– Lecture #12 –

Mass Spectrometry

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Video 1a: Introduction

analytical method:
- qualitative: kind of components
- quantitative: amount of components

chemical species:
- atoms
- molceules
- ions
- radicals

What is mass?

"gravitative mass"
- creats and interacts with gravity

$F_w = g \cdot m$

weight = grav. acc. * mass

use: gravimetry
- quantitave analysis by weight measurement

see: measurement of Ba ions (analytical chem. lab)

most precise classical analytical method

macroscopic quantitative analysis

equivalent

"inertial mass"
- mass resists acceleration, i.e. change in its velocity (velocity will be the same unless an external force is present)

$\Sigma F = a \cdot m$

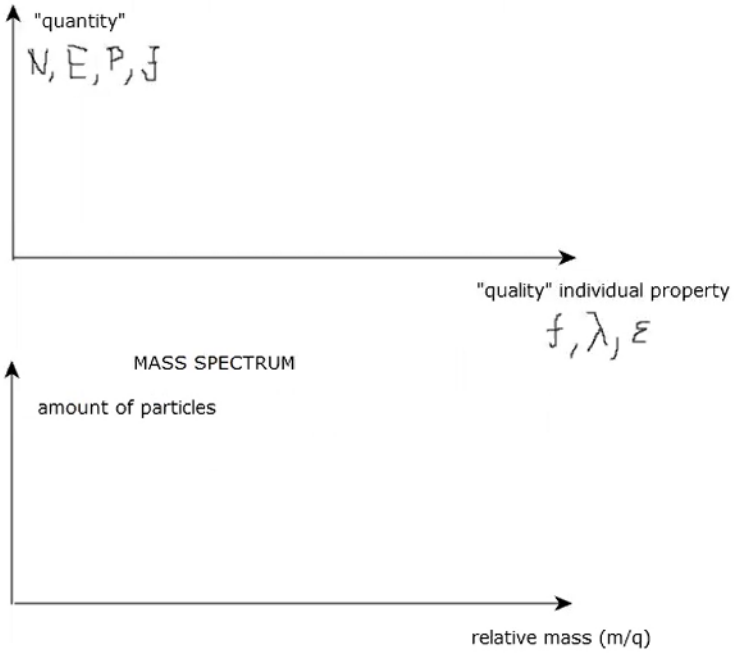
use: mass spectrometry

very sensitive method (femtomoles)

qualitative and quantitative analysis of microscopic amounts

What is a spectrum?

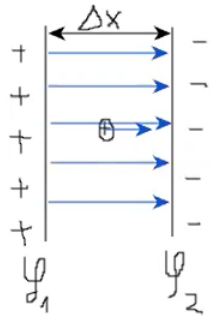
A function representing the distribution of a set of elements



Video 1b: Basic Interactions

Basic interactions of charged particles

Electric field

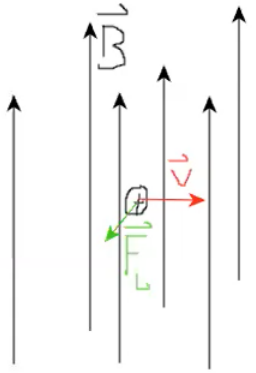


$$U = \Delta\varphi = \varphi_2 - \varphi_1$$

$$\vec{F}_el = \vec{E} \cdot q = \frac{\Delta\varphi}{\Delta x} \cdot q$$

effect: linear acceleration = |v| changes

Magnetic field



$$[B] = T \quad \text{(tesla) SI}$$

CGS: G (gauss)

$$1\,T = 10^4\,G$$

$$\vec{F}_L = q \cdot \vec{v} \times \vec{B}$$

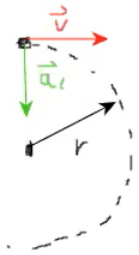
$$\downarrow \text{ if } \vec{B} \perp \vec{v}$$

$$|F_L| = q \cdot |v| \cdot |B|$$

effect:
- only affects moving charges
- the direction of v changes
- circular path

Circular motion

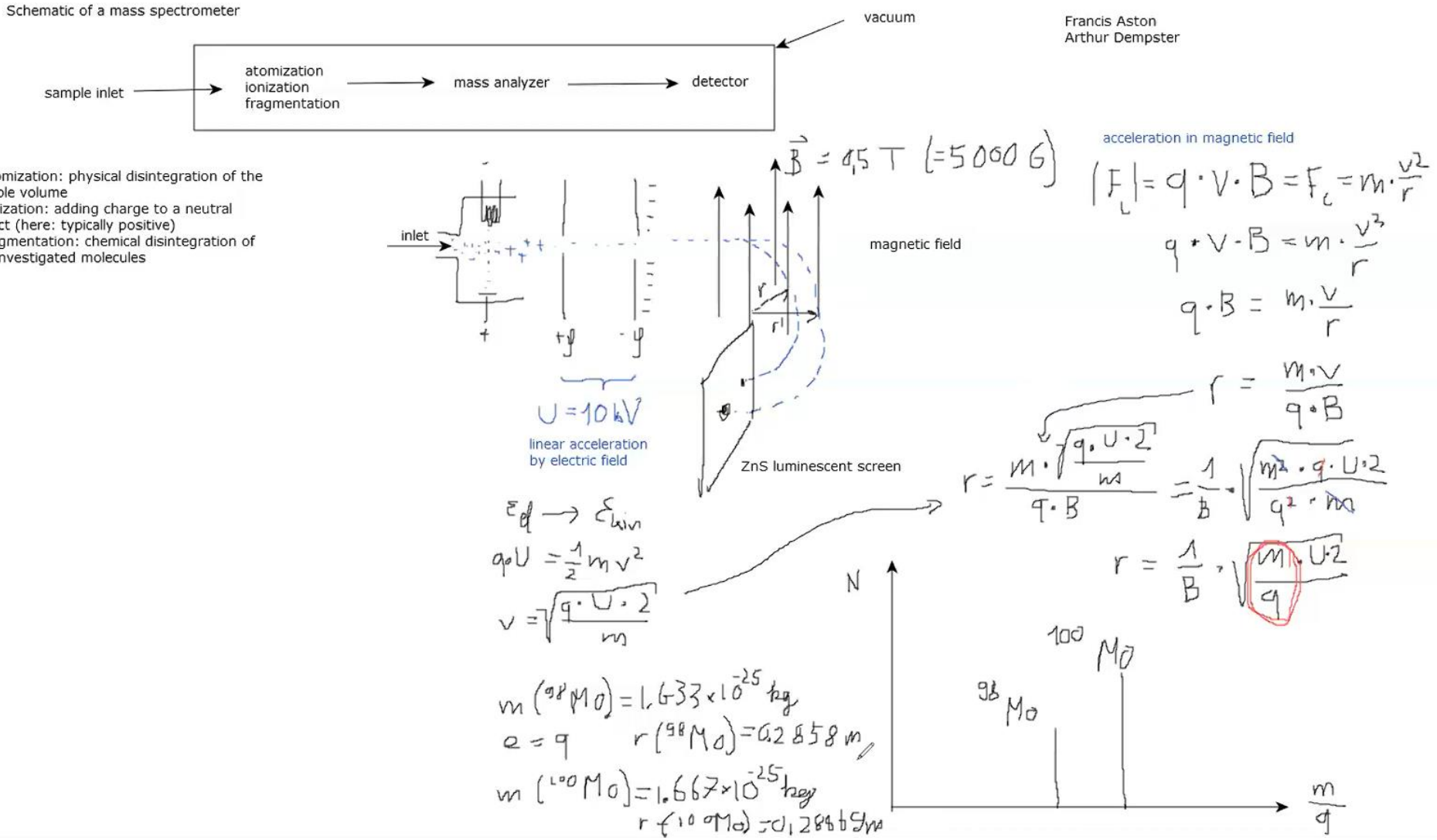
caused by acceleration perpendicular to the actual direction of motion



$$a_c = \frac{v^2}{r}$$

$$F_c = m \cdot a_c = m \cdot \frac{v^2}{r}$$

Video 2: General Description



Video 3: Ion Sources

Ion Sources

1) Electron Ionization (EI)
- electron beam flowing between a cathode and an anode will collide into the particles sprayed into the ionization chamber
- one or more electrons are removed porducing positive ions
- hard ionization: high degree of fragmentation

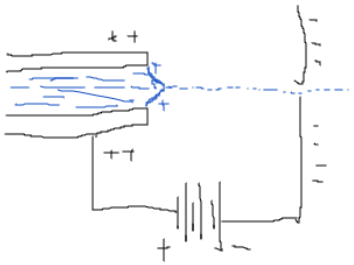
2) Chemical ionization (CI)
- an inert chemical (A) is introduduced to the ionization space
- the inert chemical is ionized: $e^- + A \rightarrow A^+ + 2e^-$ $(CH_4, NH_3 \ldots)$
- the sample (M) is introduced into the ionization space, and the charge is transferred from the "A" molecule to the sample:

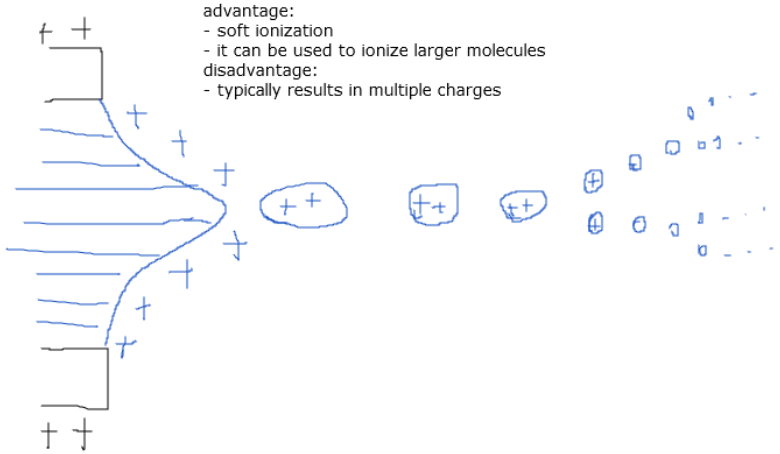
1) $M + A^+ \rightarrow M^+ + A$

2) $M + A^+ \rightarrow [MA]^+$

- soft ionization, low degree of fragmentation

3) Electro Spray Ionization (ESI)

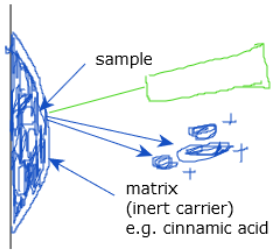




advantage:
- soft ionization
- it can be used to ionize larger molecules

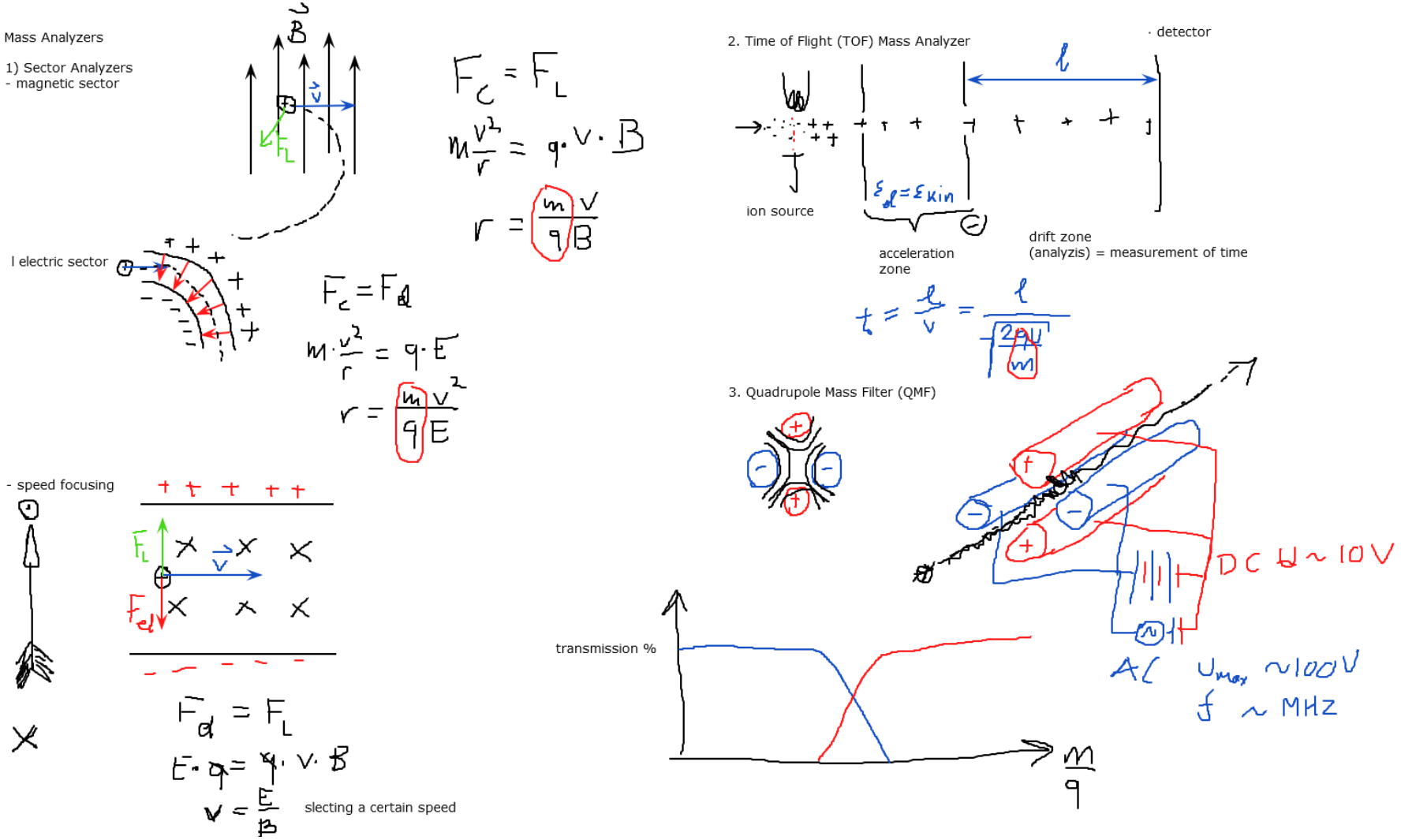
disadvantage:
- typically results in multiple charges

4) Matrix-assisted laser desorption ionization (MALDI)



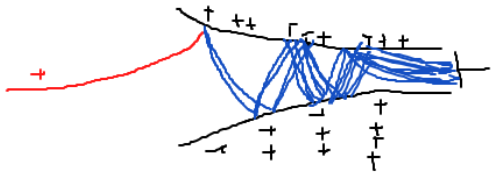
- soft ionization
- used for larger molecules

Video 4a: Mass Analyzers



Video 4b: Detectors, Applications

Detectors: electron multipliers



luminescent screen (ZnS)

Application:

- determination of isotope ratio
  - isotopic abundance of elements
  - urea breath test

$^{13}C/^{12}C$

- biomedical research: qualitative and quantitative analysis
  - TOF-MALDI
  - composition of surface oligosacchradies of cells
- iKnife, onkoknife: