

Mass Spectrometry Analysis

Chem12A, Organic Chemistry I

HOW TO ANALYZE A MASS SPECTRUM:

- (1) Locate the molecular ion peak. This is your **molar mass**.
- (2) Subtract the atomic masses of any HETEROATOMS, if applicable.
 - a. Alcohols with γ -H have distinctive 18 amu peaks
 - b. Bromine has a 50:50 ratio from Br-79 and Br-81
 - c. Chlorine has a 75:25 ratio from Cl-35 and Cl-37

(3) Divide difference from (2) 12 amu. This is your number of **carbons**.

(4) Divide the remainder by 1 amu. This is your number of **hydrogens**.

Remember that all organic compounds have SOME hydrogens, so you MUST have some remainder after (3)!

(5) Calculate your **degrees of unsaturation**.

(6) Find your **base peak**. This is your MOST stable fragment.

Remember that stability increases from $1^\circ < 2^\circ < 3^\circ$, and increases with possible resonance.

- a. Methyls ($^+\text{CH}_3$) appear at 15 amu.
- b. Ethyls ($^+\text{CH}_2\text{CH}_3$) appear at 29 amu.
- c. Propyls ($^+\text{CH}_2\text{CH}_2\text{CH}_3$ or $\text{CH}_3^+\text{CHCH}_3$) appear at 43 amu.

(7) Consider possible **cleavage**.

Remember that the first electron lost from the molecule is ALWAYS from a lone pair, if possible.

- a. Alcohols, ethers, aldehydes, and ketones undergo **homolytic** cleavage, Alcohols with γ -H can also undergo dehydration.
- b. Halogens (Br, Cl) undergo BOTH **homolytic** and **heterolytic** cleavage.
- c. All other bonds can be cleaved.

(8) Piece the structure back together from all the information above.

Watch out for structural isomers that match and give ALL possibilities.