

MASS SPECTROMETRY

analytical method: \rightarrow qualitative: kind of components
 \rightarrow quantitative: amount of components

chemical species: - atoms
- ions
- molecules
- molecule fragments

What is mass?

"gravitational mass"

- creates gravity
- interacts with gravity

$$F_w = g \cdot m_{\text{mass}}$$

weight \downarrow gravitational acceleration

use: gravimetry

- measure the weight of something to find out the amount

macroscopic quantitative analysis

"inertial mass"

- ~~change~~ mass "resists" change in its velocity (will remain the same unless external force is present)

$$\Sigma F = a \cdot m$$

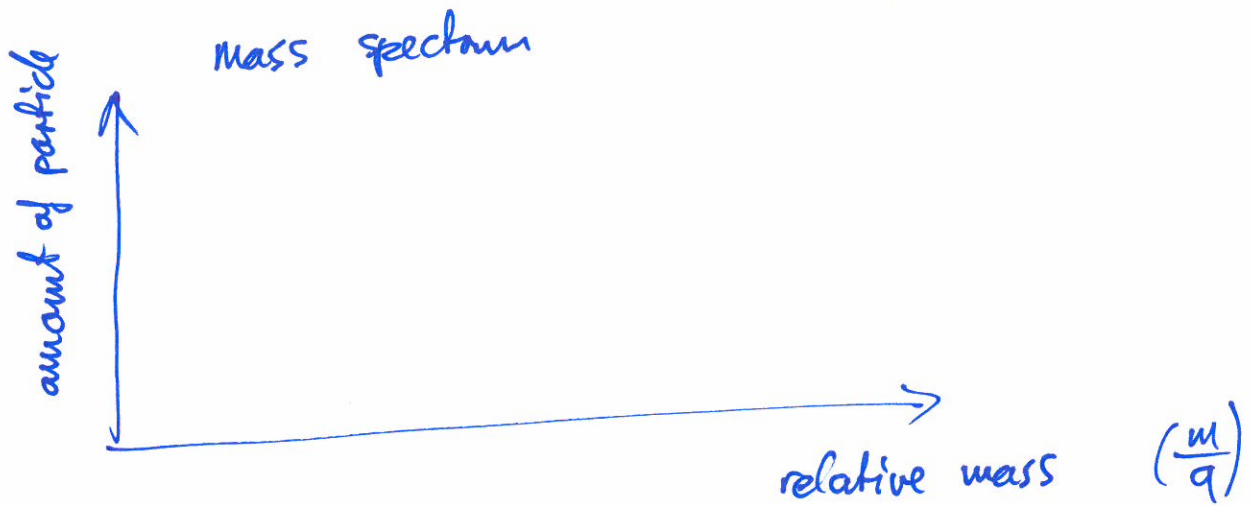
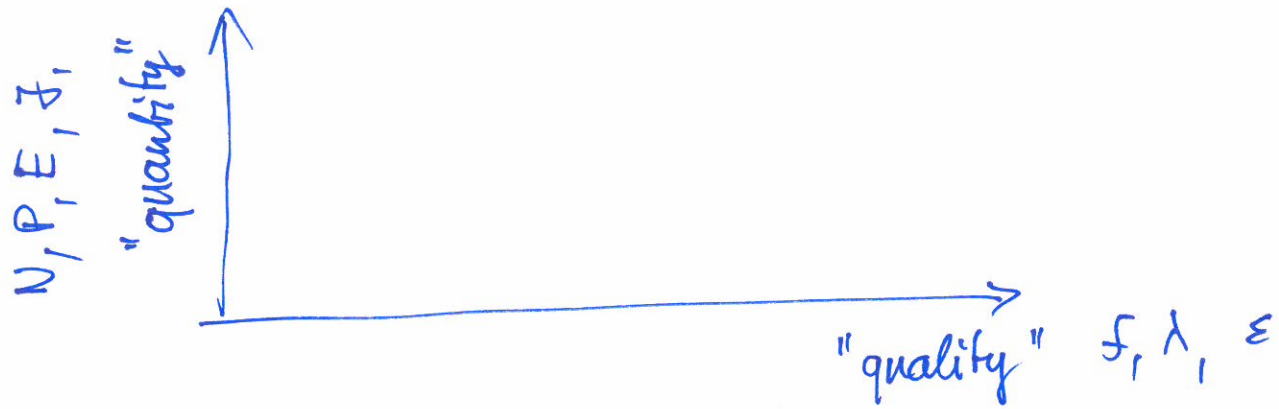
use: mass spectrometry

microscopic

qualitative & quantitative analysis

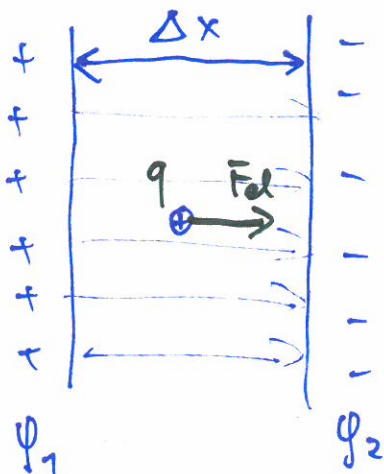
What is a spectrum?

- a special kind of distribution



basic interactions

electric field



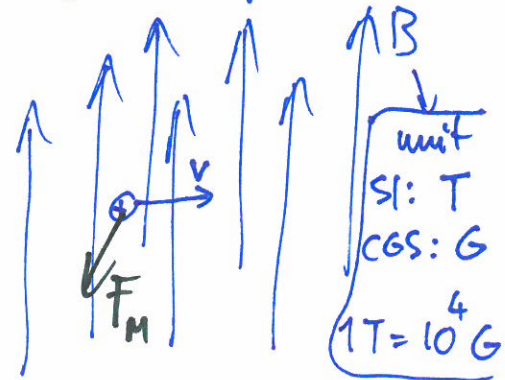
$$E = \frac{F_{el}}{q} = \frac{\Delta\varphi}{\Delta x}$$

$$\vec{F}_{el} = \vec{E} \cdot q$$

effect: linear acceleration

$|v|$ increases

magnetic field



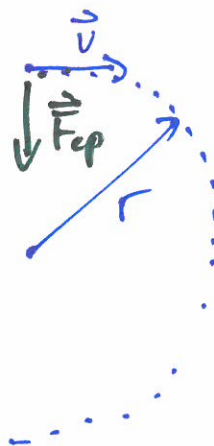
$$\vec{F}_M = q \cdot \vec{v} \times \vec{B}$$

effect: circular motion
direction of \vec{v} changes

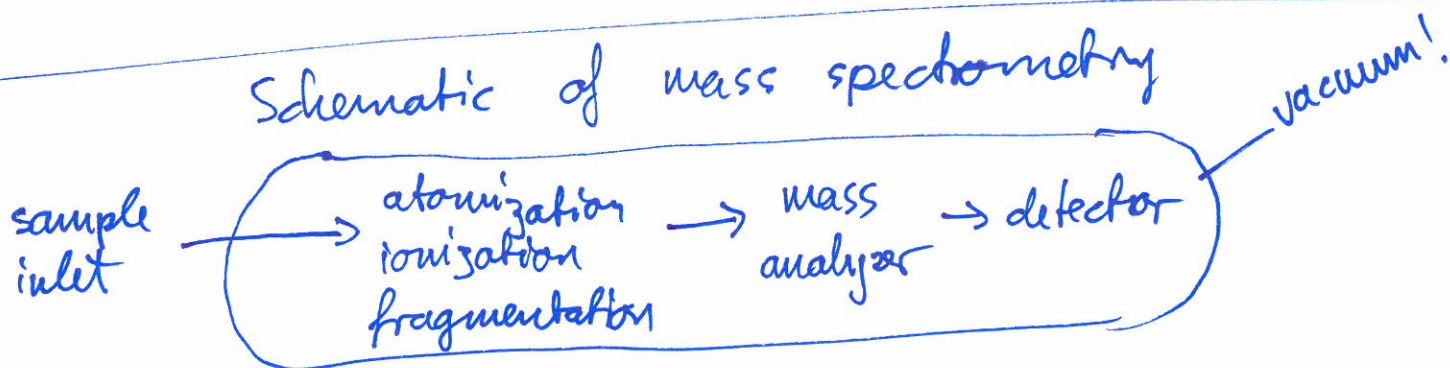
- circular motion : caused by an acceleration perpendicular to the direction of motion ($\vec{a} \perp \vec{v}$)

$$F_{cp} = a_{cp} \cdot m$$

$$a_{cp} = \frac{v^2}{r}$$



Schematic of mass spectrometry

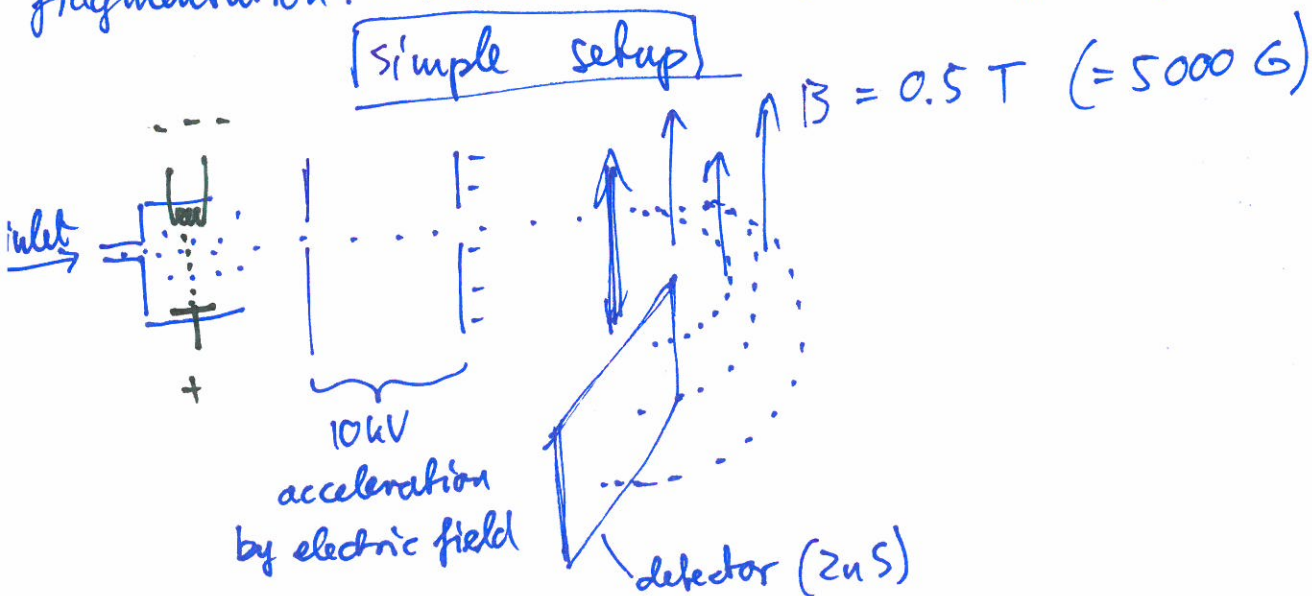


atomization : - physical disintegration of sample volume

ionization : - add charge to a neutral object

fragmentation : - chemical disintegration of bigger molecules

Simple setup



- acceleration by electric field

$$E_{el} \rightarrow E_{kin}$$

$$q \cdot U = \frac{1}{2} m v^2$$

$$v = \sqrt{\frac{q \cdot U \cdot 2}{m}} \quad \#1$$

- acceleration by magnetic field = centripetal force

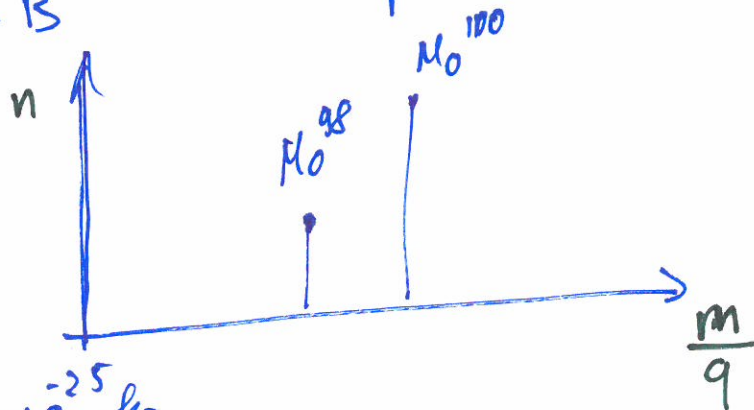
$$\vec{F}_M = q \cdot \vec{v} \times \vec{B}$$

$$|F_M| = q \cdot v \cdot B = F_{cp} = m \cdot \frac{v^2}{r}$$

$$r = \frac{m \cdot v^2}{q v B} = \frac{m v}{q B} \quad \#2$$

- combination of #1 & #2

$$r = \frac{m \cdot \sqrt{\frac{q \cdot U \cdot 2}{m}}}{q \cdot B} = \frac{1}{B} \cdot \sqrt{\frac{m^2 \cdot q \cdot U \cdot 2}{m \cdot q^2}} = \frac{1}{B} \sqrt{\frac{m \cdot U \cdot 2}{q}}$$



$$^{98}\text{Mo}^+ \quad 1.633 \times 10^{-25} \text{ kg}$$

$$^{100}\text{Mo}^+ \quad 1.667 \times 10^{-25} \text{ kg}$$

$$q = +1.6 \times 10^{-19} \text{ C}$$

$$\text{settings: } U = 10000 \text{ V} \quad B = 0.5 \text{ T}$$

$$\left. \begin{aligned} r(^{98}\text{Mo}^+) &= 0.28577 \text{ m} \\ r(^{100}\text{Mo}^+) &= 0.28868 \text{ m} \end{aligned} \right\} 0.00291 \text{ m} \approx 2.9 \text{ mm}$$

ion sources

1) Electron ionization (EI)

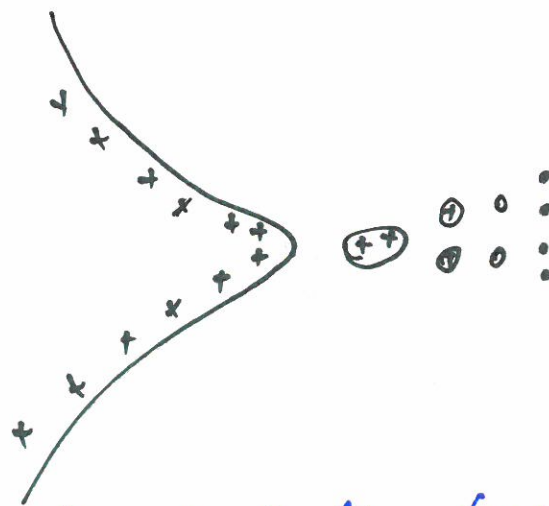
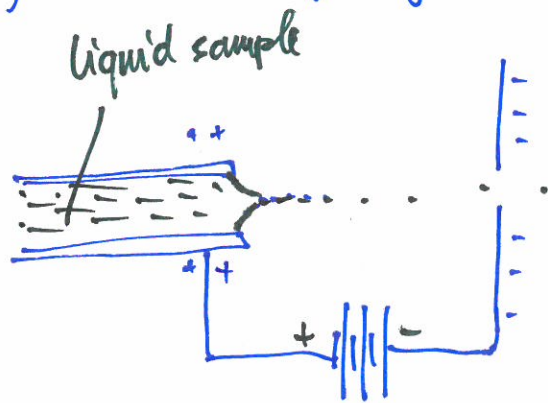
- electron beam flowing between a cathode and an anode
- hard ionization: high degree of fragmentation

2) Chemical ionization (CI)

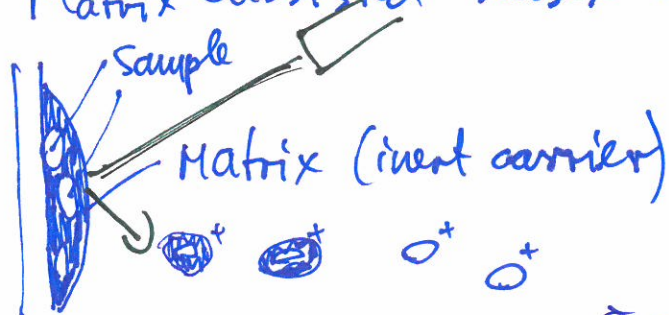
- an inert chemical is introduced into the ionization space (A)
- then it gets ionized: $e^- + A \rightarrow A^+ + 2e^-$
- the sample (M) is introduced and ~~will~~ charge will be transferred from the "A" to the sample molecules:



3) Electro spray ionization (ESI) (soft)

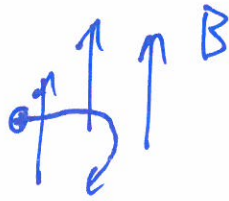


4) Matrix-assisted laser desorption ionization (MALDI) (soft)



Mass analyzers

1) Magnetic sector



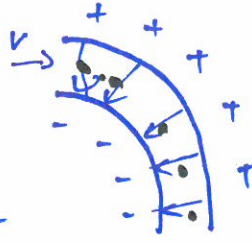
$$F_{cp} = F_M$$

$$m \frac{v^2}{r} = q \cdot v \cdot B$$

$$\frac{1}{2} m v^2 = q \cdot V$$

$$E_{kin} = E_e$$

2) Electric sector



charges are forced to follow a circular path due to the curved shape of the capacitor

$$F_{cp} = F_{el}$$

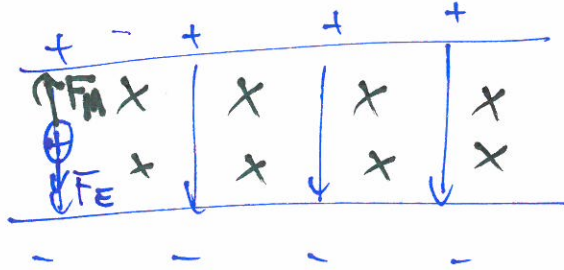
$$m \frac{v^2}{r} = E \cdot q$$

$$r = \frac{m v^2}{E \cdot q}$$

$$v^2 = \frac{e l}{q} = \frac{2 q V}{m}$$

2.b

1) speed focusing



$$F_M = q \cdot v \times B$$

$$F_{el} = q \cdot U$$

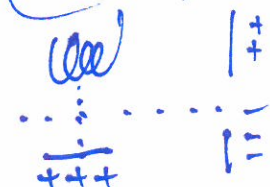
particles pass through if $F_M = F_{el}$

$$q \cdot v \cdot B = q \cdot U$$

$$v \cdot B = U$$

$$v = \frac{U}{B} \} \text{select one speed}$$

3.1 (TOF) time of flight



ion source

accelerator

analysis = measurement of time

$$v = \frac{\Delta x}{\Delta t} = \frac{l}{t}$$

$$t = \frac{l}{v} = \frac{l}{\sqrt{\frac{q \cdot U \cdot 2}{m}}}$$