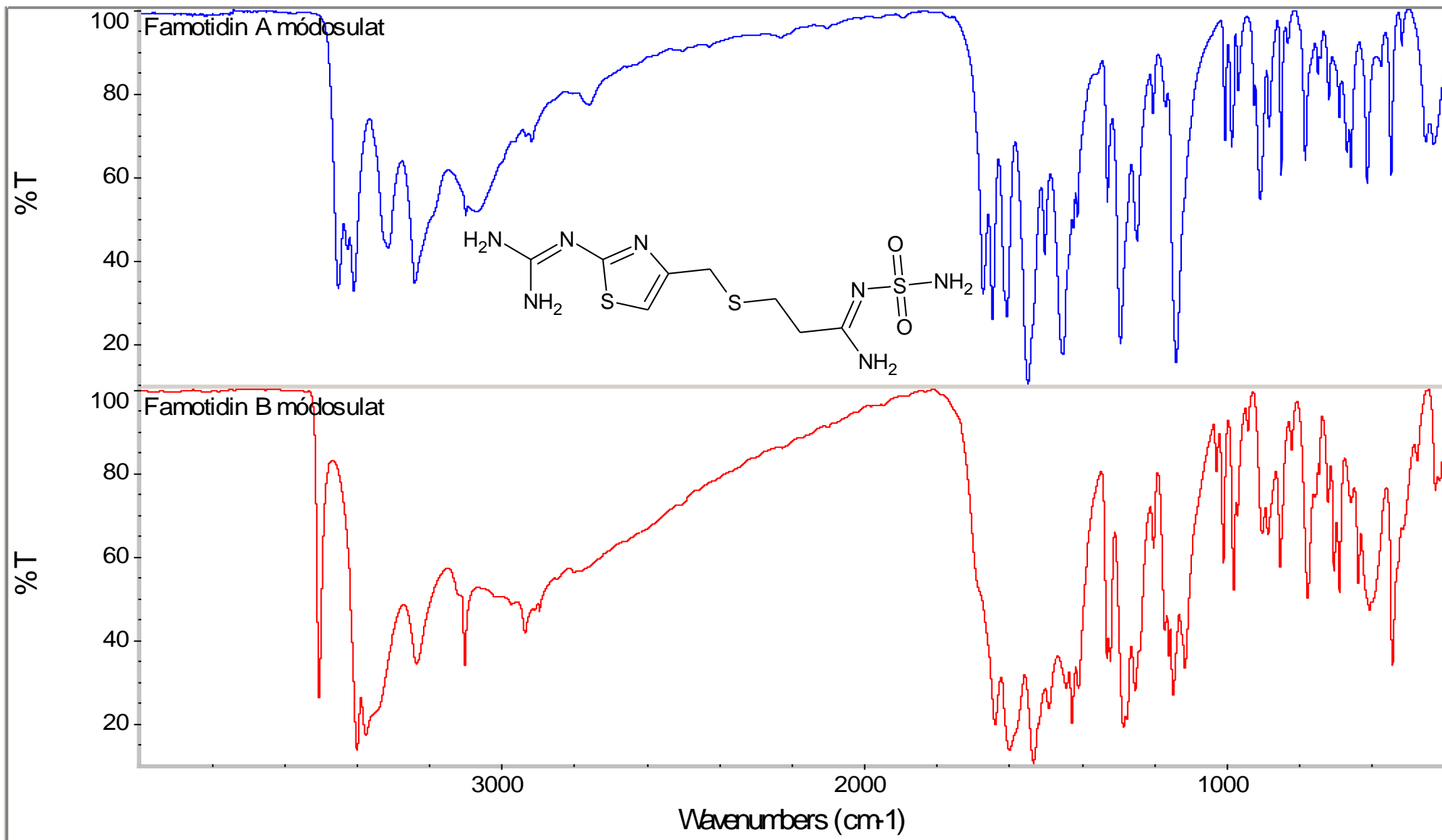


$\nu_{C=O} = 1716 \text{ cm}^{-1}$

IR in practice

1. **Verification**
Attention: spectrum is dependent on polyforms!!
2. **Structure elucidation: functional groups**
3. **Quantitation**
4. **Reaction monitoring (in-line sonda)**

Polymorphism in IR



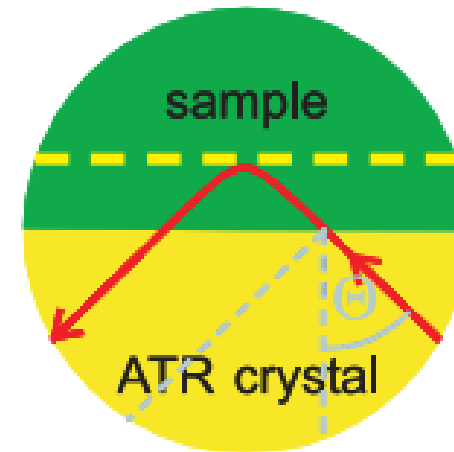
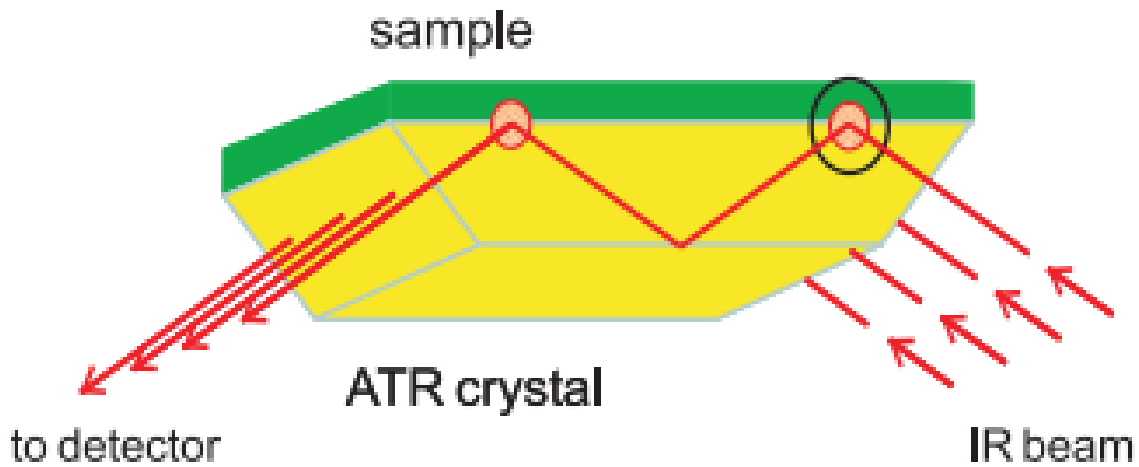
Particle size also matters!

Transmission

Solid phase: KBr pastille

Oil/Liquid: in nuyol/directly/dissolved-evaporated

Reflection: ATR head
(attenuated total reflectance)



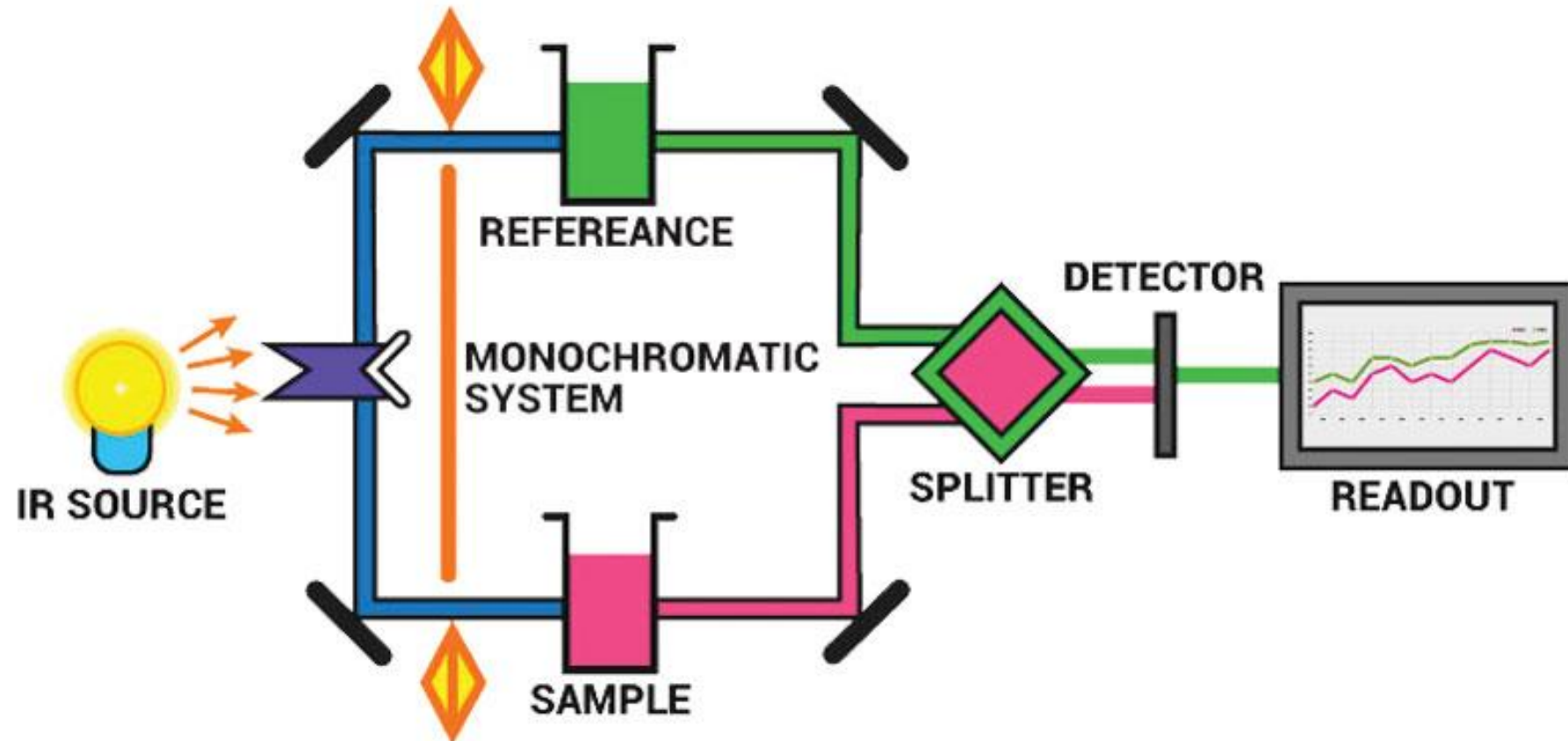
Refractive index
Crystal > Sample

Diamond, ZnSe

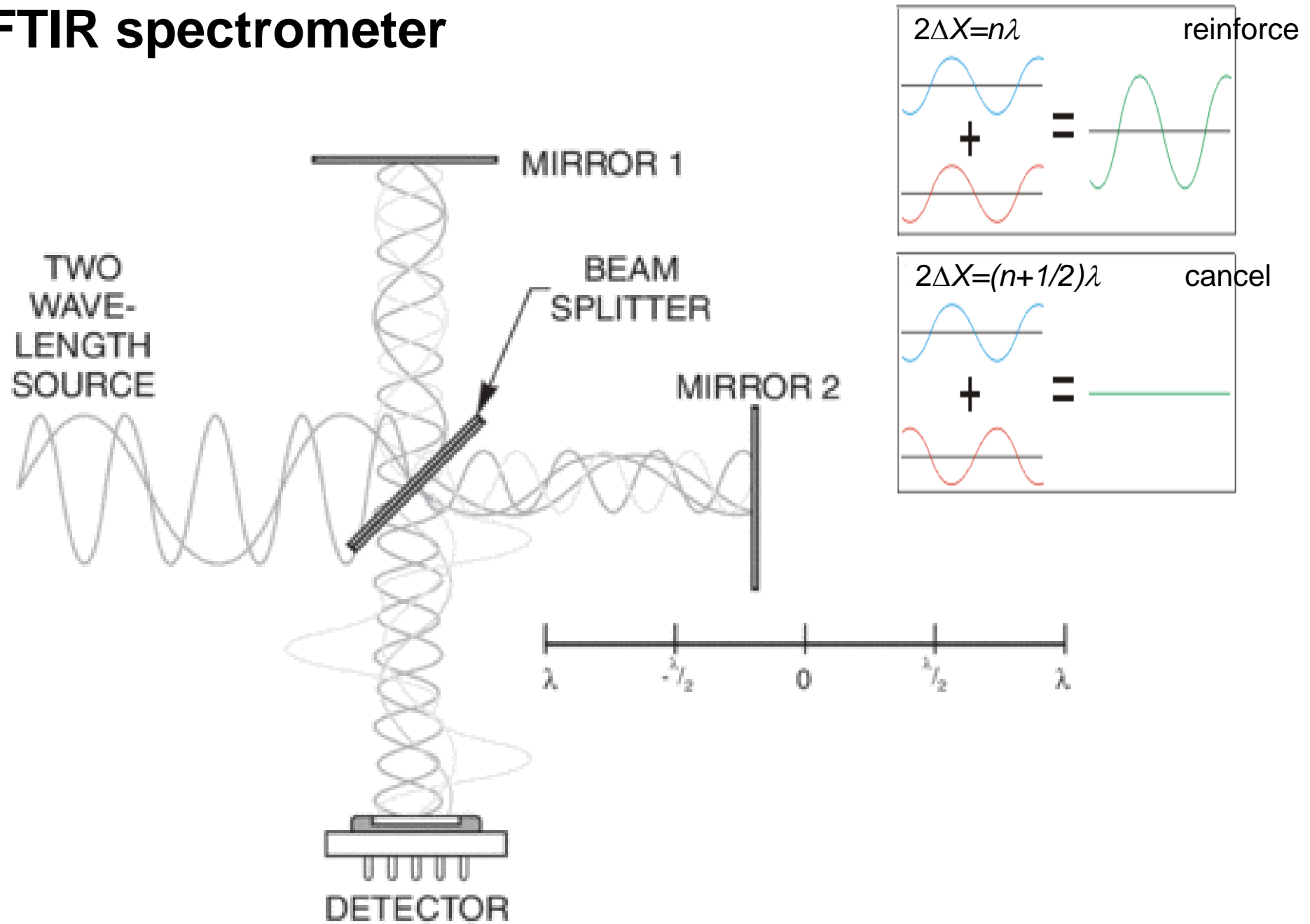
Amount: cca 1mg

The measurement is non-invasive, but with routine sample preparation it is difficult to get back the material.

Two beam IR spectrometer



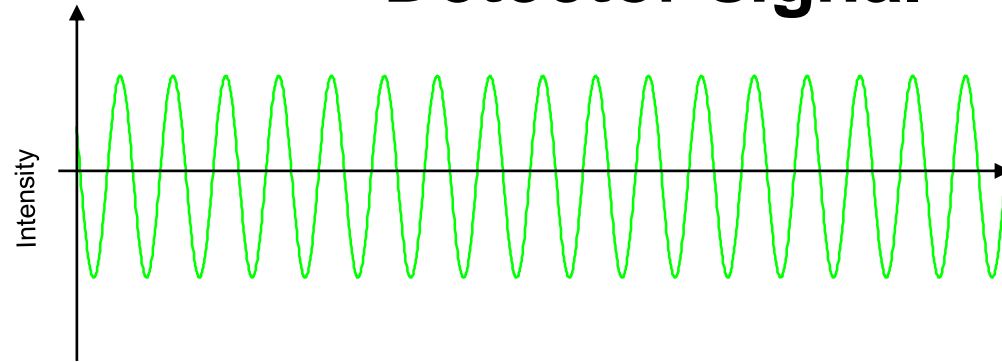
FTIR spectrometer



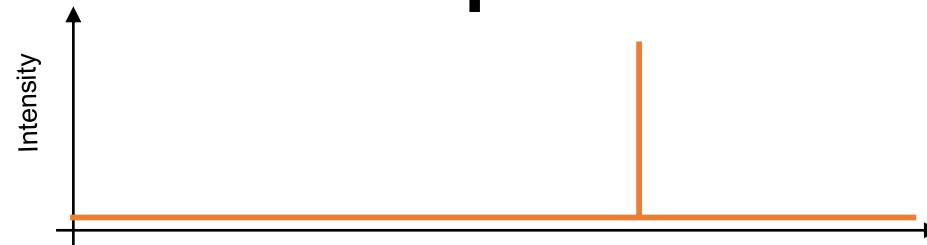
FT: Monochromatic wave



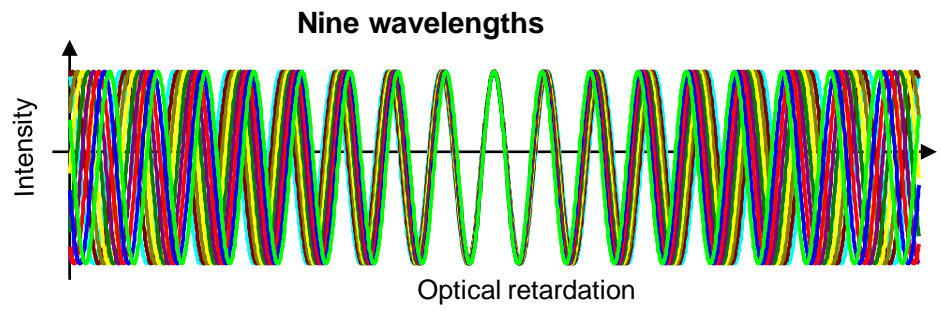
Detector signal



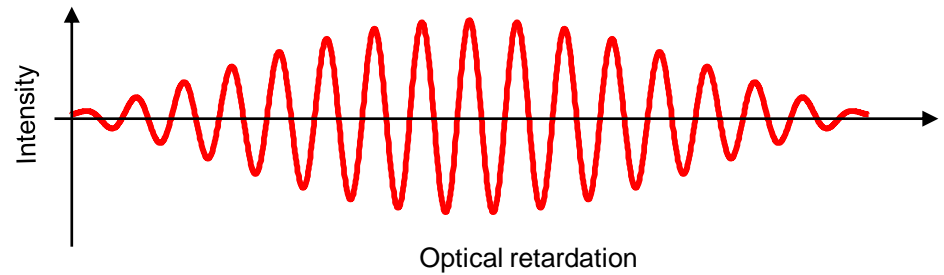
Spectrum



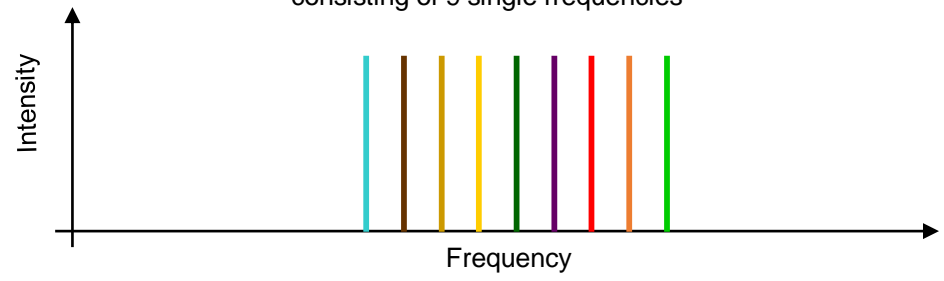
FT: more waves



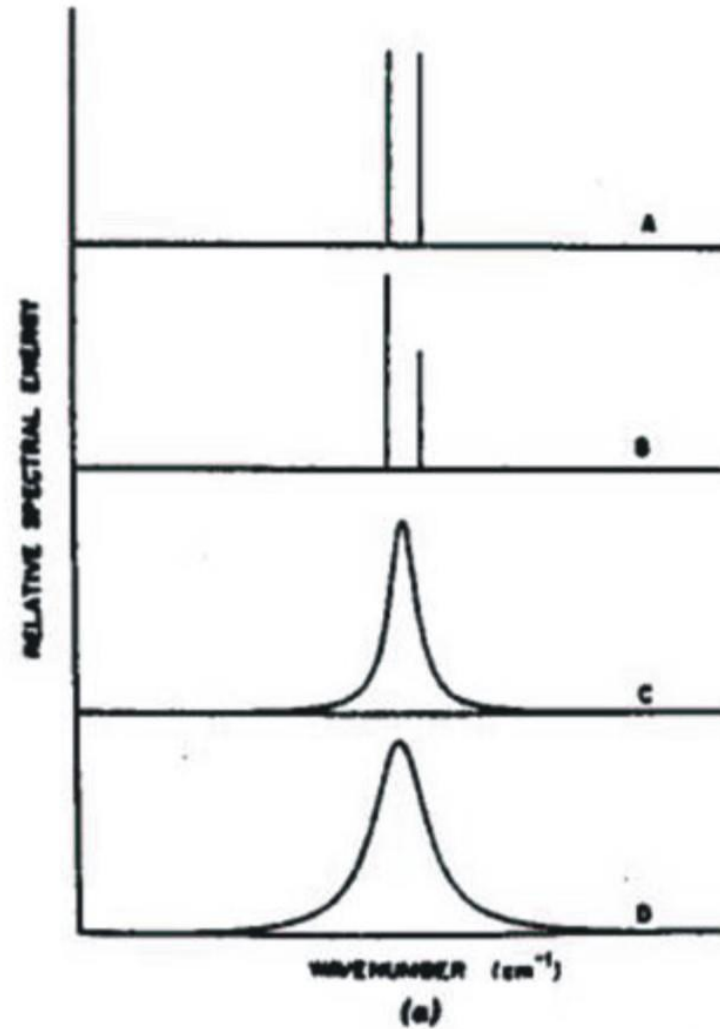
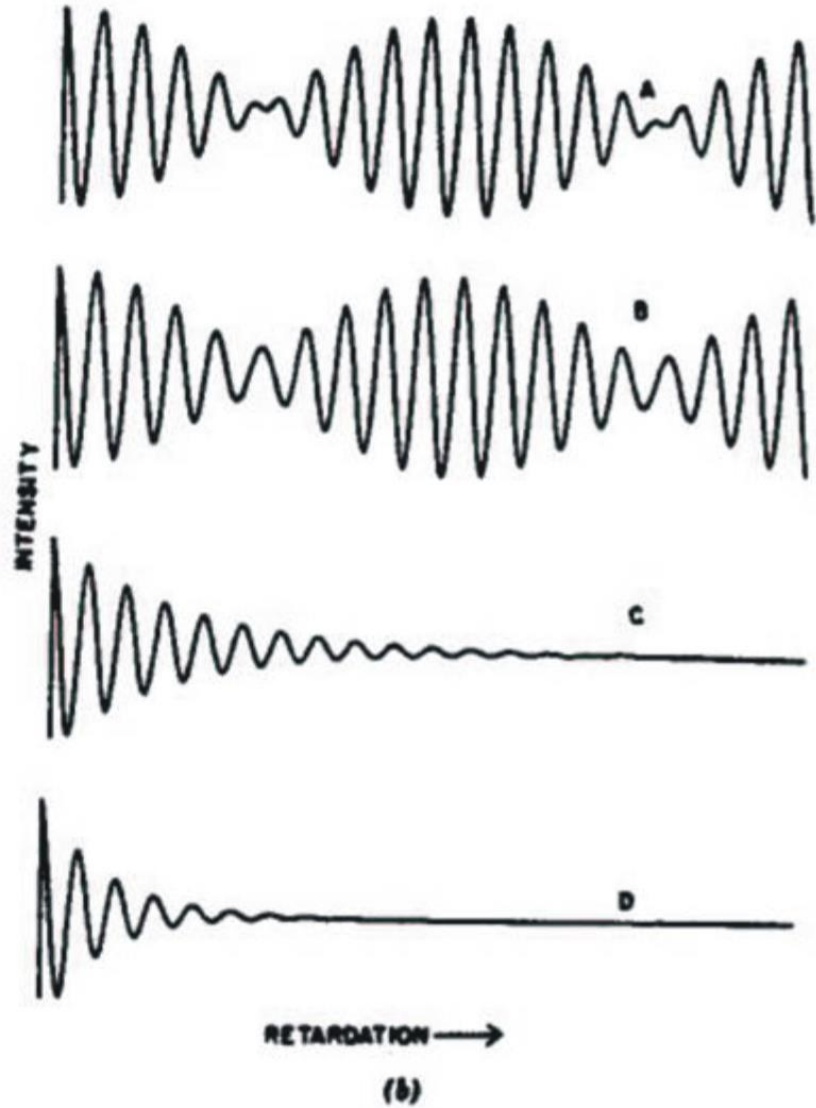
Resulting detector signal:



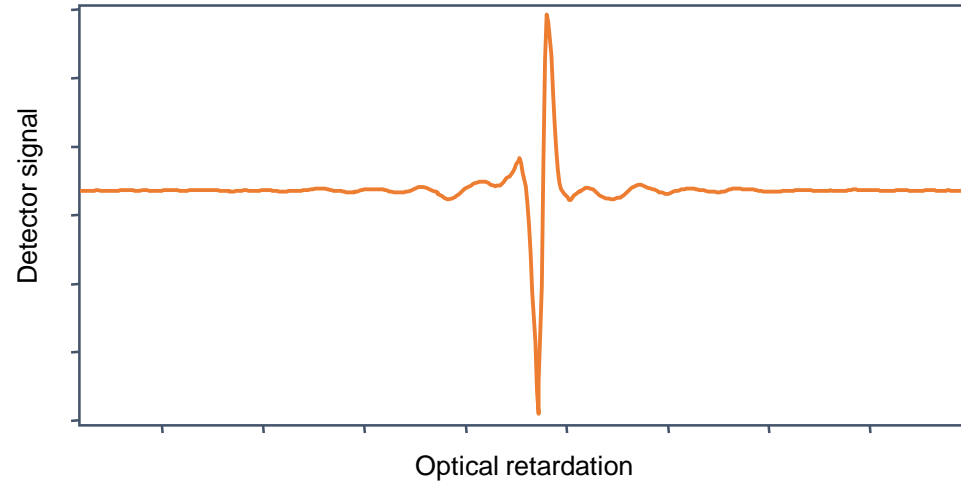
Spectrum
consisting of 9 single frequencies



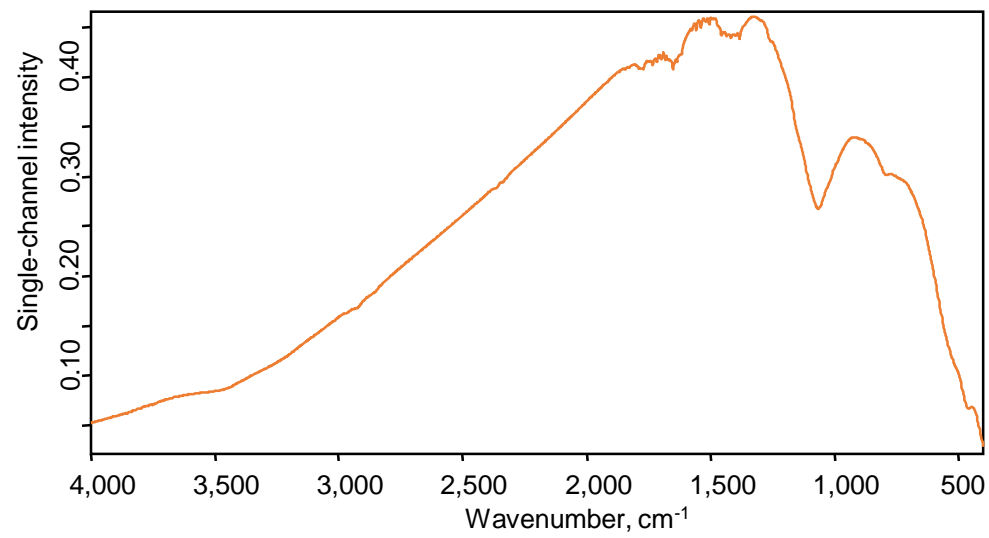
Interferogram to spectrum



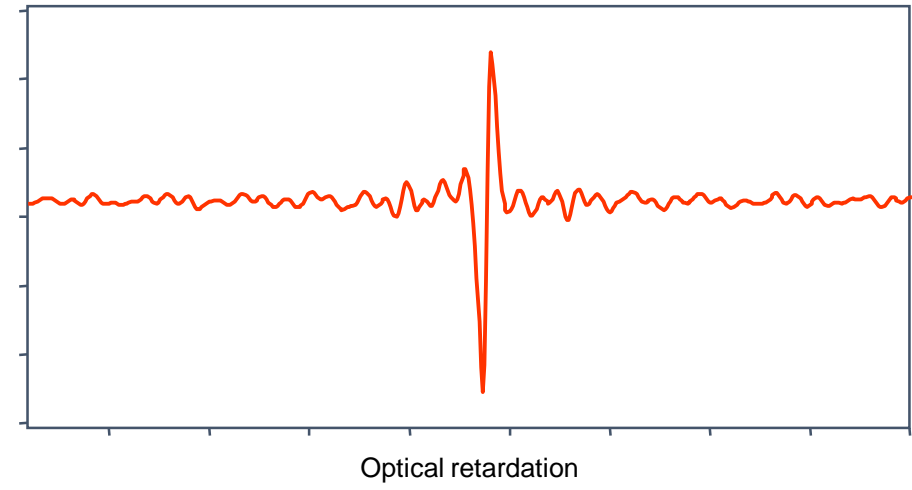
Background spectrum



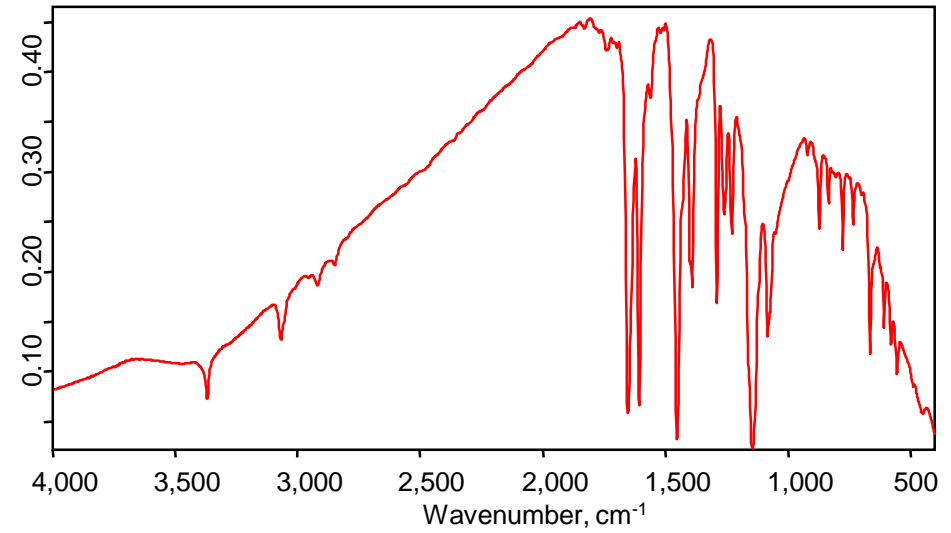
Fourier transformation

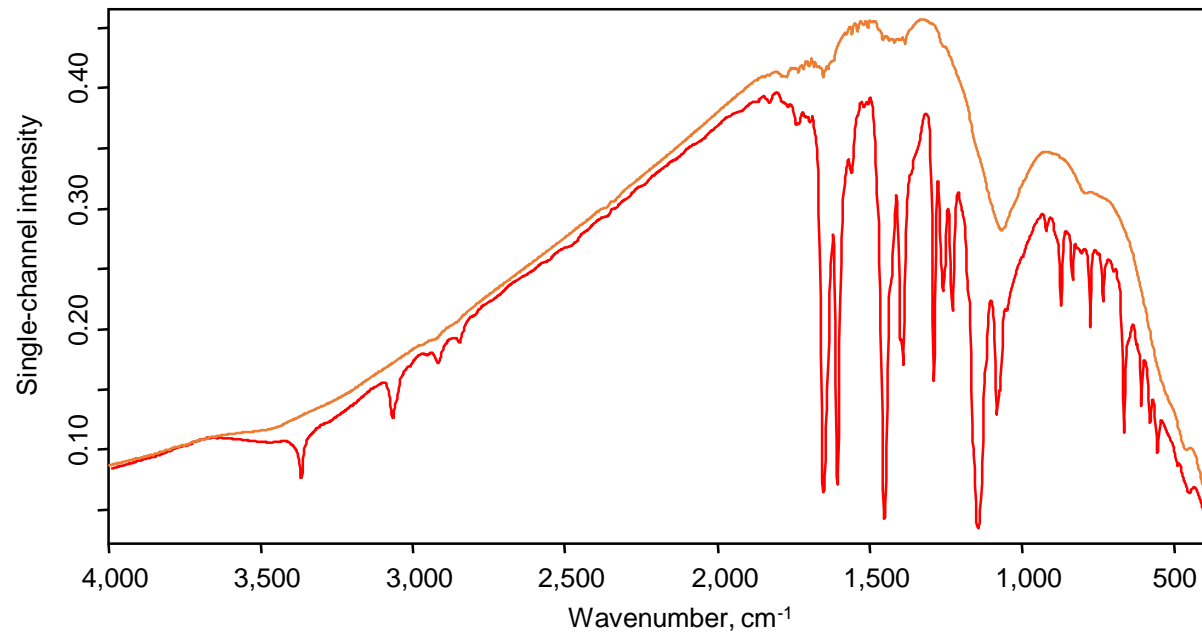


Sample spectrum

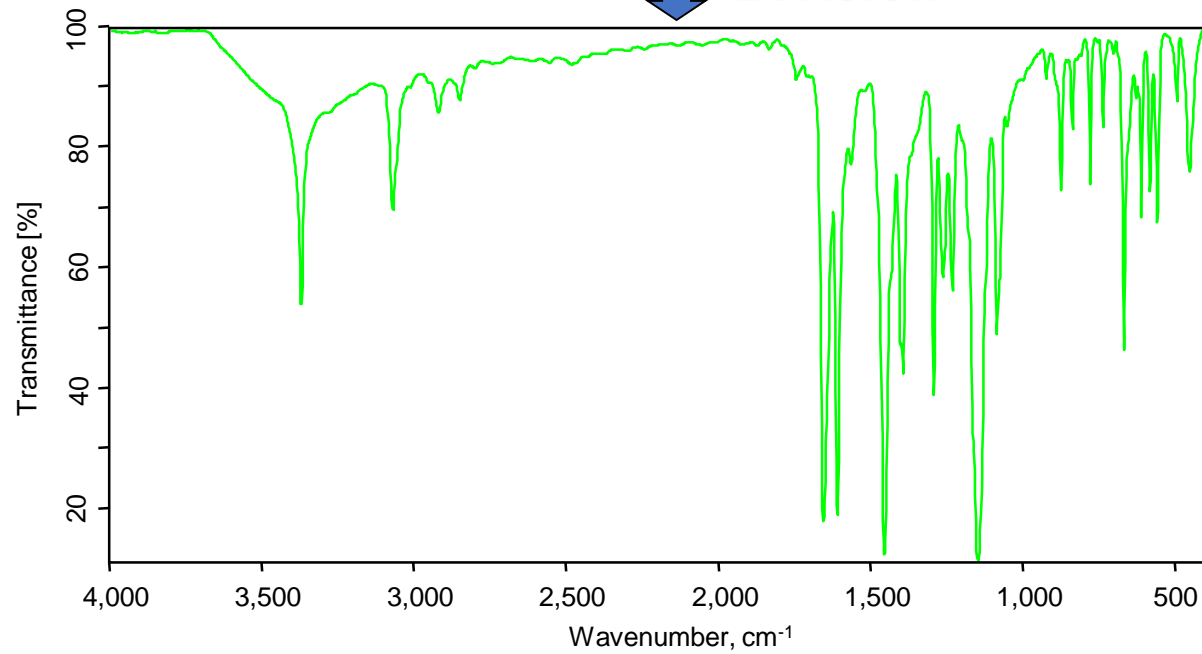


Fourier transformation





↓ **Division**



Advances of FTIR technique

Stable

Fast

Digital spectrum, easy to modify

Sensitive



Michelson (1852-1931) interferometer



Albert Abraham Michelson

