These notes can be obtained at: http://www.ndsu.nodak.edu/instruct/grcook/chem342/notes.shtml

Chapter 12: Mass Spectrometry and Infrared Spectroscopy

How do we determine the structure of organic molecules?

Probe the physical properties

Elemental Analysis (combustion analysis)
- Atomic composition (relative ratios)
- Empirical formula

Mass Spectrometry
- Molecular formula
- Elemental identification (isotopes)
- Structural features (from fragments)

Infrared (Vibrational) Spectroscopy
- Functional Group Identities

Ultraviolet (electronic) Spectroscopy
- Conjugated pi-systems

Nuclear Magnetic Resonance Spectroscopy
- Atom connectivity
- Functional groups
- stereochemistry

X-Ray Crystallography
- 3D position of atoms

Elemental Analysis

Provides empirical formula

Percent Composition by Mass

C - 63.31%
H - 6.28%
Cl - 16.99%
N - 13.42%

Assume 100g sample

$\Longrightarrow$ **%composition = grams**

Moles of C =	$\frac{63.31\ g}{12.011\ g/mol}$	=	5.27	5.27 / 0.48	=	11
Moles of H =	$\frac{6.28\ g}{1.008\ g/mol}$	=	6.23	6.23 / 0.48	=	13
Moles of N =	$\frac{13.42\ g}{14.007\ g/mol}$	=	0.96	0.96 / 0.48	=	2
Moles of Cl =	$\frac{16.99\ g}{35.45\ g/mol}$	=	0.48	0.48 / 0.48	=	1

$\Longrightarrow$ **Empirical Formula = $C_{11}H_{13}N_2Cl$**

Units of Unsaturation

The number of pi-bonds and rings in the molecule

Saturated hydrocarbon has the general formula C_nH_{2n+2}

Every pi-bond or ring removes 2 H's – each loss of 2 H's is an unsaturation

Difference in the number of H's between the saturated and the unsaturated molecule

Every halogen replaces one H and must be counted

Every nitrogren adds one H and must be counted

General Formula for Units of Unsaturation

$$UN = \frac{(2n+2) - \#H - \#X + \#N}{2}$$

2n+2 is the number of H's if completely saturated
#H is the actual number of H's in the molecule
#X is the actual number of halogens
#N is the actual numnber of nitrogens
divide by 2 because each unit of unsaturation removes 2 H's from the molecule

Empirical Formula = $C_{11}H_{13}N_2Cl$ $\quad UN = \frac{(2*11+2) - 13 - 1 + 2}{2} = 6$