

Triple Quadrupole Mass Spectrometry

Detect Mixture Analysis and
Structure Elucidation

Triple Quadrupole Mass Spectrometer

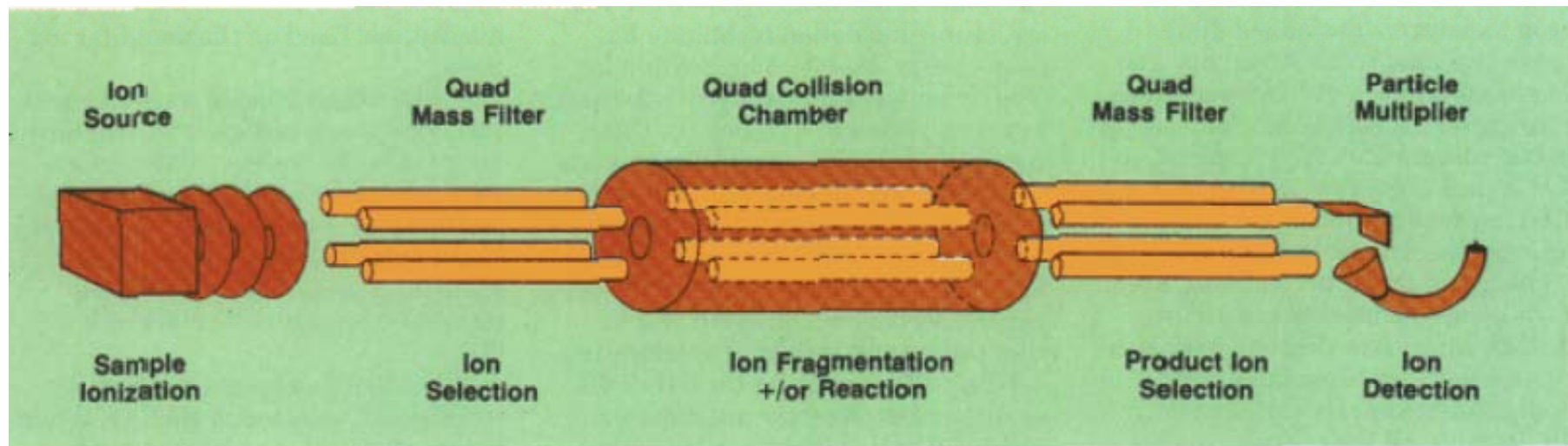


Figure 1. Conceptual diagram of the triple quadrupole mass spectrometer showing each component and its function.

- Particularly simple and efficient approach to selecting ion fragments.
- Fragmentation caused by Collision-induced dissociation (CID).

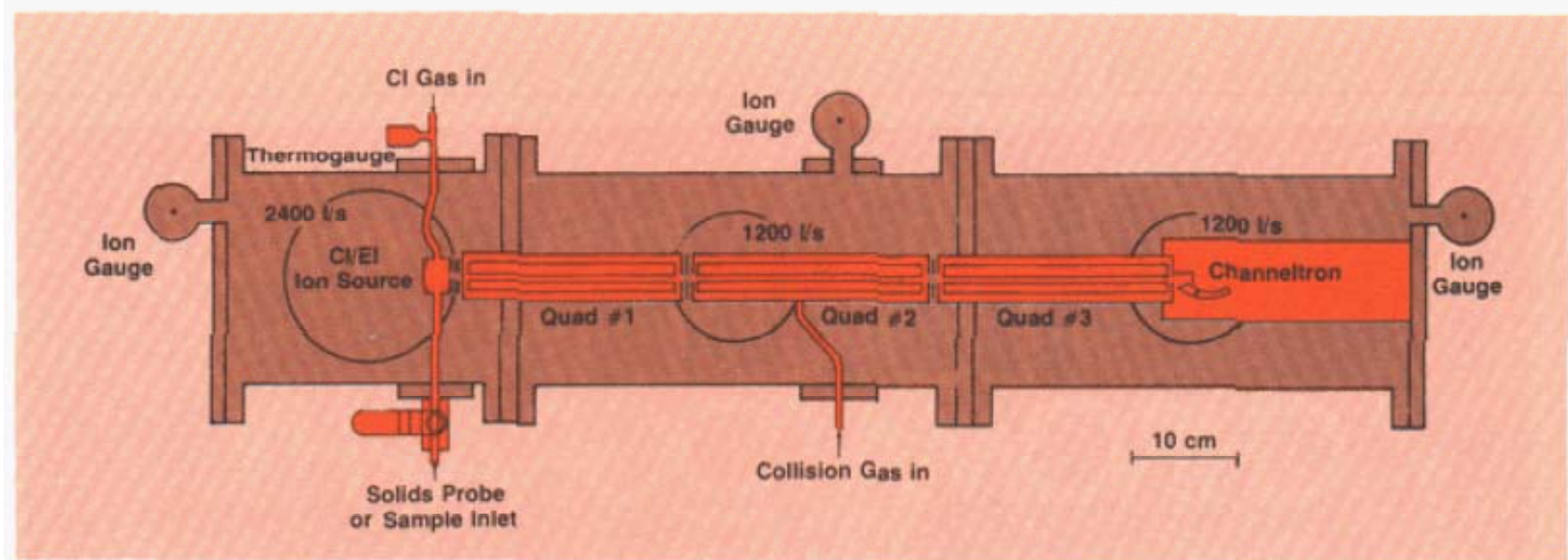


Figure 5. Scale drawing (top view) of triple quadrupole mass spectrometer

A scale drawing of the triple quadrupole spectrometer constructed at Michigan State University.

Purpose

- Complete fragmentation maps can be obtained by recording the mass spectrum of each fragment ion of a compound.
- The fragmentation process greatly eliminates the chemical noise resulting in lower limits of detection.
- The triple quadrupole method of fragmentation eliminated the time delay associated with the chromatographic separations (LC/MS and GC/MS).

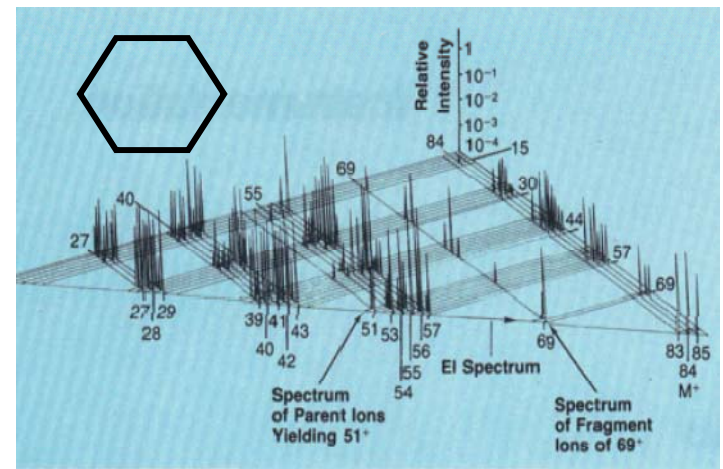


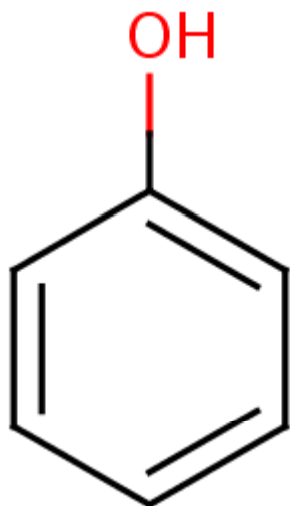
Figure 2. Three-dimensional fragmentation map for cyclohexane

The fragmentation map of cyclohexane (above).

Modes of Operation

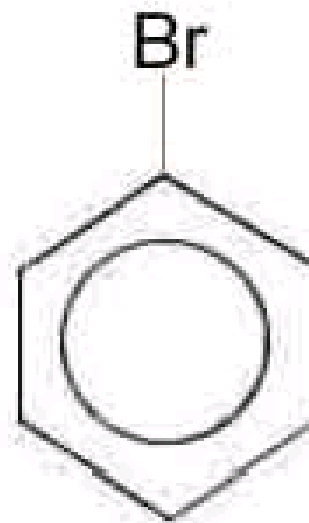
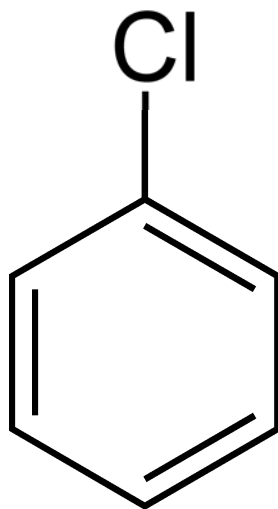
1. Normal Mass Spectrometry
 - 2nd and 3rd quadrupoles in RF-only mode
2. Scan for fragments of parent ion
 - 1st quadrupole select specific ion while 3rd quadrupole scans for fragments
3. Fragment Ion Measurement
 - 1st quadrupole select specific ion while 3rd quadrupole measures a specific fragment ion
4. Fragment Reaction
5. Specific Neutral Mass Loss
 - Scanning both mass filters with a fixed difference in mass (example following)

Specific Neutral Mass Loss



Loss of 17 (-OH)

Loss of 35 (-Cl)



Loss of 79/81 (-Br)

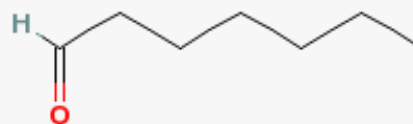
Mixture Analysis

Example: solution containing 3-heptanone, *n*-heptanal, *n*-octane, cyclohexane, and 2-pentanone all in equal concentrations.

114 g/mol



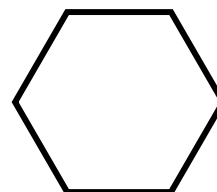
114 g/mol



114 g/mol



84 g/mol



Mixture Spectrum after fragmentation

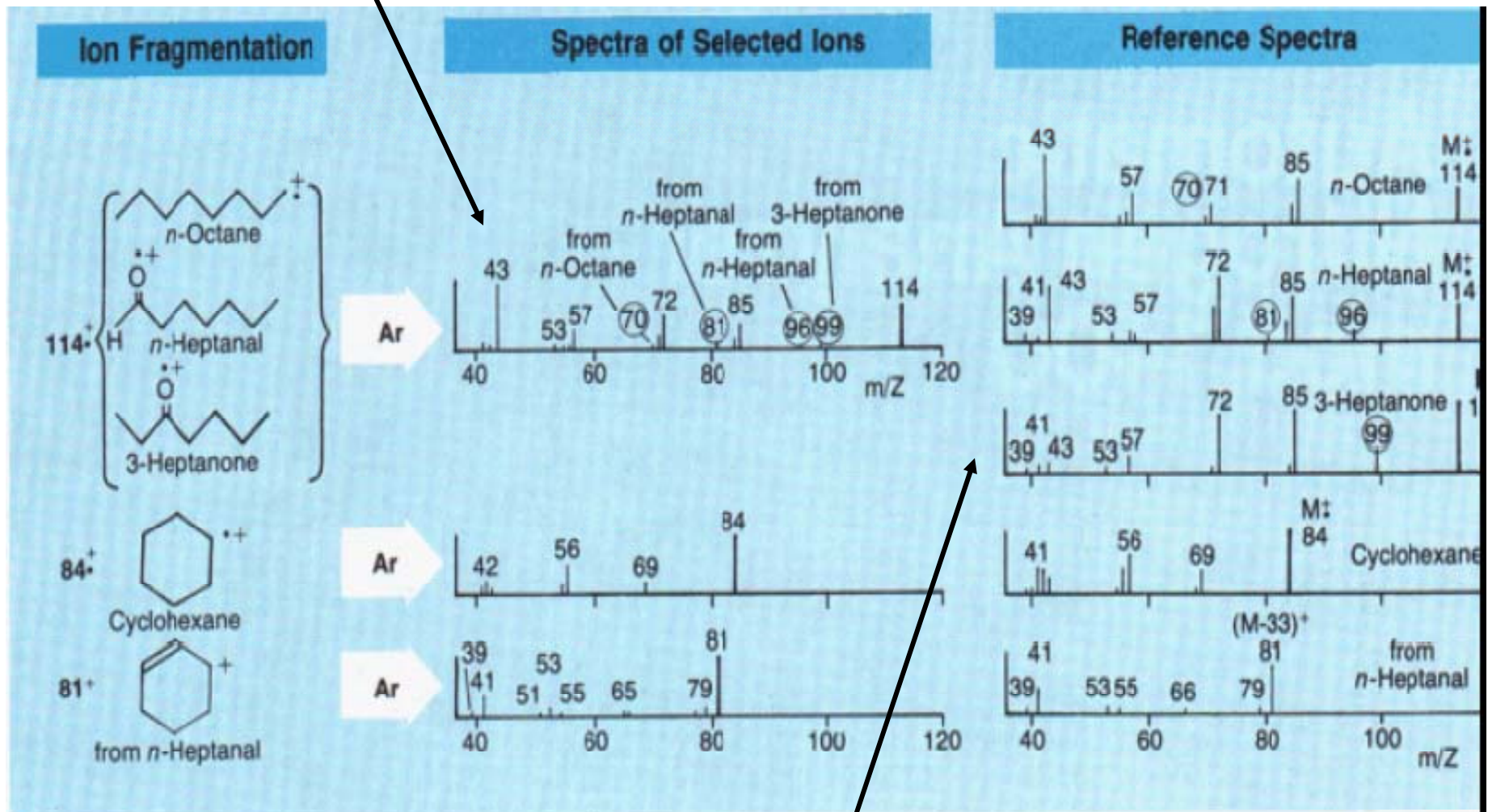
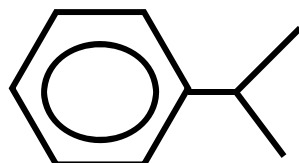
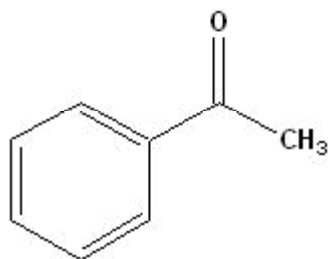


Figure 3. Comparison of CID spectra of selected ions in the EI spectrum of a five component mixture with reference CID spectra from pure components

Fragmentation Reference Spectra

Structure Elucidation

Example:



Same molar weight but they have a difference fragmentation spectra thus we can tell them apart using triple quadrupole mass spectroscopy.

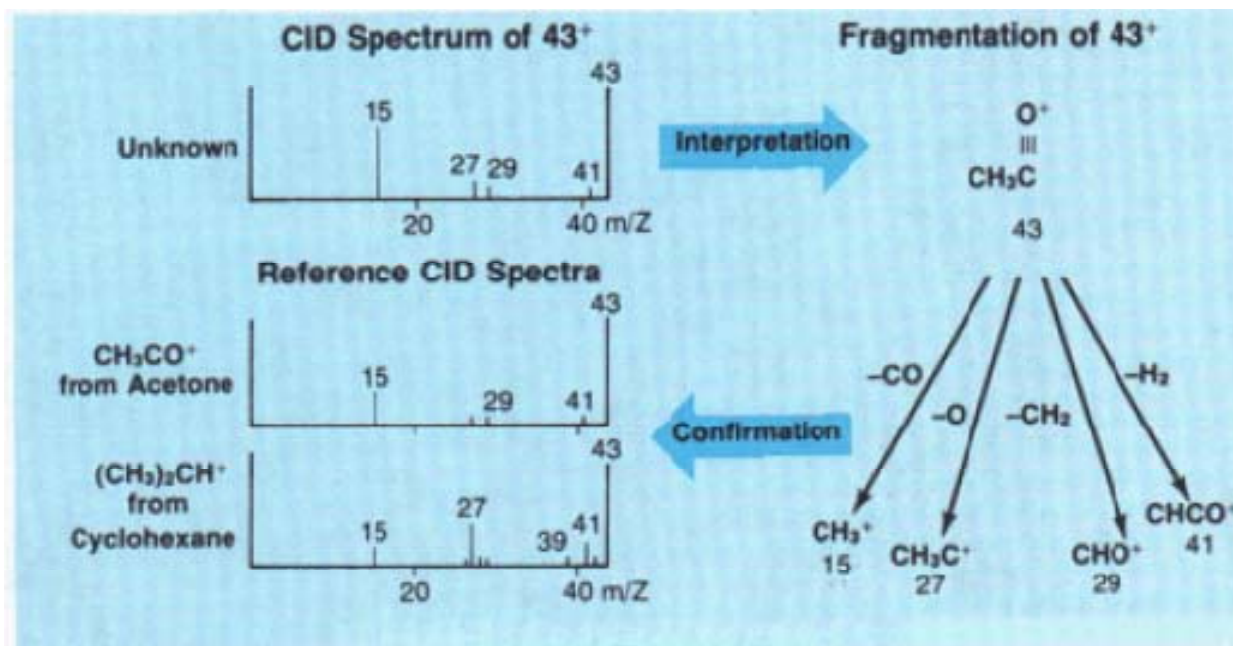


Figure 4. Structure elucidation of 43⁺ functional moiety by interpretation of CID spectrum and comparison with reference CID spectra

Reference

Yost, R. A. and C. G. Enke (1979). "Triple quadrupole mass spectrometry for direct mixture analysis and structure elucidation." *Anal. Chem.* 51(12): 1251A-1252A, 1256A, 1258A, 1260A, 1262A.