Quadrupole mass analyzer

Simulation of ionic motion in a time-varying electromagnetic field
“Mass” analysis (really mass:charge)

METHOD to determine chemical/isotopic ratios in materials

• carbon dating – ratio of $C_{12}$ and $C_{13}$ gives measure of age of biological residues

• trace gas analysis – detection of explosives

• drug characterization & quality control

• protein identification by mass

• gas safety monitors

• vacuum chamber analysis
Mass analysis:

Generate ions, accelerate them, sort by mass:charge ratio

1) magnetic sector

\[ \vec{F} = m \vec{a} = q \vec{v} \times \vec{B} \]

\[ a = \frac{v^2}{R}; \quad R = \frac{v^2}{a} = \frac{mv^2}{qvB} = \frac{m}{q} \frac{v}{B} \]

velocity determined by ion source

\[ \frac{1}{2}mv^2 = qV = qEd \]

Advantages:

simple! works well for fixed mass

Disadvantages:

difficult and slow to scan electromagnets expensive and heavy
Time of flight mass spectrometer

Pulsed source, known voltage drop

\[
\frac{1}{2}mv^2 = qV = qEd
\]

\[
v = \sqrt{\frac{2qV}{m}}; \quad time = \frac{L}{v}
\]

different masses, different velocities, different arrival times

Advantages:
- parallel detection
- sensitivity at high mass range

Disadvantages:
- Large
- require fast electronics
- (usually) need laser ionization source

http://www.docbrown.info/page06/ELmcTEST/TOFMS.gif
Quadrupole mass analyzer
4 electrodes, an ion source and a detector.

Advantages:
compact
easy to scan voltages to select different m/q

Disadvantages:
mass resolution degrades at high M

http://www.chm.bris.ac.uk/ms/images/quad-schematic.jpg
Reminder:

Electric dipole – field strongest between charges

Quadrupole – field is zero at the center - could shoot ions down the middle of this electric potential “tube”

http://hyperphysics.phy-astr.gsu.edu/hbase/electric/imgele/edip2.gif
Mass filter – need conditional stability – only some passed

add an RF field to the DC fields on the electrodes

repel ions from center part-time – light ones respond faster, get ejected

attract ions to center part time – light ones respond faster, get retained

https://users.dimi.uniud.it/~gianluca.gorni/Immagini/orientedSaddle.GIF
Equations of motion:

\[
\vec{F} = m\vec{a} = q\vec{E} \\
\vec{E} = -\nabla U
\]

\(U\) is potential; electrode surfaces correspond to known values (time dependent)

To keep it simple, assume that electrodes are rods with fixed charge density and are not affected by the moving ions

\[U(r) = \frac{\lambda}{2\pi r \varepsilon_0}\]

The electrode surfaces correspond to the values (time dependent) of the applied voltages

*Write in x- and y- coordinates (two ordinary differential equations)*
Project work:

- set up the ODEs
- code a suitable solver
- simulate motion of ions
- determine design parameters for filter
- determine parameters for ion source

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