

April 15, 2005

➤ Website updates!

- ✓ Prob Set Solutions
- ✓ Exam #3 Info Page

➤ Review Session: Monday, 5 pm, B203

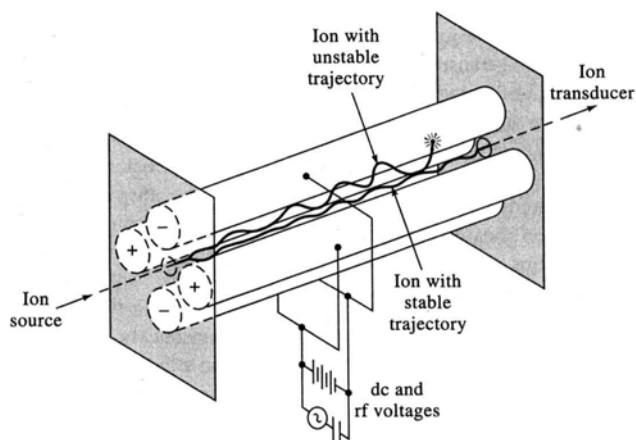
➤ Exam #3: Wednesday, 7 pm, B104

➤ Office Hours: Cancelled for today ☹

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Quadrupole Mass Analyzers

- Based on *path stability* of ions in an oscillating electric field:



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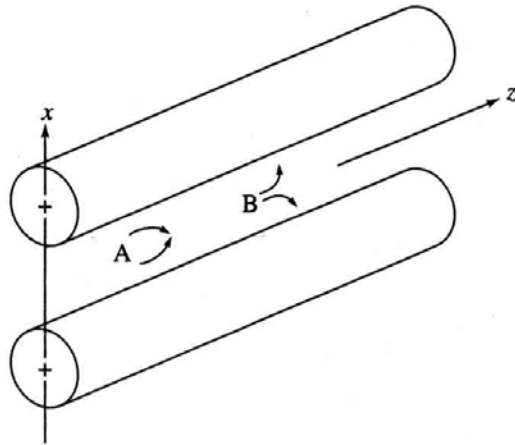
How do they work?

DC Potential:

-affects *ALL* ions
(indep of mass)

AC Potential:

-affects *LIGHT* ions

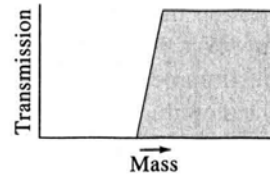
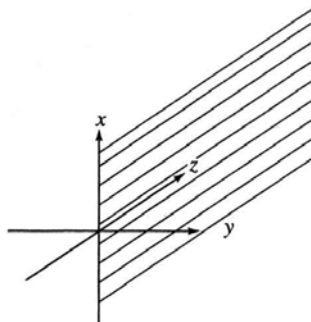


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First BiPole Pair: Pos. DC

•+ DC potential
repels ALL ions

•AC (rf) potential
attracts light ions



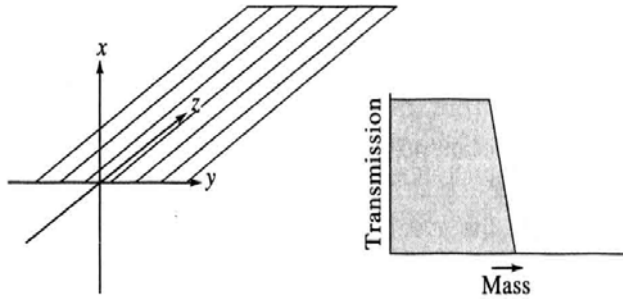
High Mass Pass Filter

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Second BiPole Pair: Neg. DC

•- DC potential
attracts ALL ions

• AC (rf) potential
repels light ions

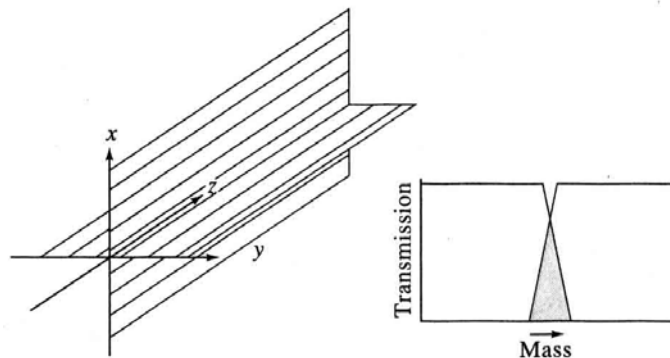


Low Mass Pass Filter

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Putting it all together

Combo of the
two filters
results in
transmission
of only a
narrow range
of masses:



• *Variable mass filter*

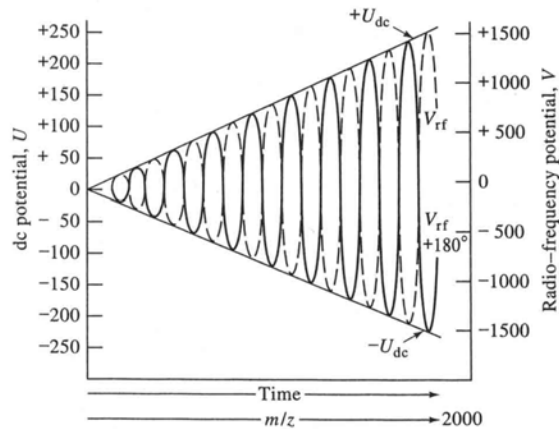
• Mass and mass range vary with ac and dc potentials

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Scanning a Quad

• Resolution:

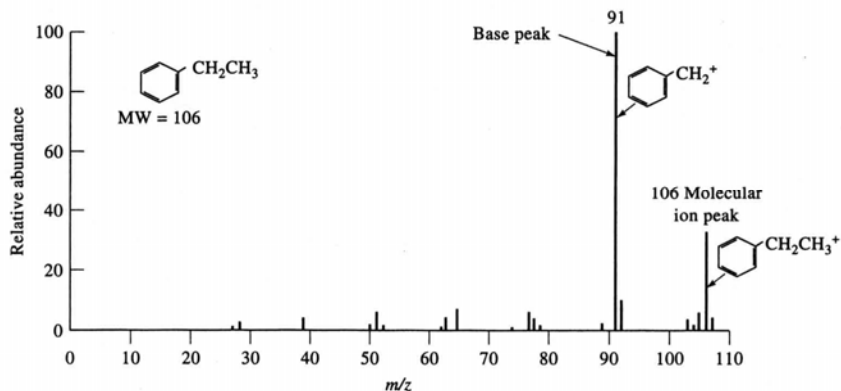
-controlled by ac/dc (max res. at ~6)



Properties of Quad Analyzers

- Resolution: up to ~1500
- Fast! can obtain spectrum in *ms*
- Small, rugged, *cheap*
- Higher ion throughput than magsectors
 - Circular versus slit aperture

A Mass Spectrum



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Applications: MW Determination

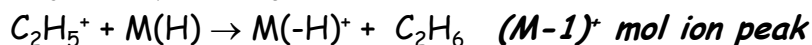
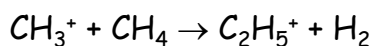
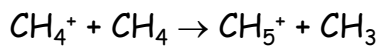
- Need *pure compound*
- Determine m/z for molecular ion
 - Vary electron gun potential to confirm molecular ion assignment
 - use a milder ionization method (e.g., *Chemical Ionization*)

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Chemical Ionization (CI)

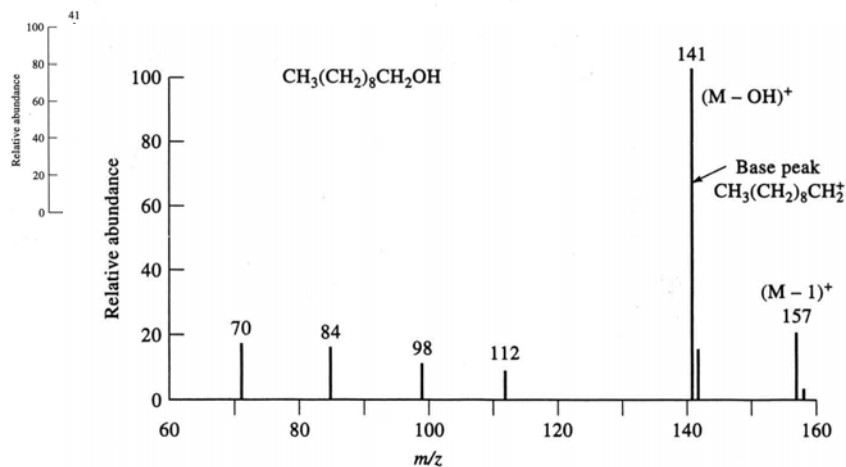
- Add a *reagent gas* to the EI source
- *Reagent ion* is formed by interaction with e^- beam
- Analyte is ionized by reaction with the *reagent ion*

➤ Example:



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EI versus CI: Decanol



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Molecular Formula Determination

■ Brute Force Method

- get molecular weight from mass spectrum
- compare MW with MWs of suspected compounds

BUT, this requires a *high-resolution* mass spectrum . . . not always an available option

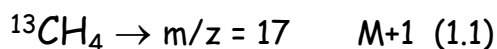
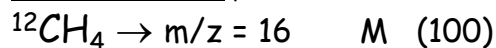
■ Isotope Ratio Method

- use isotope natural abundances to decipher multiple peaks due to *isotopomers*

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Isotope Ratio Method

➤ Consider CH₄:

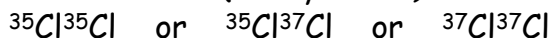


Relative abundance of $^{13}\text{C} = 1.1\%$ of ^{12}C

➤ Consider Cl₂:

-Relative abundance of $^{37}\text{Cl} = 33\%$ of ^{35}Cl

-3 possible combos (*isotopomers*):



(56.5%) (37.3%) (6.2%)

M (70) M+2 (72) M+4 (74)

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